Supporting Information for

Theoretical investigation on the atmospheric degradation of $C_6H_5C(O)O_2\cdot$ radical: reactions with NO, NO_2, $HO_2\cdot$ and NO_3

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Table S1. Summary of multireference diagnostics for the important species calculated with UHF wave functions (kcal/mol).

Species	T1[1]	%TAE$_e$[(T)][1]	The three largest CI eigenvector coefficients [2]		
Com-1 (Triplet)	0.024	2.146			
Com-3 (Triplet)	0.024	2.156			
TS-4 (Triplet)	0.031	2.282			
TS-6 (Triplet)	0.037	2.385			
$C_6H_5\cdot$ (Doublet)	0.015	1.618			
$C_6H_5C(O)O\cdot$ (Doublet)	0.025	1.886			
$C_6H_5C(O)O_2\cdot$ (Doublet)	0.021	2.044			
TS-2 (Doublet)	0.046	2.063			
$C_6H_5C(O)O_3NO_2$-cis (Singlet)	0.017	2.868			
$C_6H_5C(O)O_3NO_2$-trans (Singlet)	0.017	2.883			
TS-11 (Singlet)	0.017	2.880			
Com-2 (Singlet)	0.036	2.155	0.615	0.599	0.308
Com-4 (Singlet)	0.038	2.153	0.597	0.492	0.485
Com-5 (Singlet)	0.038	2.235	0.616	0.475	0.467
TS-5 (Singlet)	0.042	2.367	0.877	0.214	0.152
TS-7 (Singlet)	0.047	2.542	0.906	0.202	0.134
TS-8 (Singlet)	0.038	2.337	0.831	0.381	0.152
TS-9 (Singlet)	0.072	2.749	0.862	0.336	0.148
TS-10 (Singlet)	0.044	2.224	0.602	0.592	0.369
$C_6H_5C(O)O_4H$ (Singlet)	0.016	2.355	0.902	0.164	0.138

[1] The diagnostics of T1 and the triples contribution to the total atomization energy, %TAE$_e$[(T)], were calculated at the UCCSD(T)/cc-pVDZ level of theory. For T1, a value of larger than 0.02 typically indicates the closed-shell species would be marginally described by single-reference methods, while this cutoff is not as rigorous for open-shell species, but T1 < 0.04 should be OK in general. For %TAE$_e$[(T)], a value greater than 2% demonstrates more multireference character. For the calculation of %TAE$_e$[(T)], the equation can be expressed as:

$$\%TAE_e[(T)] = 100 \times \frac{\%TAE_e[CCSD(T)] - \%TAE_e[CCSD]}{\%TAE_e[CCSD(T)]}$$

The calculations of %TAE$_e$[CCSD(T)] and %TAE$_e$[CCSD] were based on following formula:

$$\%TAE_e[CCSD(T)](C_6H_5C(O)O_2\cdot) = [7 \times E_{CCSD(T)}C + 5 \times E_{CCSD(T)}H + 3 \times E_{CCSD(T)}O] - E_{CCSD(T)}(C_6H_5C(O)O_2\cdot)$$

[2] CI eigenvector coefficients were obtained for species at the CAS(16,14)/cc-pVDZ level (CAS(12,12)/cc-pVDZ for TS-9, TS-10 and $C_6H_5C(O)O_4H$), using the ORCA 4.2.1 program package. A coefficient of 1.00 for the

first eigenvector, and 0.00 for all others dedicate the perfectly single-reference system, from which the degree of deviation reflects the multireference character of different species. The absolute value of largest three CI eigenvector coefficients are listed above.

Table S2. Summary of $E_{CCSD(T)/CBS}$(triplet), E_{MR}(singlet) and E_{MR}(triplet) energies.

Species	$E_{CCSD(T)/CBS}$(triplet) (Zero-point energy obtained, kcal/mol)	E_{MR}(singlet) NEVPT2-F12/cc-pVDZ-F12 (Hartree)	E_{MR}(triplet) NEVPT2-F12/cc-pVDZ-F12 (Hartree)
Com-2	-5.28	-645.3499535	-645.3497925
Com-4	-6.73	-645.3513339	-645.3515806
Com-5	-3.73	-645.3089015	-645.3089797
TS-10	-3.52	-645.2812326	-645.2812415

Table S3. Cartesian coordinates (Angstroms) of important weak-binding complexes, stable intermediates, transition states and products on each potential energy curve coupled energies (Hartrees) at M06-2X/def2-TZVP level.

$C_6H_5C(O)O_2$·

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	2.898268	-0.271445	0.000103
6	0	2.391374	1.022875	-0.000028
6	0	1.023247	1.227258	-0.000103
6	0	0.160213	0.133321	-0.000090
6	0	0.666232	-1.164902	0.000019
6	0	2.038387	-1.361203	0.000130
1	0	3.968905	-0.430885	0.000202
1	0	3.064014	1.870083	-0.000066
1	0	0.603626	2.224674	-0.000188
1	0	-0.006003	-2.010888	0.000003
1	0	2.436502	-2.367029	0.000245
6	0	-1.288538	0.423060	-0.000058
8	0	-1.821775	1.476485	0.000170
8	0	-3.319817	-0.601473	0.000408
8	0	-2.033675	-0.792478	-0.000581

HF= -495.288519

$C_6H_5C(O)O_2NO$-trans

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-3.522487	-0.289250	0.255860
6	0	-3.022887	1.006604	0.216746
6	0	-1.670653	1.218825	0.010266
6	0	-0.818283	0.131233	-0.156951
6	0	-1.316358	-1.168498	-0.117976
6	0	-2.671406	-1.373529	0.088684
1	0	-4.579895	-0.454745	0.417232
1	0	-3.687988	1.849642	0.347535
1	0	-1.255597	2.217265	-0.024835
1	0	-0.650529	-2.009716	-0.249126
1	0	-3.063906	-2.381107	0.119069
6	0	0.618326	0.432029	-0.375909
8	0	1.115987	1.508928	-0.453763
8	0	2.681433	-0.481767	-0.772333
8	0	1.342746	-0.738404	-0.479111
7	0	3.429998	-0.124236	0.383067
8	0	2.816136	-0.050779	1.353251

HF= -625.2337602

$C_6H_5C(O)O_2NO$-cis

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.522530	-0.288976	0.255858
6	0	3.022768	1.006814	0.216621
6	0	1.670502	1.218833	0.010140
6	0	0.818266	0.131099	-0.156903
6	0	1.316503	-1.168584	-0.117756
6	0	2.671584	-1.373404	0.088847
1	0	4.579955	-0.454294	0.417218
1	0	3.687759	1.849947	0.347302
1	0	1.255333	2.217210	-0.025072
1	0	0.650808	-2.009900	-0.248863
1	0	3.064228	-2.380916	0.119281
6	0	-0.618359	0.431736	-0.376003
8	0	-1.116068	1.508575	-0.454356
8	0	-2.681384	-0.482260	-0.772177
8	0	-1.342763	-0.738773	-0.478634
7	0	-3.429950	-0.123969	0.383005
8	0	-2.816183	-0.049963	1.353202

HF= -625.2337602

TS-1

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-3.471328	-0.806195	0.000007
6	0	-3.303803	0.572814	0.000252
6	0	-2.029364	1.113800	0.000247
6	0	-0.922095	0.270875	0.000006
6	0	-1.086816	-1.111625	-0.000231
6	0	-2.365526	-1.646093	-0.000233
1	0	-4.468347	-1.227753	0.000004
1	0	-4.167094	1.224901	0.000404
1	0	-1.870168	2.183963	0.000390
1	0	-0.222908	-1.761862	-0.000387
1	0	-2.499685	-2.719551	-0.000353
6	0	0.415615	0.919953	-0.000044
8	0	0.637569	2.087042	-0.000285
8	0	2.661046	0.577459	-0.000142
8	0	1.395925	-0.044525	0.000108
7	0	3.670182	-0.381686	0.000006
8	0	3.320064	-1.483609	0.000304

HF= -625.2276271

$C_6H_5C(O)O_2\cdot$

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.508013	0.004839	0.000156
6	0	-1.824764	-1.205382	0.000063
6	0	-0.439927	-1.217062	-0.000036
6	0	0.252776	-0.012052	-0.000041
6	0	-0.426359	1.201659	0.000054
6	0	-1.812155	1.206824	0.000153
1	0	-3.590397	0.011168	0.000232
1	0	-2.373613	-2.137665	0.000068
1	0	0.120906	-2.142696	-0.000110
1	0	0.125220	2.133937	0.000057
1	0	-2.349704	2.145553	0.000229
6	0	1.734293	-0.062620	-0.000158
8	0	2.425795	-1.048872	-0.000056
8	0	2.350765	1.110429	-0.000146

HF= -420.1187886

TS-2

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.509593	-0.038026	0.006656
6	0	-1.791206	-1.220588	-0.101759
6	0	-0.399680	-1.203889	-0.107624
6	0	0.205268	0.028091	-0.008031
6	0	-0.458669	1.228477	0.090842
6	0	-1.849200	1.178620	0.106107
1	0	-3.591168	-0.065046	0.013735
1	0	-2.306539	-2.169683	-0.173387
1	0	0.186335	-2.108267	-0.170483
1	0	0.079610	2.161986	0.150043
1	0	-2.410258	2.100481	0.187337
6	0	1.968588	-0.001524	0.007960
8	0	2.353339	-1.105992	0.246466
8	0	2.277783	1.137687	-0.242986

HF= -420.018656

C_6H_5·

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.000008	1.316950	-0.000001
6	0	-1.206861	0.628587	0.000022
6	0	-1.218377	-0.766251	-0.000025
6	0	0.000012	-1.393292	-0.000002
6	0	1.218370	-0.766266	0.000027
6	0	1.206847	0.628615	-0.000020
1	0	-0.000024	2.398973	-0.000004
1	0	-2.142974	1.173050	0.000030
1	0	-2.149882	-1.317574	-0.000016
1	0	2.149906	-1.317535	0.000012
1	0	2.142985	1.173033	-0.000032

HF= -231.5388869

$C_6H_5C(O)ONO_2$

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-3.586968	-0.352688	0.000147
6	0	-2.689157	-1.412030	-0.000194
6	0	-1.325402	-1.166194	-0.000365

6	0	-0.867291	0.148205	-0.000199
6	0	-1.765876	1.211655	0.000189
6	0	-3.126494	0.958384	0.000346
1	0	-4.651228	-0.549675	0.000291
1	0	-3.051959	-2.431026	-0.000313
1	0	-0.621354	-1.986429	-0.000549
1	0	-1.380347	2.222456	0.000343
1	0	-3.828806	1.781052	0.000633
6	0	0.574053	0.486634	-0.000308
8	0	1.053419	1.575805	-0.000077
8	0	1.355563	-0.653537	-0.000685
7	0	2.758474	-0.309983	0.000158
8	0	3.230209	-0.217418	-1.078582
8	0	3.229208	-0.218637	1.079443

HF= -625.2734318

$C_6H_5C(O)O_2NO_2$-trans

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.889607	-0.287649	0.278015
6	0	3.391694	1.009270	0.252255
6	0	2.042978	1.225897	0.030139
6	0	1.193414	0.140956	-0.166856
6	0	1.689498	-1.160170	-0.141824
6	0	3.041108	-1.368917	0.081413
1	0	4.944370	-0.456857	0.452926
1	0	4.055805	1.849067	0.406943
1	0	1.629426	2.225441	0.006905
1	0	1.024732	-1.998829	-0.294099
1	0	3.432576	-2.377129	0.102481
6	0	-0.236864	0.445999	-0.395396
8	0	-0.750047	1.515088	-0.437424
8	0	-2.277933	-0.457948	-0.855470
8	0	-0.962514	-0.731269	-0.556079
7	0	-3.003256	-0.150278	0.366367
8	0	-2.393972	-0.188294	1.375466
8	0	-4.132125	0.084665	0.115231

HF= -700.4170497

$C_6H_5C(O)O_2NO_2$-cis

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

6	0	-3.894456	-0.277238	0.277061
6	0	-3.390441	1.017246	0.245398
6	0	-2.040379	1.226355	0.024298
6	0	-1.195254	0.136222	-0.164925
6	0	-1.697367	-1.162425	-0.133105
6	0	-3.050468	-1.363553	0.088292
1	0	-4.950410	-0.440095	0.450062
1	0	-4.050345	1.861370	0.393777
1	0	-1.621729	2.223508	-0.004617
1	0	-1.037612	-2.005843	-0.279758
1	0	-3.446934	-2.369627	0.113866
6	0	0.235860	0.432932	-0.398146
8	0	0.750557	1.499938	-0.468887
8	0	2.274174	-0.487100	-0.840530
8	0	0.960257	-0.749214	-0.523991
7	0	3.009060	-0.139433	0.364592
8	0	2.408457	-0.142064	1.379485
8	0	4.136385	0.084625	0.096585

HF= -700.4170271

TS-3

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-3.858911	-0.810742	-0.000002
6	0	-3.698499	0.569083	-0.000086
6	0	-2.426897	1.116403	-0.000075
6	0	-1.316190	0.277847	0.000010
6	0	-1.473129	-1.105716	0.000106
6	0	-2.749268	-1.645724	0.000102
1	0	-4.853853	-1.237133	-0.000033
1	0	-4.564952	1.216874	-0.000148
1	0	-2.273173	2.187371	-0.000126
1	0	-0.606593	-1.752730	0.000176
1	0	-2.878400	-2.719732	0.000197
6	0	0.015788	0.933820	0.000007
8	0	0.243171	2.099001	0.000051
8	0	2.253513	0.600373	0.000074
8	0	1.001680	-0.032064	-0.000064
7	0	3.241238	-0.431765	-0.000005
8	0	2.871369	-1.553534	-0.000195
8	0	4.321636	0.050959	0.000083

HF= -700.4084038

Com-1

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.232705	-1.334055	0.000079
6	0	3.435090	0.041784	0.000231
6	0	2.348371	0.896237	0.000070
6	0	1.057856	0.368753	-0.000241
6	0	0.849896	-1.010484	-0.000382
6	0	1.946985	-1.857592	-0.000230
1	0	4.084770	-2.001710	0.000192
1	0	4.439435	0.443375	0.000461
1	0	2.476845	1.970684	0.000163
1	0	-0.154163	-1.413871	-0.000659
1	0	1.796217	-2.928607	-0.000367
6	0	-0.055828	1.330673	-0.000500
8	0	-0.036726	2.508445	-0.000234
8	0	-2.343850	1.385816	-0.000288
8	0	-1.306472	0.611498	-0.000057
8	0	-3.052141	-1.859215	0.000830
8	0	-4.007125	-0.970030	0.000483
1	0	-3.563048	-0.093894	0.000173

HF= -646.2069102

TS-4

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.429279	-0.434087	0.241482
6	0	2.997459	0.861701	0.498026
6	0	1.675892	1.204178	0.274286
6	0	0.788321	0.246687	-0.212119
6	0	1.218005	-1.053127	-0.469042
6	0	2.542536	-1.388567	-0.238677
1	0	4.462998	-0.701252	0.420225
1	0	3.691255	1.601270	0.874810
1	0	1.311763	2.204228	0.469996
1	0	0.522461	-1.794027	-0.836533
1	0	2.883032	-2.397017	-0.431599
6	0	-0.606617	0.672708	-0.420086
8	0	-1.116717	1.702607	-0.150438
8	0	-2.612194	-0.051930	-1.233591
8	0	-1.354024	-0.368885	-1.062414

8	0	-1.999145	-0.784178	1.479132
8	0	-3.170285	-0.424017	1.134245
1	0	-3.121829	-0.158934	0.124419

HF= -646.2045198

$C_6H_5C(O)O_2H$

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-2.961191	0.220864	-0.000340
6	0	-2.132673	1.335854	0.001924
6	0	-0.756160	1.178469	0.002185
6	0	-0.214084	-0.104059	0.000204
6	0	-1.042061	-1.222113	-0.001766
6	0	-2.417068	-1.057241	-0.002153
1	0	-4.035952	0.349047	-0.000588
1	0	-2.560402	2.329447	0.003508
1	0	-0.104438	2.041119	0.004279
1	0	-0.592113	-2.205952	-0.003021
1	0	-3.064853	-1.923600	-0.003776
6	0	1.248089	-0.338247	0.000624
8	0	1.794801	-1.411482	0.004676
8	0	3.335290	0.569563	-0.001067
1	0	3.367649	-0.410057	0.001319
8	0	1.950034	0.809274	-0.004334

HF= -495.9485977

Com-2

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-3.232976	-1.331870	0.000024
6	0	-3.434262	0.044092	0.000228
6	0	-2.346809	0.897663	0.000205
6	0	-1.056746	0.369119	-0.000018
6	0	-0.849874	-1.010308	-0.000211
6	0	-1.947650	-1.856470	-0.000192
1	0	-4.085530	-1.998903	0.000033
1	0	-4.438246	0.446582	0.000400
1	0	-2.474472	1.972210	0.000348
1	0	0.153901	-1.414424	-0.000374
1	0	-1.797796	-2.927614	-0.000347
6	0	0.057600	1.330106	-0.000091
8	0	0.040004	2.507803	-0.000026

8	0	2.345939	1.383080	-0.000490
8	0	1.308129	0.609514	-0.000246
8	0	3.046664	-1.859004	0.000424
8	0	4.002598	-0.971091	0.000358
1	0	3.559774	-0.094258	0.000106

HF= -646.2070095

TS-5

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	3.456711	-0.410622	0.273252
6	0	3.012345	0.892952	0.460408
6	0	1.687955	1.210816	0.217757
6	0	0.808772	0.221149	-0.216200
6	0	1.251129	-1.086633	-0.403084
6	0	2.578776	-1.397038	-0.155697
1	0	4.492674	-0.658821	0.464832
1	0	3.698909	1.658282	0.796376
1	0	1.315346	2.216732	0.358492
1	0	0.563319	-1.852364	-0.731755
1	0	2.928471	-2.410879	-0.296281
6	0	-0.589602	0.626304	-0.452471
8	0	-1.092032	1.680801	-0.270974
8	0	-2.596984	-0.145124	-1.217365
8	0	-1.337951	-0.464909	-0.975927
8	0	-2.115887	-0.637583	1.528043
8	0	-3.247001	-0.327923	1.069629
1	0	-3.116390	-0.136622	-0.002709

HF= -646.1980136

Com-3

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	3.454921	-0.154369	0.393028
6	0	2.823556	-1.196755	-0.276062
6	0	1.487977	-1.086637	-0.616816
6	0	0.785247	0.071388	-0.287835
6	0	1.415383	1.117111	0.384589
6	0	2.753452	0.997591	0.722960
1	0	4.500023	-0.242055	0.660624
1	0	3.373884	-2.092993	-0.528414
1	0	0.971681	-1.884118	-1.134258

1	0	0.863671	2.009264	0.643448
1	0	3.249108	1.803491	1.246946
6	0	-0.632846	0.126795	-0.669215
8	0	-1.277858	-0.712473	-1.210122
8	0	-2.478413	1.431624	-0.548114
8	0	-1.195477	1.388784	-0.349816
8	0	-2.210514	-0.694551	1.519476
8	0	-3.164078	-1.148886	0.759805
1	0	-2.873779	-0.960307	-0.162057

HF= -646.2114806

TS-6

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.606413	-1.504036	-0.036425
6	0	-2.516022	-0.307638	0.663569
6	0	-1.303292	0.354983	0.744700
6	0	-0.182274	-0.184262	0.118497
6	0	-0.270610	-1.383910	-0.585529
6	0	-1.486373	-2.041659	-0.658469
1	0	-3.555729	-2.020585	-0.098486
1	0	-3.390930	0.107589	1.145397
1	0	-1.210548	1.287618	1.284547
1	0	0.607307	-1.789715	-1.068840
1	0	-1.562282	-2.973319	-1.202828
6	0	1.094280	0.542900	0.211270
8	0	1.170364	1.653213	0.760171
8	0	3.231284	0.739051	-0.460626
8	0	2.116454	-0.074376	-0.302769
8	0	4.122102	1.643425	1.243396
8	0	3.280287	2.548689	1.463713
1	0	2.264586	2.156458	0.982415

HF= -646.1920005

Com-4

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-3.460711	-0.166406	0.393668
6	0	-2.822735	-1.207002	-0.271935
6	0	-1.487413	-1.090281	-0.611461
6	0	-0.791483	0.072470	-0.284602
6	0	-1.428260	1.116373	0.384433

6	0	-2.766076	0.990305	0.721431
1	0	-4.505652	-0.259176	0.660179
1	0	-3.367723	-2.106970	-0.522592
1	0	-0.966097	-1.886178	-1.126298
1	0	-0.881927	2.012338	0.641535
1	0	-3.266883	1.794834	1.242619
6	0	0.626740	0.134795	-0.664813
8	0	1.275667	-0.701594	-1.205370
8	0	2.466731	1.446464	-0.535304
8	0	1.182808	1.399163	-0.344908
8	0	2.250633	-0.695660	1.511761
8	0	3.184423	-1.161052	0.734436
1	0	2.885805	-0.954924	-0.180690

HF= -646.2113843

TS-7

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-2.584032	-1.501593	-0.011516
6	0	-2.487833	-0.309788	0.695195
6	0	-1.278540	0.361106	0.756968
6	0	-0.166483	-0.167328	0.105480
6	0	-0.260376	-1.363194	-0.605029
6	0	-1.472911	-2.027636	-0.659341
1	0	-3.530870	-2.024150	-0.058516
1	0	-3.355473	0.095820	1.197819
1	0	-1.183560	1.290106	1.302392
1	0	0.610688	-1.759955	-1.107980
1	0	-1.553470	-2.955748	-1.208958
6	0	1.107012	0.560959	0.174338
8	0	1.164539	1.688462	0.720483
8	0	3.253938	0.758510	-0.463525
8	0	2.122890	-0.037817	-0.344849
8	0	3.930843	1.452098	1.402224
8	0	3.325239	2.543808	1.401276
1	0	2.160590	2.150767	0.907242

HF= -646.1819293

TS-8

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-3.646130	-0.069913	0.188317

6	0	-2.976598	-1.163413	-0.347519
6	0	-1.600117	-1.128882	-0.485533
6	0	-0.893538	0.003007	-0.086562
6	0	-1.562939	1.100585	0.450536
6	0	-2.941266	1.058503	0.585998
1	0	-4.722738	-0.097580	0.296375
1	0	-3.528797	-2.040752	-0.656365
1	0	-1.055735	-1.966601	-0.900281
1	0	-1.009173	1.975996	0.758686
1	0	-3.466354	1.907608	1.002275
6	0	0.574896	-0.014458	-0.263876
8	0	1.208181	-0.904401	-0.755599
8	0	2.448892	1.247219	-0.068438
8	0	1.149889	1.125189	0.242081
8	0	3.295978	-0.117777	0.949275
8	0	3.818728	-0.895641	0.041615
1	0	3.034669	-1.281189	-0.408898

HF= -646.2007862

$C_6H_5C(O)O_4H$

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-3.716996	-0.063359	0.156880
6	0	-3.089659	1.174409	0.091405
6	0	-1.712140	1.244113	-0.024140
6	0	-0.963495	0.071243	-0.074558
6	0	-1.590063	-1.170831	-0.009825
6	0	-2.969300	-1.232541	0.106511
1	0	-4.794423	-0.117051	0.247328
1	0	-3.674844	2.083488	0.129465
1	0	-1.199593	2.195347	-0.078755
1	0	-1.003687	-2.077919	-0.050437
1	0	-3.461978	-2.194282	0.157870
6	0	0.506813	0.211789	-0.205047
8	0	1.093021	1.250799	-0.326985
8	0	2.489192	-0.967757	-0.459112
8	0	1.116918	-1.001025	-0.142120
8	0	3.162427	-0.412286	0.629456
8	0	3.695132	0.800263	0.206589
1	0	2.890041	1.341524	0.084543

HF= -646.2311843

TS-9

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.779855	-0.013744	-0.029031
6	0	3.101568	1.197509	0.018072
6	0	1.716489	1.215176	0.033440
6	0	1.014158	0.014494	0.001610
6	0	1.691001	-1.200251	-0.048263
6	0	3.076247	-1.210834	-0.061663
1	0	4.862213	-0.024733	-0.039672
1	0	3.653066	2.127954	0.044231
1	0	1.167962	2.146225	0.072938
1	0	1.127222	-2.122732	-0.071761
1	0	3.608155	-2.152268	-0.097379
6	0	-0.476688	0.047952	0.023787
8	0	-1.051860	1.146284	0.206002
8	0	-2.842134	-0.933910	0.527436
8	0	-1.065379	-1.060371	-0.163107
8	0	-3.569349	-0.335467	-0.279542
8	0	-3.414345	1.008494	-0.236877
1	0	-2.289871	1.123493	0.032620

HF= -646.2060677

$C_6H_5C(O)OH$

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	2.554196	0.045001	0.000009
6	0	1.830070	1.229698	-0.000060
6	0	0.443956	1.195681	-0.000040
6	0	-0.214216	-0.030159	0.000007
6	0	0.511229	-1.217407	0.000034
6	0	1.895358	-1.178584	0.000057
1	0	3.636274	0.074754	-0.000006
1	0	2.345971	2.180704	-0.000081
1	0	-0.130569	2.111385	-0.000052
1	0	-0.027538	-2.155635	0.000098
1	0	2.462395	-2.099986	0.000074
6	0	-1.697617	-0.122724	-0.000020
8	0	-2.319779	-1.149735	-0.000113
8	0	-2.301491	1.080637	0.000090
1	0	-3.254225	0.912526	0.000224

HF= -420.8199896

TS-10

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.527029	-0.625726	0.370295
6	0	2.670665	-1.447089	-0.353230
6	0	1.403224	-1.000793	-0.686458
6	0	1.003741	0.270984	-0.290665
6	0	1.856552	1.097341	0.435245
6	0	3.122763	0.643614	0.764830
1	0	4.516920	-0.978026	0.629922
1	0	2.992122	-2.434754	-0.654981
1	0	0.713537	-1.618145	-1.246683
1	0	1.532670	2.085232	0.738597
1	0	3.794055	1.276968	1.328623
6	0	-0.356979	0.711426	-0.658770
8	0	-1.152212	0.096466	-1.339217
8	0	-2.308205	-0.448975	1.362350
8	0	-0.725918	1.889031	-0.201197
8	0	-3.328440	-0.923122	0.805494
8	0	-3.738744	-0.144876	-0.316478
1	0	-2.883118	0.022000	-0.770577

HF= -646.2021039

Com-5

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-2.529316	-1.529419	-0.122746
6	0	-1.393797	-1.605631	-0.921267
6	0	-0.500371	-0.549560	-0.955654
6	0	-0.751660	0.580646	-0.183451
6	0	-1.888860	0.663951	0.614978
6	0	-2.777646	-0.398668	0.643635
1	0	-3.223377	-2.359387	-0.095726
1	0	-1.205213	-2.489992	-1.514691
1	0	0.389889	-0.592198	-1.569938
1	0	-2.064648	1.542730	1.222063
1	0	-3.658851	-0.348243	1.268661
6	0	0.230104	1.687473	-0.227606
8	0	1.387386	1.624407	-0.575566
8	0	1.698593	-0.844121	1.365095
8	0	-0.257144	2.856669	0.143552

8	0	2.432968	-1.508307	0.594003
8	0	2.869360	-0.747316	-0.524854
1	0	2.382167	0.103681	-0.415539

HF= -646.2033275

$C_6H_5C(O)O_3NO_2$-trans

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.992544	-0.851438	0.300701
6	0	3.748082	0.469196	0.655652
6	0	2.498148	1.022806	0.437234
6	0	1.492528	0.251547	-0.138117
6	0	1.734979	-1.072103	-0.495038
6	0	2.988494	-1.620026	-0.272608
1	0	4.970092	-1.284013	0.471586
1	0	4.531972	1.065901	1.102800
1	0	2.280203	2.048157	0.705662
1	0	0.951557	-1.668688	-0.941106
1	0	3.181991	-2.648765	-0.546048
6	0	0.174149	0.909053	-0.331573
8	0	-0.130872	2.004777	0.006187
8	0	-1.963667	0.647377	-1.111369
8	0	-0.678623	0.057568	-1.010940
7	0	-3.027545	-0.443044	0.634089
8	0	-2.364719	0.266741	1.297451
8	0	-2.832191	-0.348860	-0.828267
8	0	-3.841996	-1.260790	0.875810

HF= -775.5532911

$C_6H_5C(O)O_3NO_2$-cis

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-4.082274	-0.888481	0.323632
6	0	-3.887146	0.461919	0.585955
6	0	-2.644101	1.033241	0.374797
6	0	-1.596047	0.249268	-0.099476
6	0	-1.789086	-1.104258	-0.364188
6	0	-3.036555	-1.669051	-0.150368
1	0	-5.054859	-1.334476	0.488363
1	0	-4.704184	1.067865	0.954221
1	0	-2.464383	2.081944	0.571621
1	0	-0.972789	-1.709177	-0.733302

1	0	-3.193114	-2.719827	-0.354425
6	0	-0.290580	0.924709	-0.299664
8	0	-0.042196	2.070797	-0.123104
8	0	1.877640	0.637455	-0.995124
8	0	0.657909	0.004481	-0.733152
7	0	3.304796	-0.548609	0.381663
8	0	3.182056	-1.375394	-0.446583
8	0	2.555249	0.705274	0.183893
8	0	3.920652	-0.491381	1.386289

HF= -775.5563836

TS-11

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	2.139227	-0.258920	0.801462
6	0	1.824182	0.977214	0.251873
6	0	0.510426	1.277143	-0.065385
6	0	-0.488346	0.337124	0.169807
6	0	-0.175782	-0.902389	0.720585
6	0	1.141616	-1.196250	1.035056
1	0	3.166790	-0.493208	1.048807
1	0	2.602722	1.706565	0.071945
1	0	0.237247	2.231752	-0.495382
1	0	-0.953393	-1.632215	0.898545
1	0	1.390087	-2.158516	1.462545
6	0	-1.873089	0.729683	-0.200904
8	0	-2.210123	1.752607	-0.706232
8	0	-4.070080	0.143051	-0.261034
8	0	-2.754442	-0.269165	0.124292
7	0	-5.304629	-1.070069	1.268371
8	0	-4.969723	-0.216195	2.002420
8	0	-4.807094	-0.972348	-0.128800
8	0	-5.975235	-2.032639	1.383079

HF= -775.5517778