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Effect of the Substituents on the Reactivity of Carbonyl Oxides. A Theoretical study on the Reaction of Substituted Carbonyl Oxides with Water.

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(Supplementary information)

Table S1. Relative energies, in kcal·mol^{-1}, of the stationary points of the reaction of the studied carbonyl oxides with water. In every case, the zero of the energy is chosen as the energy of the reactants, i.e., the energy of the carbonyl oxide plus the energy of water.

Entry		Stationary Point	ΔE	Δ (E+ZPE)	ΔH (298K)	ΔG (298K)
1		CR	-8.93	-6.88	-7.30	0.48
		TS	-0.97	1.50	-0.31	11.06
		P	-47.70	-42.69	-44.08	-33.51
2		CR	-9.42	-7.46	-7.88	0.48
	H_2O addition	TS	3.60	5.34	3.65	15.26
		P	-41.27	-36.67	-37.98	-27.13
	H transfer	TS	9.68	8.31	6.50	18.32
		CP	-26.76	-24.46	-42.15	-29.21
3		CR	-10.67	-8.54	-9.04	-0.65
		TS	-2.98	-1.20	-2.96	8.62
		P	-46.03	-41.24	-42.70	-31.62
4		CR	-10.67	-8.58	-9.06	-0.45
	H_2O addition	TS	2.40	3.57	1.94	13.61
		P	-39.29	-34.93	-36.31	-24.97
	H transfer	TS	9.15	7.52	5.84	17.19
		CP	-19.67	-19.38	-19.21	-19.62
5		CR	-9.32	-7.36	-7.74	0.53
	H_2O addition	TS	6.14	6.82	5.26	16.85
		P	-34.29	-30.46	-31.69	-20.72
	H transfer	TS	12.16	10.27	8.60	20.17
		CP	-20.78	-18.81	-19.02	-10.97
6		CR	-9.39	-7.54	-7.86	0.17
	H_2O addition	TS	4.41	5.24	3.62	15.54
		P	-35.58	-31.50	-32.82	-21.58
	H transfer	TS	10.54	8.88	7.12	19.01
		CP	-24.53	-22.32	-22.57	-14.64
7		CR	-7.73	-5.96	-6.13	0.66
		TS	5.41	5.84	4.37	15.75
		P	-35.82	-32.04	-33.33	-11.25
8		CR	-9.28	-7.40	-7.73	0.30
		TS	4.16	4.70	3.13	14.77

	P	-35.27	-31.40	-32.72	-21.50
9	CR	-9.66	-7.73	-8.04	-0.30
	TS	0.97	1.85	0.30	11.61
	P	-38.28	-34.15	-35.34	-24.82
10	CR	-9.14	-7.12	-7.52	0.87
	TS	3.75	4.69	3.06	14.82
	P	-38.84	-34.91	-36.06	-25.39
11	CR	-6.94	-5.19	-5.32	1.56
	TS	6.05	6.82	5.27	16.77
	P	-37.05	-33.12	-34.33	-23.57
12	CR	-9.38	-7.42	-7.72	-0.26
	TS	-1.22	0.16	-1.56	10.24
	P	-41.89	-37.30	-38.71	-27.59
13	CR	-11.78	-9.50	-7.21	1.94
	TS	-10.56	-8.00	-0.02	11.68
	P	-66.10	-62.19	-45.11	-34.01
14	CR	-15.14	-12.72	-13.40	-3.93
	TS	-7.99	-7.13	-8.88	3.27
	P	-44.15	-40.75	-41.98	-31.35
15	CR	-8.93	-6.88	-7.30	0.48
	TS	-0.97	1.50	-0.31	11.06
	P	-47.70	-42.69	-44.08	-33.51

Table S2. Calculated values of equilibrium constants (k_{eq} in cm^3 $molecule^{-1}$), tunneling parameters with ZCT, κ, unimolecular rate constants with TST (k_2 in s^{-1}), rate constants (k_{TS} in cm^3 $molecule^{-1}$ s^{-1}), and the overall rate constant k_{total} ($k_{Total} = k_{TS1} + k_{TS2}$ in cm^3 $molecule^{-1}$ s^{-1}) for the reaction of the carbonyl oxides with water. The (') indicates SCT tunneling and VTST unimolecular rate constant.

			Water addition			Hydrogen tranfer			
Entry	**T (K)**	k_{eq}	**κ**	k_2	k_{TS1}	**κ**	k_2	k_{TS2}	k_{Total}
1	275	4.91×10^{-20}	1.29	3.39×10^{4}	2.15×10^{-15}	--	--	--	2.15×10^{-15}
	298	2.10×10^{-20}	1.24	1.20×10^{5}	3.12×10^{-15}	--	--	--	3.12×10^{-15}
	325	9.17×10^{-21}	1.20	4.13×10^{5}	4.54×10^{-15}	--	--	--	4.54×10^{-15}
1'	275	4.91×10^{-20}	2.53	2.99×10^{3}	3.71×10^{-15}	--	--	--	3.71×10^{-15}
	298	2.10×10^{-20}	2.24	1.19×10^{5}	5.60×10^{-15}	--	--	--	5.60×10^{-15}
	325	9.17×10^{-21}	2.00	3.73×10^{5}	6.84×10^{-15}	--	--	--	6.84×10^{-15}
2	275	4.14×10^{-20}	1.48	16.0	9.80×10^{-19}	64.9	9.05×10^{-2}	2.43×10^{-19}	1.22×10^{-18}
	298	1.67×10^{-20}	1.39	89.0	2.07×10^{-18}	26.0	7.53×10^{-1}	3.27×10^{-19}	2.39×10^{-18}
	325	6.82×10^{-21}	1.32	4.86×10^{2}	4.38×10^{-18}	12.4	6.13	5.18×10^{-19}	4.90×10^{-18}
2'	275	4.14×10^{-20}	2.21	15.5	1.42×10^{-18}	90.2	9.13×10^{-2}	3.41×10^{-19}	1.76×10^{-18}
	298	1.67×10^{-20}	1.89	88.7	2.80×10^{-18}	35.1	7.26×10^{-1}	4.26×10^{-19}	3.23×10^{-1}
	325	6.82×10^{-21}	1.77	4.78×10^{2}	5.77×10^{-18}	14.6	5.77	5.74×10^{-19}	6.34×10^{-1}
3	275	3.54×10^{-19}	1.53	3.81×10^{5}	2.06×10^{-13}	--	--	--	2.06×10^{-13}
	298	1.20×10^{-19}	1.43	9.81×10^{5}	1.68×10^{-13}	--	--	--	1.68×10^{-13}
	325	4.16×10^{-20}	1.35	2.49×10^{6}	1.40×10^{-13}	--	--	--	1.40×10^{-13}
3'	275	3.54×10^{-19}	1.88	3.81×10^{5}	2.54×10^{-13}	--	--	--	2.54×10^{-13}
	298	1.20×10^{-19}	1.73	9.77×10^{5}	2.03×10^{-13}	--	--	--	2.03×10^{-13}
	325	4.16×10^{-20}	1.59	2.47×10^{6}	1.63×10^{-13}	--	--	--	1.63×10^{-13}
4	275	2.06×10^{-19}	1.97	59.9	2.43×10^{-17}	56.8	1.44×10^{-2}	1.68×10^{-19}	2.45×10^{-17}
	298	7.08×10^{-20}	1.76	3.09×10^{2}	3.84×10^{-17}	23.4	1.31×10^{-1}	2.17×10^{-19}	3.87×10^{-17}
	325	2.48×10^{-20}	1.60	1.56×10^{3}	6.19×10^{-17}	11.5	1.16	3.31×10^{-19}	6.22×10^{-17}
5	275	3.52×10^{-20}	3.68	9.94×10^{-1}	1.29×10^{-19}	83.6	1.86×10^{-3}	5.47×10^{-21}	1.34×10^{-19}
	298	1.44×10^{-20}	2.90	6.80	2.85×10^{-19}	30.7	2.04×10^{-2}	9.02×10^{-21}	2.93×10^{-19}
	325	6.05×10^{-21}	2.37	45.6	6.54×10^{-19}	13.8	2.19×10^{-1}	1.83×10^{-20}	6.72×10^{-19}
6	275	6.44×10^{-20}	2.59	5.99	9.99×10^{-19}	69.6	1.04×10^{-2}	4.66×10^{-20}	1.05×10^{-18}
	298	2.61×10^{-20}	2.20	33.1	1.90×10^{-18}	27.2	9.46×10^{-2}	6.72×10^{-20}	1.97×10^{-18}
	325	1.08×10^{-20}	1.91	1.79×10^{2}	3.69×10^{-18}	12.8	8.38×10^{-1}	1.16×10^{-19}	3.81×10^{-18}
7	275	2.61×10^{-20}	2.26	11.1	6.55×10^{-19}	--	--	--	6.55×10^{-19}
	298	1.32×10^{-20}	1.97	53.3	1.39×10^{-18}	--	--	--	1.39×10^{-18}
	325	6.79×10^{-21}	1.75	2.52×10^{2}	2.99×10^{-18}	--	--	--	2.99×10^{-18}

8	275	5.94×10^{-20}	3.07	26.2	4.78×10^{-18}	--	--	--	4.78×10^{-18}
	298	2.46×10^{-20}	2.52	1.34×10^{2}	8.31×10^{-18}	--	--	--	8.31×10^{-18}
	325	1.04×10^{-20}	2.13	6.71×10^{2}	1.49×10^{-17}	--	--	--	1.49×10^{-17}
9	275	1.69×10^{-19}	3.03	3.23×10^{3}	1.65×10^{-15}	--	--	--	1.65×10^{-15}
	298	6.59×10^{-20}	2.50	1.15×10^{4}	1.89×10^{-15}	--	--	--	1.89×10^{-15}
	325	2.62×10^{-20}	2.12	4.00×10^{4}	2.22×10^{-15}	--	--	--	2.22×10^{-15}
10	275	1.76×10^{-20}	1.94	76.3	2.61×10^{-18}	--	--	--	2.61×10^{-18}
	298	7.53×10^{-21}	1.74	3.71×10^{2}	4.86×10^{-18}	--	--	--	4.86×10^{-18}
	325	3.28×10^{-21}	1.58	1.77×10^{3}	8.17×10^{-18}	--	--	--	8.17×10^{-18}
11	275	7.03×10^{-21}	1.80	17.9	2.27×10^{-19}	--	--	--	2.27×10^{-19}
	298	3.93×10^{-21}	1.63	87.2	5.58×10^{-19}	--	--	--	5.58×10^{-19}
	325	2.23×10^{-21}	1.50	4.17×10^{2}	1.39×10^{-18}	--	--	--	1.39×10^{-18}
12	275	1.53×10^{-19}	1.98	4.71×10^{4}	1.43×10^{-14}	--	--	--	1.43×10^{-14}
	298	6.26×10^{-20}	1.77	1.23×10^{5}	1.36×10^{-14}	--	--	--	1.36×10^{-14}
	325	2.61×10^{-20}	1.61	3.16×10^{5}	1.33×10^{-14}	--	--	--	1.33×10^{-14}
13	275	3.67×10^{-19}	1.06	3.39×10^{10}	1.32×10^{-8}	--	--	--	1.32×10^{-8}
	298	1.12×10^{-19}	1.05	3.95×10^{10}	4.65×10^{-9}	--	--	--	4.65×10^{-9}
	325	3.51×10^{-20}	1.04	4.55×10^{-10}	1.66×10^{-9}	--	--	--	1.66×10^{-9}
14	275	3.73×10^{-17}	2.03	2.47×10^{6}	1.87×10^{-10}	--	--	--	1.87×10^{-10}
	298	6.62×10^{-18}	1.81	5.89×10^{6}	7.06×10^{-11}	--	--	--	7.06×10^{-11}
	325	1.19×10^{-18}	1.63	1.39×10^{7}	2.70×10^{-11}	--	--	--	2.70×10^{-11}
15	275	8.26×10^{-16}	2.48	1.13×10^{4}	2.31×10^{-11}	--	--	--	2.31×10^{-11}
	298	1.36×10^{-16}	2.12	4.26×10^{4}	1.23×10^{-11}	--	--	--	1.23×10^{-11}
	325	2.30×10^{-17}	1.86	1.59×10^{5}	6.80×10^{-12}	--	--	--	6.80×10^{-12}

(a) Using CCSD(T)/aug-cc-ρVQZ results are:

Entry	T (K)	k_{eq}	κ	k_2	k_{TS1}	κ	k_2	k_{TS2}	k_{Total}
1	275	5.69×10^{-20}	1.29	1.79×10^{4}	1.31×10^{-15}	--	--	--	1.31×10^{-15}
	298	2.41×10^{-20}	1.24	5.55×10^{4}	1.66×10^{-15}	--	--	--	1.66×10^{-15}
	325	1.04×10^{-20}	1.20	1.69×10^{5}	2.11×10^{-15}	--	--	--	2.11×10^{-15}

Table S3. Calculated values of equilibrium constants (k_{eq} in cm^3 $molecule^{-1}$), tunneling parameters, κ, unimolecular rate constants (k_2 in s^{-1}), rate constants (k_{TS} in cm^3 $molecule^{-1}$ s^{-1}), and the overall rate constant k_{total} ($k_{Total} = k_{TS1} + k_{TS2}$ in cm^3 $molecule^{-1}$ s^{-1}) for the reaction of carbonyl oxides **2**, **4**, **5** and **6** with deuterated water.

			Deuterated Water addition			Hydrogen/Deuterium tranfer			
Entry	**T (K)**	k_{eq}	**κ**	k_2	k_{TS1}	**κ**	k_2	k_{TS2}	k_{Total}
2	275	2.27×10^{-20}	1.39	7.13	2.25×10^{-19}	25.8	1.94×10^{-2}	1.14×10^{-20}	2.36×10^{-19}
	298	9.37×10^{-21}	1.31	47.4	5.82×10^{-19}	12.7	1.73×10^{-1}	2.06×10^{-20}	6.03×10^{-19}
	325	3.95×10^{-21}	1.26	2.34×10^{2}	1.16×10^{-18}	7.22	1.51	4.31×10^{-20}	1.20×10^{-18}
4	275	1.11×10^{-19}	1.62	19.0	3.42×10^{-18}	19.4	2.36×10^{-2}	5.08×10^{-20}	3.47×10^{-18}
	298	3.91×10^{-20}	1.50	1.05×10^{2}	6.16×10^{-18}	10.2	2.28×10^{-1}	9.09×10^{-20}	6.25×10^{-18}
	325	1.41×10^{-20}	1.40	5.66×10^{2}	1.12×10^{-17}	6.18	2.16	1.88×10^{-19}	1.14×10^{-17}
5	275	4.62×10^{-22}	2.15	2.50×10^{-1}	2.48×10^{-22}	27.7	5.50×10^{-4}	7.04×10^{-24}	2.55×10^{-22}
	298	1.65×10^{-22}	1.89	1.85	5.77×10^{-22}	13.2	6.51×10^{-3}	1.42×10^{-23}	5.91×10^{-22}
	325	5.99×10^{-23}	1.69	13.5	1.37×10^{-21}	7.36	7.54×10^{-2}	3.32×10^{-23}	1.40×10^{-21}
6	275	3.59×10^{-20}	1.84	1.63	1.08×10^{-19}	24.0	3.01×10^{-3}	2.59×10^{-21}	1.11×10^{-19}
	298	1.49×10^{-20}	1.67	97.3	2.42×10^{-19}	11.9	2.94×10^{-2}	5.21×10^{-21}	2.47×10^{-19}
	325	6.32×10^{-21}	1.52	56.9	5.47×10^{-19}	6.89	2.81×10^{-1}	1.22×10^{-20}	5.59×10^{-19}

Table S4. Branching ratios at different temperatures of the reactions of carbonyl oxides **2**, **4**, **5** and **6** with water.

Entry	T (K)	Water Addition	Hydrogen Transfer
2	275	80.1	19.9
	298	86.3	13.7
	325	89.4	10.6
4	275	99.3	0.7
	298	99.4	0.6
	325	99.5	0.5
5	275	95.9	4.1
	298	96.9	3.1
	325	97.3	2.7
6	275	95.5	4.5
	298	96.6	3.4
	325	97.0	3.0

Table S5. Branching ratios at different temperatures of the reactions of carbonyl oxides **2**, **4**, **5** and **6** with deuterated water.

Entry	T (K)	Water Addition	Hydrogen Transfer
2	275	95.2	4.6
	298	96.6	3.4
	325	96.5	3.5
4	275	98.5	1.5
	298	98.5	1.5
	325	98.3	1.7
5	275	97.2	2.8
	298	97.6	2.4
	325	97.6	2.4
6	275	97.6	2.4
	298	97.9	2.1
	325	97.8	2.2

Cartesian coordinates in Ångstroms for all structures studied in this work

H2O B3LYP/6-311+G(2df,2p)

H	0.000000	0.763192	-0.466890
O	0.000000	0.000000	0.116723
H	0.000000	-0.763192	-0.466890

1 B3LYP/6-311+G(2df,2p)

C	1.069372	-0.196934	0.000000
O	0.000000	0.457253	0.000000
O	-1.177507	-0.198929	0.000000
H	1.030080	-1.279279	0.000000
H	1.973742	0.394290	0.000000

1 CASSCF(8,8)/6-311+G(2df,2p)

O	0.001774	-0.000720	0.000054
O	1.358679	0.003136	-0.000075
C	1.951894	1.134194	-0.000008
H	1.373003	2.033649	-0.000020
H	3.019149	1.080319	0.000048

1 CASPT2(8,8)/6-311+G(2df,2p)

O	0.015766	-0.001277	-0.000251
O	1.349704	0.004884	0.000209
C	1.951491	1.136819	0.000040
H	1.363778	2.039869	-0.000241
H	3.023760	1.070283	0.000243

1 CR B3LYP/6-311+G(2df,2p)

O	0.366626	-1.170952	-0.016672
O	1.290071	-0.170057	0.022554
C	0.922996	1.026217	-0.004236
H	-0.131748	1.280411	-0.050167
H	1.734746	1.740605	0.030412
O	-2.021743	0.264198	-0.031084
H	-1.362872	-0.456667	-0.011546
H	-2.857736	-0.107169	0.258341

1 CR CASSCF(8,8)/6-311+G(2df,2p)

O	0.441161	-1.160038	-0.006544
O	1.392662	-0.160115	0.014966
C	0.993144	1.039152	0.000329
H	-0.054327	1.263722	-0.020882
H	1.777529	1.767369	0.016253
O	-2.143827	0.237081	-0.071213
H	-1.507090	-0.465149	-0.029355
H	-2.958910	-0.115436	0.294048

1 CR CASPT2(8,8)/6-311+G(2df,2p)

O	0.0000	0.0000	0.0000
O	1.3526	0.0000	0.0000
C	1.9759	1.1074	0.0000
H	1.4310	2.0403	0.0077
H	3.0466	0.9962	-0.0019
O	-0.5898	2.7699	0.0048
H	-0.6706	1.8014	0.0257
H	-1.4121	3.1091	0.3628

1 TS-add B3LYP/6-311+G(2df,2p)

O	-0.952600	-0.940575	0.167499

O	-0.882159	0.403458	-0.374742
C	0.056648	0.996342	0.245719
H	0.193625	0.821812	1.304664
H	0.410256	1.915556	-0.210811
O	1.437134	-0.381739	-0.006433
H	0.542137	-0.952060	0.076490
H	1.695092	-0.412506	-0.935247

1 TS CASSCF(8,8)/6-311+G(2df,2p)

O	-0.9831814666	-0.9537691617	0.1970812116
O	-0.8938012923	0.4106406234	-0.3929365922
C	0.0888026400	0.9576407847	0.2392222654
H	0.1674960654	0.8232945341	1.2985522281
H	0.4715698937	1.8551310558	-0.2103672188
O	1.3944452955	-0.3325832393	-0.0188650144
H	0.5880995992	-0.9484537301	0.0772456848
H	1.6667022652	-0.3616138668	-0.9227935646

1 TS CASPT2(8,8)/6-311+G(2df,2p)

O	-0.961368	-0.926978	0.176301
O	-0.876207	0.408202	-0.387255
C	0.046225	1.003118	0.246900
H	0.187336	0.799201	1.296770
H	0.396922	1.925373	-0.197438
O	1.449972	-0.378462	-0.009615
H	0.569504	-0.935972	0.083426
H	1.687748	-0.444194	-0.941949

1 HHP B3LYP/6-311+G(2df,2p)

C	0.612635	0.541510	0.284956

O	1.380002	-0.593716	-0.014340
O	-0.613251	0.575757	-0.402026
O	-1.484452	-0.418967	0.183095
H	0.442660	0.527104	1.359563
H	1.099275	1.469113	-0.028606
H	-1.189399	-1.227495	-0.260028
H	1.713261	-0.522367	-0.914495

2 B3LYP/6-311+G(2df,2p)

C	0.000000	0.847343	0.000000
O	-0.970509	0.043046	0.000000
O	-0.683812	-1.290821	0.000000
H	-0.310976	1.885252	0.000000
C	1.391356	0.386050	0.000000
H	2.087246	1.219809	0.000000
H	1.555079	-0.261606	0.866740
H	1.555079	-0.261606	-0.866740

2 CR B3LYP/6-311+G(2df,2p)

O	-0.138543	-1.207915	0.647882
O	0.771511	-0.975330	-0.364863
C	1.229339	0.189741	-0.484070
C	0.864512	1.301203	0.395807
H	-0.180335	1.576835	0.209039
H	0.898682	0.962207	1.433853
H	1.511821	2.157440	0.229520
H	1.927193	0.272353	-1.310671
H	-1.603693	-0.256902	0.128187
O	-2.148915	0.466677	-0.241916
H	-2.989201	0.074947	-0.489175

2 TS-add B3LYP/6-311+G(2df,2p)

O	-1.236084	-0.623307	-0.667600
O	-0.610389	-0.795485	0.634189
C	0.508396	-0.159414	0.627738
C	1.539255	-0.276705	-0.437528
H	0.852530	0.060387	1.637258
O	-0.262795	1.525304	-0.069294
H	-0.877751	0.759546	-0.540486
H	-0.809015	1.921666	0.619127
H	2.194940	0.589639	-0.425570
H	2.136789	-1.161664	-0.194791
H	1.090751	-0.404959	-1.415162

2 HHP B3LYP/6-311+G(2df,2p)

C	1.053235	-1.164304	-0.183700
C	0.527914	0.111327	0.433824
O	0.844548	1.185348	-0.421389
O	-0.861086	0.085222	0.734549
O	-1.610788	-0.282616	-0.446164
H	0.942702	0.271063	1.435218
H	-1.659631	0.560522	-0.918543
H	0.692828	2.012203	0.047381
H	2.139161	-1.118011	-0.242683
H	0.764355	-2.017157	0.427225
H	0.652296	-1.294394	-1.185317

2 TS-absH B3LYP/6-311+G(2df,2p)

C	1.146529	0.398105	-0.297632
O	0.931598	-0.869706	-0.299838
O	-0.154069	-1.310969	0.519569

H	1.911265	0.648880	-1.027942
C	0.422959	1.359484	0.413269
H	-0.777297	1.092490	-0.087012
H	0.135791	1.057144	1.418006
H	0.787232	2.372942	0.315954
O	-1.752694	0.245714	-0.403170
H	-1.112518	-0.613164	0.050005
H	-2.560075	0.375865	0.104677

2 Cp-absH B3LYP/6-311+G(2df,2p)

C	1.220050	0.293212	-0.452556
O	0.675509	-0.947690	-0.501630
O	-0.104922	-1.238767	0.671353
H	1.797495	0.432285	-1.359132
C	1.104886	1.223180	0.490475
H	-1.493319	1.166977	-0.332108
H	0.565224	1.049892	1.407308
H	1.622841	2.160093	0.358590
O	-2.141146	0.453133	-0.280380
H	-0.970528	-0.859524	0.411948
H	-2.906858	0.818525	0.171134

2 P-absH B3LYP/6-311+G(2df,2p)

C	1.422900	-0.560289	0.009904
H	0.969324	-1.536708	-0.026185
H	2.498536	-0.485249	0.033726
C	0.710172	0.555353	0.012455
H	1.139672	1.549603	0.031619
O	-0.646081	0.707558	-0.018257
O	-1.305048	-0.574164	-0.095523

H -1.796938 -0.565185 0.736926

3 B3LYP/6-311+G(2df,2p)

C -1.362066 1.130219 0.000000

C 0.000000 0.558910 0.000000

O 0.142465 -0.686902 0.000000

O 1.405487 -1.209315 0.000000

H 0.908252 1.155463 0.000000

H -2.113569 0.344735 0.000000

H -1.502953 1.767381 0.876991

H -1.502953 1.767381 -0.876991

3 CR B3LYP/6-311+G(2df,2p)

O -0.901079 1.376308 0.105673

O 0.360120 0.914138 -0.242676

C 0.777230 -0.133311 0.299658

H 0.131766 -0.619592 1.023962

C 2.100648 -0.658922 -0.083574

H 2.582392 -0.022396 -0.820903

H 2.735040 -0.747980 0.801677

H 1.982520 -1.667706 -0.487763

H -1.839871 -0.161785 0.013066

O -1.980261 -1.133233 -0.011349

H -2.689354 -1.284850 -0.639723

3 TS-add B3LYP/6-311+G(2df,2p)

O 1.668970 -0.584904 0.085367

O 0.317622 -0.939838 -0.312326

C -0.478714 -0.198440 0.364759

H -0.212877 0.010062 1.394336

C -1.897156 -0.135253 -0.062302

O	0.466511	1.507091	-0.004355
H	1.270407	0.752354	0.016897
H	0.348247	1.753625	-0.928878
H	-2.313368	0.834026	0.205093
H	-1.999858	-0.308419	-1.130562
H	-2.462160	-0.898289	0.478883

3 HHP B3LYP/6-311+G(2df,2p)

C	-1.686414	-0.653923	-0.008464
C	-0.383963	0.042787	0.332186
O	-0.365717	1.406299	-0.027619
O	0.625841	-0.675169	-0.350569
O	1.907622	-0.234028	0.144619
H	-0.167321	0.027776	1.400143
H	1.992306	0.636524	-0.272265
H	-0.715019	1.497747	-0.921391
H	-2.510916	-0.134956	0.476423
H	-1.850956	-0.649456	-1.087338
H	-1.667796	-1.687638	0.330648

4 B3LYP/6-311+G(2df,2p)

C	0.000000	0.378238	0.000000
O	-0.775650	-0.620260	0.000000
O	-0.205867	-1.874440	0.000000
C	1.458148	0.168600	0.000000
C	-0.655135	1.711697	0.000000
H	1.999548	1.110633	0.000000
H	1.730069	-0.442070	0.865185
H	1.730069	-0.442070	-0.865185
H	-0.344109	2.284030	0.877335
H	-0.344109	2.284030	-0.877335

H -1.737410 1.611836 0.000000

4 CR B3LYP/6-311+G(2df,2p)

C 0.895792 -0.024667 0.062910

O 0.270406 1.050271 -0.152613

O -0.910136 1.268615 0.555092

O -2.310370 -0.759515 -0.642011

C 0.409527 -1.004029 1.048566

C 2.128927 -0.214528 -0.742700

H -1.992286 0.070224 -0.224093

H -3.107931 -0.531431 -1.123934

H 1.152413 -1.774511 1.235671

H 0.129360 -0.479408 1.963788

H -0.514044 -1.456072 0.672043

H 2.040531 -1.130211 -1.331941

H 2.298349 0.629159 -1.405915

H 2.988929 -0.343371 -0.082019

4 TS-add B3LYP/6-311+G(2df,2p)

C 0.457353 0.123337 -0.162871

O -0.429511 -0.119327 -1.078105

O -1.748000 0.179312 -0.550760

O -0.559372 -0.867712 1.255101

C 0.456929 1.400952 0.614189

C 1.761455 -0.567776 -0.395589

H -1.363117 -0.460321 0.580516

H -0.509559 -1.812157 1.070343

H 0.961827 1.270431 1.566758

H 1.017059 2.131191 0.022076

H -0.550334 1.767469 0.767745

H 2.224246 -0.805067 0.560204

H	1.626056	-1.473567	-0.980337
H	2.434464	0.104751	-0.931579

4 HHP B3LYP/6-311+G(2df,2p)

C	0.374291	0.033204	0.036864
O	-0.697456	-0.648570	-0.625276
O	-1.965531	-0.097027	-0.214385
O	0.293785	-0.205505	1.431155
C	0.314917	1.537415	-0.161278
C	1.613528	-0.608290	-0.576802
H	-2.056120	-0.457239	0.680112
H	0.526369	-1.124797	1.600889
H	1.195777	1.999796	0.280407
H	0.282744	1.770319	-1.223740
H	-0.571341	1.947092	0.314148
H	2.502909	-0.203372	-0.097779
H	1.593924	-1.689544	-0.433836
H	1.662925	-0.407410	-1.644855

4 TS-absH B3LYP/6-311+G(2df,2p)

O	1.075487	1.260179	0.390256
O	-0.274222	1.108141	-0.063250
C	-0.821203	-0.045476	0.156075
C	-0.162584	-1.104921	0.802917
H	0.863439	-1.226947	-0.007882
H	0.443923	-0.797660	1.651551
H	-0.765503	-1.989246	0.962370
C	-2.171319	-0.157094	-0.471486
H	-2.414243	0.735596	-1.041143
H	-2.193798	-1.025145	-1.131222

H	-2.924089	-0.314277	0.301909
H	1.623443	0.346720	-0.191137
O	1.891907	-0.722868	-0.707620
H	2.752085	-1.047705	-0.424579

4 Cp-absH B3LYP/6-311+G(2df,2p)

C	-0.513669	-0.776152	1.235988
C	-0.901798	-0.081248	0.165502
O	-0.275527	1.021241	-0.344304
O	0.887211	1.402606	0.409021
O	2.247517	-0.847116	-0.615491
H	1.531547	-1.353085	-0.207813
H	0.320487	-0.467567	1.844006
H	-1.098338	-1.626306	1.549630
H	1.566212	0.825034	0.003152
H	3.065854	-1.256067	-0.321006
C	-2.095130	-0.376191	-0.690431
H	-1.798318	-0.538255	-1.727267
H	-2.608793	-1.261564	-0.325398
H	-2.788680	0.465508	-0.675460

4 P-absH B3LYP/6-311+G(2df,2p)

H	-2.211761	-0.355135	0.786221
O	-1.865271	-0.138466	-0.090256
O	-0.573575	-0.773120	-0.028128
C	0.450406	0.147993	0.000371
C	0.306261	1.467657	0.007024
H	-0.660978	1.939499	-0.022897
H	1.186722	2.089879	0.028062

C	1.741442	-0.609951	0.011718
H	1.832033	-1.230446	-0.880882
H	2.577003	0.084367	0.043090
H	1.799089	-1.269671	0.878795

5 B3LYP/6-311+G(2df,2p)

C	0.000000	0.023464	0.000000
O	0.850073	0.980871	0.000000
O	0.374152	2.255399	0.000000
C	-1.437500	0.349553	0.000000
C	0.602005	-1.286040	0.000000
H	-2.060983	-0.537913	0.000000
H	-1.657929	0.976174	0.867257
H	-1.657929	0.976174	-0.867257
C	-0.067414	-2.443975	0.000000
H	1.685240	-1.283030	0.000000
H	0.462014	-3.385513	0.000000
H	-1.146757	-2.494064	0.000000

5 CR B3LYP/6-311+G(2df,2p)

O	-1.502556	1.199039	0.404084
O	-0.246779	1.177213	-0.160036
C	0.543699	0.229128	0.168324
C	0.111030	-0.791725	1.138441
C	1.824149	0.305146	-0.497340
O	-2.554154	-1.113440	-0.688123
H	-2.361162	-0.219957	-0.337736
H	-3.305869	-1.015507	-1.276279
H	-0.680429	-1.399290	0.690088
H	0.932572	-1.425818	1.453452

H	-0.346136	-0.288602	1.992098
C	2.815875	-0.577286	-0.346489
H	1.938346	1.150602	-1.164216
H	3.745055	-0.457916	-0.884554
H	2.737021	-1.437586	0.302121

5 TS-add B3LYP/6-311+G(2df,2p)

O	-2.123296	-0.246006	-0.373760
O	-0.834423	-0.754417	-0.770182
C	0.103698	0.013583	-0.275059
C	0.046483	1.500604	-0.424851
C	1.380955	-0.699247	-0.188426
O	-0.758039	0.079766	1.552952
H	-1.644212	-0.056520	0.814998
H	-0.609901	-0.770762	1.980446
H	0.588767	1.995551	0.374374
H	0.513196	1.752817	-1.380428
H	-0.982538	1.838127	-0.429165
C	2.545439	-0.123910	0.100107
H	1.313932	-1.766625	-0.358705
H	3.451760	-0.709364	0.163906
H	2.635605	0.935852	0.291876

5 HHP B3LYP/6-311+G(2df,2p)

O	-2.249272	-0.456428	-0.175795
O	-0.905853	-0.738690	-0.618257
C	0.022096	0.151345	0.024922
C	-0.359033	1.613689	-0.159019
C	1.319315	-0.194381	-0.671978
O	0.047448	-0.106553	1.408969
H	-2.259442	-0.868344	0.700298

H	0.440302	-0.976762	1.545237
H	0.398172	2.244147	0.301549
H	-0.423758	1.849583	-1.219251
H	-1.321471	1.809728	0.305107
C	2.486315	-0.333393	-0.060207
H	1.239692	-0.300503	-1.746792
H	3.384257	-0.560878	-0.617437
H	2.591508	-0.207166	1.009644

5 TS-absH B3LYP/6-311+G(2df,2p)

O	1.688608	-1.084654	0.357710
O	0.323634	-1.213381	-0.029519
C	-0.444208	-0.182784	0.205248
C	-1.772469	-0.405581	-0.361581
C	-2.817430	0.399115	-0.178400
H	-2.759951	1.297975	0.418820
H	-3.773573	0.171938	-0.627700
H	-1.868404	-1.306943	-0.953436
C	0.028286	0.996483	0.810093
H	0.984756	1.302884	-0.039527
H	-0.712436	1.763766	0.985476
H	0.706324	0.817176	1.641230
O	2.061760	1.010516	-0.769567
H	2.845129	1.504444	-0.508143
H	2.021059	-0.094489	-0.237867

5 Cp-absH B3LYP/6-311+G(2df,2p)

O	-1.506064	1.301857	0.341716
O	-0.269298	1.115305	-0.360979

C 0.518150 0.142986 0.201121

C 1.719574 -0.005360 -0.635448

C 2.912399 -0.392612 -0.194670

H 3.096375 -0.607937 0.849269

H 3.746566 -0.499605 -0.873546

H 1.584244 0.249395 -1.680226

C 0.220198 -0.562541 1.296851

H -1.694435 -1.554671 -0.202998

H 0.899474 -1.331312 1.627971

H -0.651759 -0.344269 1.890423

O -2.464447 -1.160696 -0.633954

H -3.226472 -1.659388 -0.326556

H -2.057449 0.601218 -0.065734

5 P-absH B3LYP/6-311+G(2df,2p)

O -2.273360 -0.160597 -0.172207

O -0.979501 -0.784626 -0.086100

C 0.025848 0.149842 0.072438

C 1.294368 -0.581801 0.199976

C 2.482066 -0.123823 -0.183627

H 2.597440 0.839090 -0.662527

H 3.378217 -0.707669 -0.028555

H 1.213209 -1.572521 0.632920

C -0.147327 1.468890 0.114216

H 0.706115 2.104387 0.285887

H -1.115954 1.920532 -0.013069

H -2.685867 -0.500684 0.633779

6 B3LYP/6-311+G(2df,2p)

C 0.000000 0.327369 0.000000

O	0.634162	-0.778265	0.000000
O	2.000455	-0.728163	0.000000
C	0.763054	1.590035	0.000000
C	-1.448164	0.257193	0.000000
H	0.106297	2.454927	0.000000
H	1.430045	1.605705	0.865798
H	1.430045	1.605705	-0.865798
C	-2.171121	-0.867839	0.000000
H	-1.947462	1.217498	0.000000
H	-3.250634	-0.828521	0.000000
H	-1.707846	-1.844436	0.000000

6 CR B3LYP/6-311+G(2df,2p)

O	-1.183030	-0.862753	-1.077478
O	0.097315	-0.782635	-0.557723
C	0.536647	0.365405	-0.231745
C	-0.291241	1.567860	-0.436100
C	1.875189	0.409235	0.333289
O	-2.613652	-0.062282	1.141923
H	-2.248607	-0.473964	0.331355
H	-3.227515	-0.698616	1.514479
H	-1.143169	1.540812	0.250896
H	0.285930	2.473690	-0.275111
H	-0.721121	1.538921	-1.439063
C	2.629922	-0.660684	0.599272
H	2.246088	1.402554	0.547539
H	3.618029	-0.547061	1.020975
H	2.282194	-1.665868	0.406853

6 TS-add B3LYP/6-311+G(2df,2p)

O	-1.680183	-1.011056	-0.503009

O	-0.277953	-0.775777	-0.773633
C	0.082253	0.346558	-0.214261
C	-0.697661	1.605625	-0.416579
C	1.524917	0.455232	0.046192
O	-0.858365	-0.064894	1.531395
H	-1.468907	-0.616345	0.739063
H	-0.330098	-0.724493	1.993672
H	-0.535047	2.292261	0.409147
H	-0.320993	2.069285	-1.333913
H	-1.754374	1.398062	-0.529065
C	2.361523	-0.578967	-0.005365
H	1.883807	1.448020	0.283513
H	3.419384	-0.447337	0.173026
H	2.012036	-1.576322	-0.233390

6 HHP B3LYP/6-311+G(2df,2p)

O	-1.875629	-1.050185	-0.153815
O	-0.440125	-1.006788	-0.049699
C	-0.003480	0.348374	0.041247
C	-0.536373	1.211588	-1.092407
C	1.506512	0.289456	0.050118
O	-0.478572	0.918364	1.254007
H	-2.143932	-0.846255	0.754510
H	0.013872	0.526509	1.984278
H	-0.086125	2.201096	-1.040851
H	-0.289375	0.755113	-2.048189
H	-1.615142	1.311938	-1.012045
C	2.257886	-0.786085	-0.138900
H	1.962940	1.254773	0.239067
H	3.336636	-0.716763	-0.104525
H	1.828472	-1.757528	-0.336544

6 TS-absH B3LYP/6-311+G(2df,2p)

C	-0.423216	0.283556	-0.338506
C	-1.796392	0.564918	0.078719
H	-2.091431	1.601990	-0.006198
C	-2.657599	-0.351974	0.519342
H	-3.666036	-0.075874	0.792495
H	-2.381383	-1.392282	0.615938
C	0.493784	1.298718	-0.676481
H	1.365012	1.120202	0.281470
H	1.188324	1.024267	-1.467006
H	0.067973	2.289465	-0.760887
O	-0.095813	-0.973370	-0.269537
O	1.277623	-1.278372	-0.522368
H	1.842317	-0.570873	0.290590
O	2.176447	0.337234	1.021564
H	3.109715	0.547864	0.917883

6 Cp-absH B3LYP/6-311+G(2df,2p)

C	0.549176	0.512392	0.182880
C	1.862480	0.289884	-0.423347
H	2.305147	1.179066	-0.854483
C	2.513664	-0.870999	-0.467652
H	3.486980	-0.938494	-0.932409
H	2.101221	-1.774667	-0.043188
C	-0.061363	1.704236	0.196586
H	-1.874619	0.247707	-1.491473
H	-1.005585	1.858343	0.690273
H	0.439129	2.548833	-0.249971

O	0.046284	-0.642802	0.714791
O	-1.237386	-0.450503	1.327703
H	-1.829056	-0.605305	0.561981
O	-2.488668	-0.434978	-1.194936
H	-3.368809	-0.102299	-1.391988

6 P-absH B3LYP/6-311+G(2df,2p)

C	0.011636	0.458593	-0.000473
C	-1.448714	0.402560	0.020008
H	-1.921495	1.375961	0.055662
C	-2.194781	-0.700879	-0.003110
H	-3.273270	-0.635872	0.013726
H	-1.759243	-1.688615	-0.043413
C	0.709943	1.596069	0.000380
H	1.785322	1.613078	-0.031760
H	0.174965	2.532120	0.020857
O	0.551502	-0.806476	-0.027957
O	1.988264	-0.765439	-0.083109
H	2.207084	-1.159417	0.772616

7 B3LYP/6-311+G(2df,2p)

C	0.000000	0.573418	0.000000
O	1.188769	0.103160	0.000000
O	1.405150	-1.243472	0.000000
C	-1.212442	-0.193090	0.000000
C	-0.046061	2.067795	0.000000
H	-0.581003	2.432121	0.880000
H	0.959396	2.479300	0.000000
H	-0.581003	2.432121	-0.880000
C	-1.344730	-1.531642	0.000000

H	-2.106436	0.419871	0.000000
H	-2.338217	-1.962216	0.000000
H	-0.484694	-2.177591	0.000000

7 CR B3LYP/6-311+G(2df,2p)

O	0.966378	0.032213	1.119097
O	-0.031247	-0.804494	0.668463
C	-1.014878	-0.331180	0.009851
C	-1.225338	1.044293	-0.345003
C	-2.003331	-1.372522	-0.403043
O	2.977521	-0.345132	-0.827423
H	2.345229	-0.239002	-0.092171
H	3.694598	-0.872280	-0.468433
H	-2.089365	-1.395278	-1.491011
H	-1.697638	-2.352481	-0.048641
H	-2.991098	-1.135462	-0.003682
C	-0.447716	2.101810	-0.055995
H	-2.131260	1.202740	-0.917985
H	-0.744946	3.083267	-0.402976
H	0.460846	1.993382	0.508941

7 TS-add B3LYP/6-311+G(2df,2p)

O	0.432548	1.702945	-0.474447
O	-0.339472	0.607178	-1.038741
C	-0.349211	-0.387143	-0.201827
C	0.859363	-0.940562	0.431220
C	-1.504086	-1.318857	-0.395237
O	-0.764563	0.789781	1.392678
H	-0.163475	1.454567	0.692154
H	-1.680145	1.084621	1.326211
H	-1.742042	-1.808939	0.546389

H	-2.373298	-0.786818	-0.771848
H	-1.222711	-2.092746	-1.112499
C	2.101248	-0.665403	0.048047
H	0.663497	-1.675589	1.200348
H	2.938342	-1.187539	0.490540
H	2.307835	0.085007	-0.700436

7 HHP B3LYP/6-311+G(2df,2p)

O	0.588304	1.878302	-0.133179
O	-0.187747	0.869859	-0.815555
C	-0.429346	-0.233916	0.052286
C	0.823883	-0.916969	0.543973
C	-1.292759	-1.165743	-0.795854
O	-1.126386	0.216925	1.204945
H	-0.000078	2.114587	0.601000
H	-2.034706	0.418324	0.953859
H	-1.542587	-2.052863	-0.217064
H	-2.212980	-0.660490	-1.094328
H	-0.755103	-1.469056	-1.690845
C	2.006757	-0.839670	-0.043385
H	0.676253	-1.528519	1.425874
H	2.855533	-1.387149	0.342340
H	2.169089	-0.217726	-0.912639

8 B3LYP/6-311+G(2df,2p)

C	0.000000	0.352992	0.000000
O	1.267608	0.525276	0.000000
O	2.112567	-0.543327	0.000000
C	-0.561736	-0.971029	0.000000
C	-0.787520	1.618530	0.000000
H	-1.429846	1.675673	0.880000

H	-0.113871	2.471146	0.000000
H	-1.429846	1.675673	-0.880000
C	-1.877855	-1.211271	0.000000
H	0.166203	-1.769491	0.000000
H	-2.255707	-2.223815	0.000000
H	-2.615664	-0.420113	0.000000

8 CR B3LYP/6-311+G(2df,2p)

O	-1.389198	-0.888805	-0.960880
O	-0.282942	-1.289707	-0.238668
C	0.663468	-0.465732	-0.012420
C	0.621703	0.881011	-0.519223
C	1.775780	-1.035920	0.799842
O	-2.381572	0.955081	0.847996
H	-2.191924	0.269852	0.174608
H	-3.221947	0.704545	1.237929
H	1.879983	-0.487891	1.737536
H	1.572132	-2.079492	1.022695
H	2.723040	-0.962493	0.264454
C	1.593172	1.770308	-0.291032
H	-0.255186	1.131844	-1.095781
H	1.526361	2.773536	-0.687106
H	2.472500	1.539543	0.295073

8 TS-add B3LYP/6-311+G(2df,2p)

O	1.779726	-0.879822	-0.434860
O	1.099254	0.327890	-0.846547
C	-0.065456	0.357316	-0.249433
C	-0.919499	-0.834675	-0.310254
C	-0.647799	1.730198	-0.156368
O	0.711048	-0.095069	1.547741

H	1.396487	-0.631739	0.789099
H	1.207756	0.669738	1.861590
H	-1.320999	1.798362	0.694254
H	0.143286	2.467999	-0.055372
H	-1.219085	1.945135	-1.060546
C	-2.201276	-0.854573	0.041713
H	-0.425838	-1.710371	-0.706068
H	-2.793438	-1.749605	-0.086714
H	-2.704218	-0.003099	0.479135

8 HHP B3LYP/6-311+G(2df,2p)

O	1.766890	-1.149200	-0.333295
O	1.055813	0.005255	-0.825015
C	0.001030	0.357637	0.085679
C	-0.898703	-0.817864	0.374576
C	-0.658230	1.542869	-0.604020
O	0.569079	0.722606	1.332348
H	2.290044	-0.765368	0.385794
H	0.992607	1.582900	1.238124
H	-1.458660	1.930607	0.021626
H	0.080628	2.328104	-0.766023
H	-1.061895	1.257843	-1.572336
C	-2.141279	-0.966144	-0.057614
H	-0.440672	-1.580968	0.988670
H	-2.711279	-1.850055	0.193314
H	-2.641940	-0.231351	-0.673191

9 B3LYP/6-311+G(2df,2p)

C	2.204456	-0.224874	0.000000
C	0.882868	-0.469580	0.000000
C	0.290189	-1.850979	0.000000

C	0.000000	0.663036	0.000000
O	-1.252055	0.481970	0.000000
O	-2.063334	1.575437	0.000000
H	0.348489	1.690929	0.000000
H	2.926085	-1.029264	0.000000
H	2.593021	0.784512	0.000000
H	-0.341670	-2.003047	0.875580
H	-0.341670	-2.003047	-0.875580
H	1.073784	-2.604961	0.000000

9 CR B3LYP/6-311+G(2df,2p)

O	-1.699382	-1.380839	-0.056385
O	-0.348742	-1.118551	-0.012238
C	0.045944	0.082374	-0.046678
H	-0.701362	0.869501	-0.097847
C	1.458414	0.350254	-0.004718
O	-2.876027	1.127042	0.013376
H	-2.671193	0.168618	0.006344
H	-3.719719	1.227261	0.459181
C	1.828050	1.641591	-0.041516
C	2.422203	-0.799214	0.075918
H	2.869284	1.930821	-0.014383
H	1.095989	2.435562	-0.099464
H	2.240663	-1.396826	0.969767
H	2.303739	-1.466738	-0.778142
H	3.448131	-0.439440	0.098485

9 TS-add B3LYP/6-311+G(2df,2p)

O	-2.295084	-0.451317	-0.405241
O	-0.916947	-0.887079	-0.384781
C	-0.181795	0.173357	-0.463720

H	-0.505690	0.966688	-1.124551
C	1.234062	0.036324	-0.135990
O	-1.204345	1.212452	0.907179
H	-1.979261	0.513940	0.407817
H	-1.023265	0.862488	1.786481
C	2.049086	1.015152	-0.539560
C	1.680367	-1.177486	0.627250
H	3.109965	0.989425	-0.331434
H	1.674722	1.873602	-1.080429
H	1.173000	-1.242542	1.590954
H	1.437565	-2.091360	0.084508
H	2.753649	-1.148770	0.801511

9 HHP B3LYP/6-311+G(2df,2p)

O	2.420861	-0.322346	-0.561979
O	1.046720	0.050840	-0.798322
C	0.289138	-0.321861	0.340954
H	0.527693	-1.349668	0.607738
C	-1.163178	-0.167165	-0.050200
O	0.668068	0.452176	1.460540
H	2.691748	0.328906	0.102774
H	0.320145	1.345051	1.361999
C	-1.972055	-1.217691	0.030007
C	-1.617332	1.191651	-0.508026
H	-3.020550	-1.143656	-0.226814
H	-1.615691	-2.186149	0.354346
H	-1.468679	1.955377	0.261282
H	-1.061220	1.513539	-1.389258
H	-2.678074	1.181640	-0.750393

10 B3LYP/6-311+G(2df,2p)

O	0.506604	-1.988032	0.000000
O	-0.750583	-1.466800	0.000000
C	-0.948604	-0.214046	0.000000
C	0.000000	0.873119	0.000000
H	-2.009022	0.011119	0.000000
C	-0.553935	2.101236	0.000000
C	1.490104	0.667727	0.000000
H	0.058294	2.991923	0.000000
H	-1.626017	2.245054	0.000000
H	1.805114	0.094109	0.868536
H	1.805114	0.094109	-0.868536
H	1.992960	1.634136	0.000000

10 CR B3LYP/6-311+G(2df,2p)

O	-1.373738	0.813259	0.847005
O	-0.562689	1.507154	-0.025973
C	0.561726	1.044940	-0.373066
C	1.243250	-0.166215	0.015422
H	1.054126	1.716826	-1.068191
O	-2.192412	-1.229400	-0.821880
H	-2.070774	-0.485428	-0.197722
H	-3.117327	-1.207048	-1.076534
C	2.447443	-0.318164	-0.569970
C	0.686544	-1.175124	0.980592
H	3.065175	-1.180554	-0.362821
H	2.840960	0.407485	-1.268927
H	0.388152	-0.703510	1.913220
H	-0.201680	-1.651105	0.568629
H	1.438299	-1.937401	1.181266

10 TS-add B3LYP/6-311+G(2df,2p)

O	-0.290791	0.243364	0.215742
O	0.074089	0.160122	1.617060
C	1.368513	0.119425	1.702651
C	2.262465	-0.844059	1.048448
H	1.714281	0.492938	2.663364
O	1.655490	1.628927	0.425689
H	0.703721	1.156178	0.072502
H	1.407813	2.443750	0.877528
C	3.426284	-1.046625	1.677034
C	1.861552	-1.601042	-0.183369
H	4.141848	-1.771051	1.313631
H	3.699881	-0.497987	2.568454
H	0.867621	-2.029939	-0.074812
H	1.819667	-0.941219	-1.048107
H	2.581742	-2.394541	-0.378011

10 HHP B3LYP/6-311+G(2df,2p)

O	-1.509680	0.492468	-1.205036
O	-1.302738	-0.753427	-0.500286
C	-0.302826	-0.588702	0.502432
C	1.033122	-0.088038	-0.005270
H	-0.206796	-1.623146	0.845487
O	-0.756188	0.253276	1.533538
H	-2.147490	0.938131	-0.630174
H	-1.474182	-0.187790	1.998286
C	1.937807	-0.988465	-0.376696
C	1.282606	1.391841	-0.050064
H	2.904670	-0.690932	-0.759866
H	1.742523	-2.051724	-0.322952
H	0.595057	1.880746	-0.739970
H	1.127727	1.840827	0.931152

H	2.303087	1.595527	-0.370096

11 B3LYP/6-311+G(2df,2p)

C	-1.348771	0.767775	0.000000
C	0.000000	0.806281	0.000000
C	0.824568	-0.365094	0.000000
O	0.496687	-1.597291	0.000000
O	-0.806550	-1.968871	0.000000
C	0.767253	2.110624	0.000000
H	-1.906013	1.696392	0.000000
H	-1.877913	-0.168622	0.000000
H	1.408287	2.196067	0.879287
H	1.408287	2.196067	-0.879287
H	0.083701	2.956563	0.000000
H	1.904255	-0.264679	0.000000

11 CR B3LYP/6-311+G(2df,2p)

O	-1.210541	0.485737	-0.133502
O	-0.636384	-0.751083	-0.106548
C	0.628177	-0.871255	-0.042187
C	1.653124	0.128755	0.014456
O	-3.999180	-0.038197	0.218861
H	-3.051486	0.150034	0.093271
H	-4.410152	0.180337	-0.620272
C	1.397970	1.453587	0.008451
H	2.222960	2.153287	0.056737
H	0.390778	1.826992	-0.041336
C	3.060421	-0.422091	0.085745
H	3.200687	-1.041970	0.972905
H	3.290746	-1.040137	-0.783743
H	3.785963	0.386894	0.123883

H	0.901192	-1.921074	-0.030718

11 TS-add B3LYP/6-311+G(2df,2p)

O	-1.807447	-0.684311	-0.468067
O	-1.343709	-0.337869	0.868174
C	-0.185150	0.225060	0.768639
C	1.005552	-0.288318	0.073077
O	-0.737530	1.470728	-0.696064
H	-1.351065	0.558712	-0.866258
H	-1.333667	2.129963	-0.321798
C	1.027907	-1.528266	-0.417058
H	1.943460	-1.940092	-0.820364
H	0.141952	-2.144379	-0.429275
C	2.188508	0.638694	0.071258
H	1.972443	1.524895	-0.526368
H	2.436052	0.977928	1.080158
H	3.064719	0.145726	-0.343945
H	0.014693	0.875848	1.620008

11 HHP B3LYP/6-311+G(2df,2p)

O	1.862978	0.681988	-0.667518
O	1.460163	0.206550	0.638251
C	0.226628	-0.478942	0.541432
C	-0.961208	0.342649	0.085872
O	0.352533	-1.617596	-0.286017
H	2.068833	-0.147583	-1.123602
H	0.897177	-2.268473	0.168011
C	-0.909625	1.668441	0.054673
H	-1.782627	2.248739	-0.212912
H	-0.003753	2.209468	0.281395
C	-2.204089	-0.443158	-0.225977

H	-2.059227	-1.076254	-1.101551
H	-2.470605	-1.109498	0.598928
H	-3.044328	0.223502	-0.410631
H	0.078895	-0.781375	1.586632

12 B3LYP/6-311+G(2df,2p)

C	0.003428	-1.852580	0.000000
C	-0.674565	-0.694952	0.000000
C	0.000000	0.585443	0.000000
O	1.261761	0.663149	0.000000
O	1.838086	1.895253	0.000000
C	-2.180572	-0.623428	0.000000
H	-0.518042	-2.799063	0.000000
H	1.083462	-1.878741	0.000000
H	-2.615164	-1.620452	0.000000
H	-2.550548	-0.092384	0.878976
H	-2.550548	-0.092384	-0.878976
H	-0.537678	1.528906	0.000000

12 CR B3LYP/6-311+G(2df,2p)

O	1.822236	-1.317978	0.075519
O	0.454781	-1.192634	0.006009
C	-0.064692	-0.042819	0.059826
C	-1.504383	0.118415	-0.004283
O	2.741571	1.296718	-0.032517
H	2.639372	0.322843	-0.012348
H	3.577765	1.479660	-0.466023
C	-2.326145	-0.936476	-0.103083
H	-3.397508	-0.801598	-0.148182
H	-1.949817	-1.948605	-0.139563
C	-1.988040	1.544516	0.052114

H	-3.073244	1.587631	-0.002909
H	-1.672684	2.030193	0.977268
H	-1.579537	2.131262	-0.772486
H	0.606500	0.807949	0.144714

12 TS-add B3LYP/6-311+G(2df,2p)

O	-2.360195	-0.306629	-0.385480
O	-1.046946	-0.913080	-0.296855
C	-0.187265	0.036115	-0.447653
C	1.205359	-0.188165	-0.048154
O	-1.067701	1.327179	0.803503
H	-1.907327	0.715768	0.370419
H	-0.922364	1.011100	1.702501
C	1.533262	-1.271412	0.660586
H	2.559404	-1.462354	0.943145
H	0.788731	-1.992862	0.965135
C	2.182550	0.864927	-0.488904
H	3.183951	0.645625	-0.125331
H	2.221877	0.934686	-1.577926
H	1.884627	1.845831	-0.114474
H	-0.413604	0.793652	-1.188066

12 HHP B3LYP/6-311+G(2df,2p)

O	2.494306	0.208225	-0.443421
O	1.201244	0.730332	-0.077853
C	0.266562	-0.317596	-0.204871
C	-1.129724	0.247673	-0.060852
O	0.523029	-1.335221	0.749194
H	2.697808	-0.363397	0.312753
H	0.216473	-1.022370	1.608620
C	-1.356170	1.464148	0.425372

H	-2.366936	1.833316	0.539750
H	-0.552168	2.127583	0.707468
C	-2.222097	-0.691369	-0.491106
H	-3.203808	-0.262796	-0.299038
H	-2.147396	-0.907905	-1.559821
H	-2.152024	-1.648167	0.028986
H	0.407983	-0.800080	-1.173335

13 B3LYP/6-311+G(2df,2p)

C	0.000000	0.387109	0.000000
O	-0.745716	-0.585649	0.000000
O	-0.137246	-1.871369	0.000000
F	1.277043	0.343760	0.000000
F	-0.492188	1.582184	0.000000

13 CASSCF(8,8)/6-311+G(2df,2p)

C	-0.008077	0.388319	-0.000000
O	-0.779464	-0.555384	-0.000000
O	-0.090864	-1.876321	0.000000
F	1.239717	0.330254	0.000000
F	-0.459418	1.569170	-0.000000

13 CASPT2(12,12)/6-311+G(2df,2p)

C	0.000503	0.385522	-0.000000
O	-0.754056	-0.586332	-0.000000
O	-0.127529	-1.851719	0.000000
F	1.271587	0.332470	0.000000
F	-0.488611	1.576093	-0.00000

13 CR B3LYP/6-311+G(2df,2p)

C	0.717401	0.074085	0.016880
O	0.072720	0.945732	-0.559000
O	-1.091608	1.422522	0.139643
O	-1.583186	-1.301431	-0.184354
F	0.556703	-0.303062	1.219672
F	1.712665	-0.478088	-0.584822
H	-1.834810	-0.371570	-0.025112
H	-2.077309	-1.577167	-0.960133

13 TS-add B3LYP/6-311+G(2df,2p)

C	-0.462683	-0.263465	-0.009056
O	0.453287	-0.831676	-0.636219
O	1.737670	-0.558430	0.027121
O	0.388518	1.610741	-0.027310
F	-0.561064	-0.234254	1.271722
F	-1.603366	-0.123734	-0.603509
H	1.230233	1.056950	0.049115
H	0.389931	1.980648	-0.917428

13 HHP B3LYP/6-311+G(2df,2p)

C	-0.383831	-0.002059	0.020188
O	0.734285	-0.376029	-0.729694
O	1.906503	-0.070891	0.044579
O	-0.477018	1.328786	0.284048
F	-0.420942	-0.643593	1.185797
F	-1.410003	-0.427056	-0.749717
H	2.152056	0.799198	-0.301673
H	-0.680726	1.794071	-0.535644

14 B3LYP/6-311+G(2df,2p)

C	-0.344365	-0.263761	-0.013552
O	-1.523380	-0.640044	-0.014385
O	-2.508105	0.423423	0.027890
O	0.059516	0.983080	0.065322
O	0.635676	-1.159692	-0.098601
C	1.885083	-0.464820	0.122992
C	1.498823	0.999174	-0.097632
H	2.213423	-0.671482	1.140193
H	2.612017	-0.842780	-0.588850
H	1.911167	1.681410	0.638691
H	1.716498	1.355165	-1.102690

14 CR B3LYP/6-311+G(2df,2p)

C	-0.052413	-0.611916	-0.019891
O	1.011613	-1.229617	-0.208559
O	2.124333	-0.734420	0.596685
O	1.611054	1.659081	-0.625477
O	-0.274362	0.238787	0.943716
O	-1.075118	-0.816751	-0.831250
H	2.003559	0.902120	-0.125342
H	2.219621	1.830572	-1.347526
C	-1.512006	0.929825	0.635940
C	-2.194777	-0.041888	-0.326307
H	-2.046683	1.087662	1.566309
H	-1.241975	1.876868	0.174350
H	-2.883334	-0.726484	0.165629
H	-2.676173	0.436490	-1.172793

14 TS-add B3LYP/6-311+G(2df,2p)

C	-0.162368	-0.376195	-0.081999
O	-1.282224	-0.992255	-0.226917
O	-2.311435	0.019099	-0.503578
O	-0.911604	1.097459	1.080715
O	0.328471	0.445620	-0.995465
O	0.765532	-0.977662	0.644039
H	-1.785622	0.785981	0.389703
H	-1.109002	0.736461	1.951431
C	1.645052	0.819663	-0.541040
C	2.048472	-0.392616	0.301017
H	2.265776	0.980190	-1.416174
H	1.555853	1.729930	0.047614
H	2.614881	-1.137957	-0.254019
H	2.561253	-0.137805	1.223220

14 HHP B3LYP/6-311+G(2df,2p)

C	0.238035	0.341941	0.092012
O	1.122639	-0.216695	-0.878750
O	2.141485	-0.976690	-0.201474
O	0.895823	1.270668	0.871496
O	-0.311432	-0.623499	0.908480
O	-0.766331	0.923552	-0.669891
H	2.745964	-0.282502	0.099363
H	1.128026	2.015793	0.305056
C	-1.708768	-0.734103	0.612410
C	-1.834537	-0.030596	-0.734255
H	-1.976707	-1.787660	0.580529
H	-2.281451	-0.231593	1.394015
H	-1.676021	-0.709821	-1.573083
H	-2.765666	0.513644	-0.865761

15 B3LYP/6-311+G(2df,2p)

C	0.000000	0.342423	0.000000
O	-1.085311	-0.248333	0.000000
O	-0.920375	-1.701714	0.000000
C	1.395995	0.341155	0.000000
C	0.752795	1.516633	0.000000
H	2.329595	-0.192709	0.000000
H	0.823151	2.591818	0.000000

15 CR B3LYP/6-311+G(2df,2p)

C	-0.780082	-0.352209	-0.056667
O	-0.041643	-1.324504	-0.291837
O	1.264241	-1.202537	0.366751
O	1.576637	1.378028	-0.221507
C	-1.025328	0.878301	0.536856
C	-1.980342	0.324748	-0.226059
H	1.641867	0.406817	-0.004475
H	2.305536	1.574774	-0.813535
H	-2.957880	0.409332	-0.669940
H	-0.668886	1.696133	1.135915

15 TS-add B3LYP/6-311+G(2df,2p)

C	-0.418185	-0.255335	-0.145115
O	0.601071	-0.980853	-0.443609
O	1.706992	-0.543371	0.413072
O	0.631709	1.490854	-0.152075
C	-1.383396	0.058830	0.825261
C	-1.792835	-0.176978	-0.415158
H	1.386573	0.660882	0.191717

H	0.884487	1.751451	-1.044055
H	-2.607435	-0.237015	-1.115562
H	-1.615303	0.332543	1.838878

15 HHP B3LYP/6-311+G(2df,2p)

C	-0.317604	0.152421	-0.082230
O	0.803516	-0.407430	-0.708989
O	1.866199	-0.537615	0.277482
O	-0.090774	1.497642	0.253045
C	-1.225572	-0.645656	0.739456
C	-1.632580	-0.381135	-0.465818
H	2.163245	0.379828	0.367219
H	0.047964	1.996487	-0.559966
H	-2.386591	-0.457961	-1.228978
H	-1.401611	-1.092914	1.700976