- SUPPORTING INFORMATION -

Psychiatric Disorders and Oxidative Injury: Antioxidant Effects of Zolpidem Therapy disclosed *in silico*

Marco Bortoli,[a] Marco Dalla Tiezza,[a] Cecilia Muraro,[a] Chiara Pavan,[b] Giovanni Ribaudo,[c]

Anna Rodighiero,[a] Cristina Tubaro,[a] Giuseppe Zagotto,[c] Laura Orian*,[a]

[a] Dipartimento di Scienze Chimiche, Università degli Studi di Padova, Via Marzolo 1, 35131 Padova, Italy.
[b] Dipartimento di Medicina, Università degli Studi di Padova, Via Giustiniani 2, 35128 Padova, Italy.
[c] Dipartimento di Scienze del Farmaco, Università degli Studi di Padova, Via Marzolo 5, 35131 Padova, Italy.

LIST of TABLES and FIGURES:

Table S1. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO$^{\bullet}$, HOO$^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and $CH_2CHOO^{\bullet}$ radicals through HAT from all the sites of **1** (Scheme 1). Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G°_{HAT,gas}$					$\Delta G°_{HAT,water}$					$\Delta G°_{HAT,benzene}$				
	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	CH_2=$CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	CH_2=$CHOO^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	CH_2=$CHOO^{\bullet}$
C1	-21.7	9.9	-7.2	11.5	8.6	-25.9	6.5	-10.8	7.8	4.3	-23.1	9.0	-8.0	10.8	7.5
C2	-22.6	8.9	-8.1	10.5	7.7	-25.4	7.0	-10.4	8.3	4.7	-23.8	8.2	-8.8	10.1	6.7
C4	-33.3	-1.7	-18.8	-0.1	-3.0	-34.4	-1.9	-19.3	-0.7	-4.2	-33.8	-1.7	-18.7	-0.1	-3.2
C6	-1.2	30.4	13.3	31.9	29.0	-5.2	27.3	9.9	28.5	25.0	-2.8	29.2	12.3	31.1	27.8
C8	-25.2	6.4	-10.7	8.0	5.1	-29.5	3.0	-14.4	4.2	0.7	-26.3	5.8	-11.2	7.6	4.3
C9	-3.9	27.7	10.6	29.3	26.4	-7.7	24.8	7.4	26.0	22.5	-5.2	26.9	9.9	28.8	25.4
C10	-1.2	30.4	13.3	31.9	29.0	-5.6	26.9	9.5	28.1	24.6	-2.7	29.4	12.4	31.2	27.9
C14	-6.8	24.8	7.7	26.4	23.5	-9.8	22.7	5.3	24.0	20.4	-7.6	24.4	7.4	26.3	22.9
C15	-3.9	27.6	10.6	29.2	26.4	-7.9	24.6	7.2	25.8	22.3	-5.3	26.8	9.8	28.6	25.3
C17	-24.7	6.9	-10.2	8.5	5.6	-29.3	3.2	-14.2	4.4	0.9	-25.9	6.1	-10.8	8.0	4.7
C18	-4.2	27.4	10.3	29.0	26.1	-8.4	24.1	6.7	25.4	21.8	-5.6	26.5	9.5	28.3	25.0
C19	-2.9	28.7	11.6	30.3	27.4	-8.7	23.8	6.4	25.1	21.5	-4.8	27.3	10.3	29.2	25.8

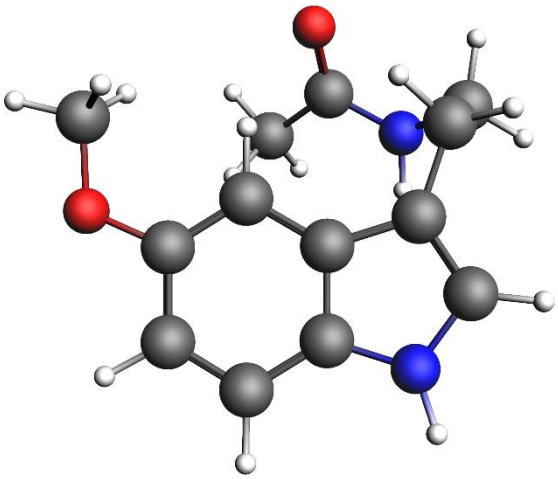
Table S2. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of $HO^{\bullet}$, $HOO^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and $CH_2{=}CHOO^{\bullet}$ radicals through HAT from C4 for **1** and its metabolites. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G°_{HAT,gas}$					$\Delta G°_{HAT,water}$					$\Delta G°_{HAT,benzene}$				
	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$
1	-33.3	-1.7	-18.8	-0.1	-3.0	-34.4	-1.9	-19.3	-0.7	-4.2	-33.8	-1.7	-18.7	-0.1	-3.2
MI	-35.4	-3.8	-20.8	-2.2	-5.1	-34.6	-2.1	-19.5	-0.9	-4.4	-34.8	-2.7	-19.7	-0.9	-4.2
MII	-34.9	-3.3	-20.4	-1.7	-4.6	-34.2	-1.8	-19.2	-0.5	-4.1	-34.3	-2.3	-19.3	-0.4	-3.8
MIII	-34.7	-3.1	-20.2	-1.5	-4.4	-34.0	-1.5	-18.9	-0.2	-3.8	-34.1	-2.1	-19.1	-0.2	-3.6
MIV	-35.5	-3.9	-20.1	-2.3	-5.2	-35.2	-2.7	-20.1	-1.4	-5.0	-35.0	-3.0	-20.0	-1.1	-4.5
MX	-36.4	-4.8	-21.9	-3.2	-6.8	-35.7	-3.3	-20.7	-2.0	-5.6	-35.9	-3.8	-20.8	-2.0	-5.3
MXI	-37.0	-5.4	-22.5	-3.8	-6.7	-36.5	-4.0	-21.4	-2.7	-6.3	-36.1	-4.1	-21.0	-2.2	-5.6

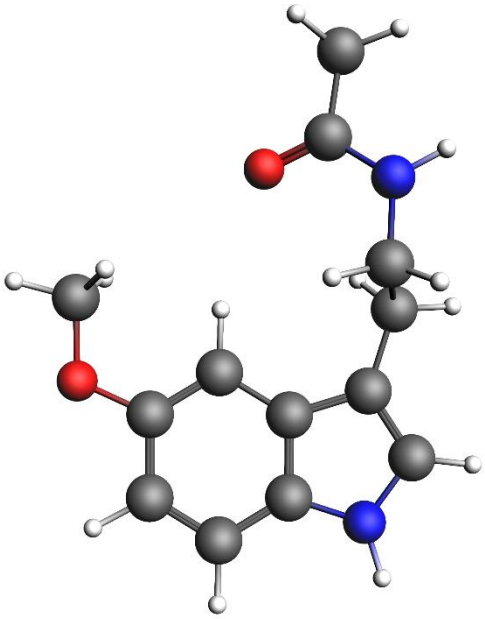
Table S3. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of $HO^{\bullet}$, $HOO^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and $CH_2{=}CHOO^{\bullet}$ radicals through HAT from neutral Trolox (see Scheme 1 in the text). For comparison the values of HAT from C4 of zolpidem **1** are also included. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G°_{HAT,gas}$					$\Delta G°_{HAT,water}$					$\Delta G°_{HAT,benzene}$				
	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$
C1	-28.3	3.3	-13.8	4.9	2.0	-31.0	1.5	-15.9	2.8	-0.8	-28.6	3.5	-13.5	5.3	2.0
C2	-27.4	4.2	-12.9	5.8	2.9	-29.5	2.9	-14.4	4.2	0.6	-27.3	4.7	-12.3	6.6	3.3
C3	-27.7	3.9	-13.2	5.4	2.6	-30.4	2.1	-15.3	3.3	-0.2	-27.9	4.1	-12.9	6.0	2.6
C4	-16.6	15.0	-2.1	16.6	13.7	-19.0	13.5	-3.9	14.7	11.2	-16.9	15.2	-1.8	17.0	13.7
C5	-19.4	12.2	-4.9	13.8	10.9	-21.7	10.7	-6.6	12.0	8.5	-19.7	12.4	-4.6	14.2	10.9
C6	-31.4	0.2	-16.9	1.8	-1.2	-33.5	-1.0	-18.4	0.2	-3.3	-31.7	0.3	-16.7	2.2	-1.2
O1	-38.7	-7.1	-24.2	-5.5	-8.4	-41.7	-9.3	-26.7	-8.0	-11.6	-39.9	-7.8	-24.8	-6.0	-9.3
O2	-6.6	25.0	8.0	26.6	23.7	-5.6	26.9	9.5	28.2	24.6	-7.2	24.9	7.9	26.7	23.4
1	-33.3	-1.7	-18.8	-0.1	-3.0	-34.4	-1.9	-19.3	-0.7	-4.2	-33.8	-1.7	-18.7	-0.1	-3.2

Figure S1. Conformers of melatonin **2** considered in this work.



Conformer 2a



Conformer 2b

Table S4. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of $HO^{\bullet}$, $HOO^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and $CH_2{=}CHOO^{\bullet}$ radicals through HAT from C4 site of melatonin **2** (see Scheme 1 in the text). Two lowest energy conformers of melatonin, **2a** and **2b**, have been considered (Figure S1)[a]. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G°_{HAT,gas}$					$\Delta G°_{HAT,water}$					$\Delta G°_{HAT,benzene}$				
	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$
2a	-28.9	2.8	-14.3	4.3	1.5	-33.8	-1.3	-18.7	-0.1	-3.6	-31.3	0.8	-16.2	2.7	-0.7
2b	-28.6	3.0	-14.1	4.5	1.7	-31.0	1.4	-16.0	2.7	-0.9	-29.1	3.0	-14.0	4.9	1.5
1	-33.3	-1.7	-18.8	-0.1	-3.0	-34.4	-1.9	-19.3	-0.7	-4.2	-33.8	-1.7	-18.7	-0.1	-3.2

[a] Fogueri UR, Kozuch S, Karton A, Martin JML. The Melatonin Conformer Space: Benchmark and Assessment of Wave Function and DFT Methods for a Paradigmatic Biological and Pharmacological Molecule. J Phys Chem A 2013;117:2269–77.

Table S5. $\Delta G°_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of $HO^{\bullet}$, $HOO^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and $CH_2{=}CHOO^{\bullet}$ radicals through HAT from the OH or COOH sites of zolpidem metabolites (see Scheme 3 in the text). For comparison the values of HAT from C4 of zolpidem **1** are also included. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G°_{HAT,gas}$					$\Delta G°_{HAT,water}$					$\Delta G°_{HAT,benzene}$				
	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	$CH_2{=}CHOO^{\bullet}$
1	-33.3	-1.7	-18.8	-0.1	-3.0	-34.4	-1.9	-19.3	-0.7	-4.2	-33.8	-1.7	-18.7	-0.1	-3.2
MI	-5.0	26.6	9.5	28.2	25.3	-5.3	27.2	9.8	28.4	25.3	-5.6	26.4	9.4	28.3	25.0
MII	5.6	37.2	20.1	38.8	35.9	4.4	36.8	19.4	38.1	34.5	5.1	37.1	20.2	39.0	35.6
MIII	-14.1	17.5	0.4	19.1	16.2	-15.0	17.4	0.08	18.7	15.2	-14.8	17.2	0.2	19.1	15.7
MIV	-14.5	17.1	0.01	18.7	15.8	-15.2	17.2	-0.1	18.5	15.0	-15.2	16.8	-0.1	18.7	15.4
MX	-37.3	-5.7	-22.8	-4.1	-7.0	-40.8	-8.3	-25.7	-7.1	-10.6	-38.6	-6.5	-23.5	-4.7	-8.0
MXI	-14.0	17. 6	0.5	19.2	16.3	-14.6	17.9	0.5	19.2	15.6	-14.5	17.6	0.6	19.4	16.1

Table S6. $\Delta G^{\ddagger}_{HAT}$ (kcal mol^{-1}) in gas-phase, water and benzene, for the scavenging of HO$^{\bullet}$, HOO$^{\bullet}$, $CH_3O^{\bullet}$, $CH_3OO^{\bullet}$ and CH_2=$CHOO^{\bullet}$ through HAT from the OH or COOH sites of zolpidem metabolites (see Scheme 3 in the text). For comparison the values of HAT from C4 of zolpidem **1** are also included. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

	$\Delta G^{\ddagger}_{HAT,gas}$			$\Delta G^{\ddagger}_{HAT,water}$			$\Delta G^{\ddagger}_{HAT,benzene}$		
	HO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	HO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$	HO$^{\bullet}$	$CH_3O^{\bullet}$	$CH_3OO^{\bullet}$
MI	8.9	22.9	35.6	13.7	26.8	39.9	10.6	24.7	37.7
MII	12.6	21.5	33.7	19.7	26.3	37.3	15.0	23.4	35.6
MIII	9.9	16.2	27.3	14.2	20.4	30.9	11.3	18.1	29.3
MIV	8.6	15.9	30.9	14.2	20.9	33.3	10.5	17.9	32.6
MX	4.0	8.7	19.8	5.6	16.1	15.1	5.3	10.2	21.1
MXI	9.8	16.0	-	14.6	20.5		11.9	18.7	
1	5.4	9.4	19.3	7.8	11.4	21.7	7.2	11.9	22.9

Table S7. Coordinates and energies of the structures of melatonin and melatonin radicals at the C4 site. Level of theory: M06-2X/6-31G(d).

Melatonin

Conformer 2a
E = -764.661776389 Ha

N	-0.186892000	3.158686000	0.348801000
C	1.027742000	2.856951000	-0.228284000
C	1.029094000	1.559062000	-0.666709000
C	-0.268349000	1.028496000	-0.346754000
C	-0.849285000	-0.235918000	-0.558760000
C	-2.139458000	-0.445991000	-0.104076000
C	-2.865321000	0.587222000	0.537163000
C	-2.313807000	1.836441000	0.734219000
C	-1.003267000	2.049703000	0.286273000
H	-0.452884000	4.061685000	0.706699000
H	1.806614000	3.605436000	-0.284977000
H	-0.279149000	-1.017553000	-1.049555000
H	-3.874228000	0.363001000	0.866202000
H	-2.882059000	2.622020000	1.223192000
O	-2.803339000	-1.633037000	-0.216355000
C	-2.148286000	-2.659301000	-0.930437000
H	-1.191602000	-2.933627000	-0.467408000
H	-1.958183000	-2.358484000	-1.968190000
H	-2.820953000	-3.516970000	-0.915399000
C	2.146990000	0.771194000	-1.278663000
C	3.048887000	0.099942000	-0.226611000
N	2.320971000	-0.620136000	0.803814000
C	1.686147000	-1.795303000	0.535486000
C	0.828794000	-2.333053000	1.663911000
H	2.774853000	1.405656000	-1.914600000
H	1.729516000	-0.012859000	-1.918872000
H	3.658145000	0.855109000	0.278847000
H	3.720687000	-0.609567000	-0.717104000
H	2.011546000	-0.095817000	1.610190000
O	1.790409000	-2.364637000	-0.541363000
H	-0.165371000	-1.875825000	1.601778000
H	1.252591000	-2.111605000	2.646874000
H	0.727656000	-3.411781000	1.541215000

Conformer 2b
E = -764.659393102 Ha

N	-2.498515000	-2.484134000	-0.043777000
C	-1.205918000	-2.919814000	-0.240694000
C	-0.360501000	-1.847183000	-0.319845000
C	-1.177808000	-0.674954000	-0.160506000
C	-0.859523000	0.695594000	-0.154397000
C	-1.894358000	1.596544000	0.027540000
C	-3.229071000	1.154433000	0.194454000
C	-3.550414000	-0.187774000	0.185839000
C	-2.506839000	-1.105205000	0.007813000
H	-3.308156000	-3.077940000	0.030866000
H	-0.989243000	-3.976806000	-0.314955000
H	0.171765000	1.011682000	-0.282559000
H	-3.994787000	1.910577000	0.331081000
H	-4.578576000	-0.512706000	0.314508000
O	-1.727597000	2.949974000	0.064899000
C	-0.406158000	3.422665000	-0.084629000
H	0.012866000	3.138904000	-1.057738000
H	0.252302000	3.030567000	0.699845000
H	-0.462395000	4.509118000	-0.011640000
C	1.124162000	-1.804598000	-0.498237000
C	1.823122000	-1.306134000	0.778658000
N	3.179923000	-0.843562000	0.542219000
C	3.405418000	0.395199000	0.030075000
C	4.853641000	0.748035000	-0.245900000
H	1.371669000	-1.102364000	-1.304124000
H	1.519552000	-2.785171000	-0.786468000
H	1.846944000	-2.092945000	1.537575000
H	1.262595000	-0.463220000	1.190904000
H	3.950787000	-1.487478000	0.632689000
O	2.500110000	1.186277000	-0.195150000
H	4.980182000	0.888896000	-1.322227000
H	5.560925000	-0.008177000	0.102306000
H	5.075471000	1.700333000	0.239744000

Melatonin radical (C4)

Conformer 2a
E = -764.004880659 Ha

N	-0.522161000	2.985347000	0.199040000
C	0.614264000	2.225066000	0.290763000
C	0.327525000	0.897199000	-0.050722000
C	-1.095472000	0.886316000	-0.373480000
C	-1.962222000	-0.136183000	-0.785141000
C	-3.292933000	0.183057000	-1.016932000
C	-3.764496000	1.502452000	-0.842363000
C	-2.920779000	2.517087000	-0.437788000
C	-1.580959000	2.193123000	-0.206222000
H	-0.573243000	3.974656000	0.381971000
H	1.549205000	2.675451000	0.589179000
H	-1.588829000	-1.145090000	-0.918325000
H	-4.814206000	1.691010000	-1.039166000
H	-3.291190000	3.529154000	-0.306956000
O	-4.241389000	-0.709936000	-1.421093000
C	-3.827106000	-2.040380000	-1.620748000
H	-3.439427000	-2.481677000	-0.693752000
H	-3.055331000	-2.106245000	-2.398040000
H	-4.711740000	-2.590828000	-1.941110000
C	1.189958000	-0.206666000	-0.082988000
C	2.644470000	-0.148627000	0.245593000
N	2.981944000	-1.086842000	1.308657000
C	4.136628000	-1.808885000	1.302167000
C	4.323878000	-2.751789000	2.476887000
H	0.793214000	-1.173243000	-0.380203000
H	2.942436000	0.868860000	0.529537000
H	3.271888000	-0.434788000	-0.606591000
H	2.326489000	-1.191368000	2.069145000
O	4.970395000	-1.712815000	0.417924000
H	4.507356000	-3.755365000	2.087318000
H	3.470434000	-2.779226000	3.158375000
H	5.214754000	-2.445341000	3.030211000

Conformer 2b
E = -764.011241254 Ha

N	-2.191873000	-2.404178000	-0.609581000
C	-1.120280000	-3.002777000	-0.011268000
C	-0.218184000	-2.035520000	0.443701000
C	-0.821494000	-0.750034000	0.091007000
C	-0.445885000	0.590128000	0.299115000
C	-1.288347000	1.593726000	-0.163195000
C	-2.493856000	1.286369000	-0.831487000
C	-2.881712000	-0.021540000	-1.033093000
C	-2.037447000	-1.030102000	-0.560859000
H	-2.982172000	-2.885443000	-1.008018000
H	-1.046515000	-4.078893000	0.054787000
H	0.466288000	0.842652000	0.825169000
H	-3.107588000	2.113739000	-1.170661000
H	-3.814785000	-0.255379000	-1.536757000
O	-1.045076000	2.924490000	-0.017626000
C	0.114677000	3.295240000	0.700217000
H	1.029695000	2.939881000	0.214151000
H	0.095953000	2.896317000	1.721645000
H	0.111899000	4.384861000	0.732543000
C	0.999571000	-2.321774000	1.088103000
C	2.034767000	-1.296091000	1.419954000
N	2.568264000	-0.671764000	0.207178000
C	2.839623000	0.654835000	0.126014000
C	3.158844000	1.166280000	-1.264310000
H	1.230474000	-3.362671000	1.291791000
H	2.849844000	-1.754753000	1.989827000
H	1.641451000	-0.478965000	2.036640000
H	2.543890000	-1.221299000	-0.640334000
O	2.769414000	1.402376000	1.093116000
H	2.220276000	1.470289000	-1.741189000
H	3.638958000	0.412604000	-1.893456000
H	3.803350000	2.041201000	-1.178487000

Table S8. Coordinates and energies of the structures of zolpidem and zolpidem radicals at each available site. Level of theory: M06-2X/6-31G(d).

ZPD
E = -975.763621119 Ha

C	4.290733000	-0.700993000	0.137452000
N	0.537576000	-2.298214000	-0.378156000
C	-0.179679000	-1.192718000	-0.029876000
C	0.644796000	-0.139296000	0.335987000
C	4.204305000	-2.068153000	-0.278904000
C	2.998670000	-2.672626000	-0.483054000
C	1.806075000	-1.940139000	-0.257723000
N	1.924350000	-0.617558000	0.168061000
C	3.140569000	-0.001233000	0.341537000
H	-1.830669000	0.849750000	-0.718635000
H	2.906923000	-3.700748000	-0.812674000
C	5.634341000	-0.047069000	0.314434000
H	6.209751000	-0.077055000	-0.616540000
H	5.530087000	0.998993000	0.612416000
H	6.223320000	-0.562067000	1.080759000
C	-1.649255000	-1.187912000	-0.047444000
C	-2.360273000	-2.351828000	0.266879000
C	-3.747778000	-2.350715000	0.264405000
C	-4.472663000	-1.196046000	-0.053046000
C	-3.760258000	-0.045347000	-0.390092000
C	-2.367505000	-0.040371000	-0.395899000
H	-1.802771000	-3.251621000	0.507513000
H	-4.285620000	-3.262753000	0.513214000
H	-6.376011000	-2.053382000	-0.604365000
H	-4.301861000	0.854226000	-0.673870000
C	-5.979917000	-1.207974000	-0.033221000
H	-6.359717000	-1.300052000	0.990236000
H	-6.389872000	-0.289123000	-0.460432000
C	0.331492000	1.174331000	0.970212000
H	-0.672180000	1.110451000	1.393145000
H	1.020216000	1.355635000	1.808562000
C	0.500493000	2.347533000	0.005114000
H	0.465232000	4.201065000	-1.624181000
H	-0.085876000	5.329311000	-0.362419000
N	-0.493190000	3.282718000	-0.032369000
H	-2.265014000	2.476366000	0.826219000
O	1.501435000	2.414834000	-0.693971000
C	-0.337835000	4.421742000	-0.923851000
H	-1.269365000	4.591999000	-1.471559000
C	-1.588257000	3.331022000	0.928438000
H	-1.225796000	3.374353000	1.961004000
H	-2.162798000	4.238945000	0.738349000
H	5.125308000	-2.619000000	-0.448159000
H	3.105744000	1.054185000	0.582346000

C1
E = -975.103960631 Ha

C	4.286065000	-0.676534000	0.138266000
N	0.532738000	-2.279802000	-0.361188000
C	-0.184314000	-1.169984000	-0.027530000
C	0.640207000	-0.112916000	0.326680000
C	4.199643000	-2.048487000	-0.262167000
C	2.994206000	-2.655612000	-0.459531000
C	1.801401000	-1.920680000	-0.243574000
N	1.919674000	-0.593244000	0.166691000
C	3.135658000	0.025095000	0.333940000
H	-1.825341000	0.859974000	-0.766646000
H	2.902878000	-3.687532000	-0.777140000
C	5.629587000	-0.020696000	0.308292000
H	6.204849000	-0.060890000	-0.622348000
H	5.525557000	1.028544000	0.594913000
H	6.218377000	-0.527530000	1.080133000
C	-1.653894000	-1.161613000	-0.047793000
C	-2.370010000	-2.315411000	0.290820000
C	-3.757548000	-2.308529000	0.285970000
C	-4.477277000	-1.158311000	-0.058356000
C	-3.759843000	-0.018189000	-0.420040000
C	-2.367137000	-0.019330000	-0.422916000
H	-1.816768000	-3.212098000	0.552082000
H	-4.299553000	-3.212680000	0.553716000
H	-6.382653000	-2.020719000	-0.593925000
H	-4.297346000	0.876364000	-0.726483000
C	-5.984571000	-1.164014000	-0.041371000
H	-6.366660000	-1.231358000	0.983147000
H	-6.390175000	-0.253645000	-0.490282000
C	0.325096000	1.207882000	0.944780000
H	-0.683265000	1.146921000	1.356963000
H	1.003424000	1.392131000	1.791907000
C	0.501338000	2.369058000	-0.027985000
H	0.492695000	4.363803000	-1.619370000
N	-0.460728000	3.362739000	-0.034735000
H	-2.270033000	2.556351000	0.732840000
O	1.473669000	2.420508000	-0.765280000
C	-0.308525000	4.425459000	-0.902741000
H	-1.121229000	5.129524000	-0.984790000
C	-1.572349000	3.379042000	0.915133000
H	-1.209477000	3.319984000	1.944266000
H	-2.105343000	4.322003000	0.797681000
H	5.120756000	-2.601152000	-0.424594000
H	3.101770000	1.082713000	0.565533000

C2
E = -975.105411808 Ha

C	4.268362000	-0.746509000	0.156597000
N	0.487113000	-2.239667000	-0.450451000
C	-0.213194000	-1.140330000	-0.051982000
C	0.631026000	-0.118553000	0.359924000
C	4.156504000	-2.088481000	-0.328884000
C	2.939620000	-2.656504000	-0.567715000
C	1.761394000	-1.911124000	-0.311925000
N	1.903314000	-0.612124000	0.174572000
C	3.131704000	-0.033073000	0.388336000
H	-1.880692000	0.969909000	-0.524133000
H	2.827701000	-3.665584000	-0.946265000
C	5.623861000	-0.131909000	0.378439000
H	6.208718000	-0.129667000	-0.547103000
H	5.539067000	0.900563000	0.725878000
H	6.193076000	-0.696197000	1.124697000
C	-1.683361000	-1.125321000	-0.053881000
C	-2.391747000	-2.313302000	0.165029000
C	-3.778688000	-2.311489000	0.185082000
C	-4.506208000	-1.131289000	-0.010467000
C	-3.796892000	0.044850000	-0.249814000
C	-2.405052000	0.049454000	-0.281810000
H	-1.831910000	-3.231185000	0.314217000
H	-4.314181000	-3.242419000	0.357236000
H	-6.422312000	-1.942246000	-0.588012000
H	-4.337110000	0.971448000	-0.429170000
C	-6.012839000	-1.143089000	0.037718000
H	-6.373107000	-1.312084000	1.058504000
H	-6.428324000	-0.193687000	-0.310005000
C	0.341131000	1.179143000	1.040329000
H	-0.672420000	1.119471000	1.436047000
H	1.020649000	1.314280000	1.893751000
C	0.553156000	2.369835000	0.111272000
H	0.385733000	3.958469000	-1.816305000
H	0.229731000	5.217152000	-0.572558000
N	-0.459820000	3.298373000	-0.025289000
O	1.599904000	2.486419000	-0.509708000
C	-0.252503000	4.345739000	-1.025094000
H	-1.222907000	4.635775000	-1.431410000
C	-1.610401000	3.354624000	0.737695000
H	-1.658761000	2.837624000	1.681785000
H	-2.298213000	4.156800000	0.519445000
H	5.066772000	-2.649774000	-0.520301000
H	3.119765000	1.007908000	0.686477000

C4
E = -975.125687502 Ha

C	3.871632000	-1.594305000	0.026502000
N	-0.164215000	-2.369661000	0.025471000
C	-0.625621000	-1.113104000	-0.032800000
C	0.434314000	-0.149150000	-0.055943000
C	3.459405000	-2.957875000	0.077398000
C	2.132381000	-3.291229000	0.069742000
C	1.167707000	-2.267477000	0.015529000
N	1.588938000	-0.943602000	-0.048621000
C	2.924225000	-0.612857000	-0.034672000

H	-1.984449000	0.843230000	-1.397676000
H	1.780293000	-4.314828000	0.111966000
C	5.334926000	-1.241663000	0.028076000
H	5.846082000	-1.691179000	-0.829483000
H	5.479599000	-0.160182000	-0.021192000
H	5.826301000	-1.611174000	0.934217000
C	-2.069457000	-0.847567000	-0.064040000
C	-2.931609000	-1.710485000	0.627417000
C	-4.302129000	-1.504133000	0.606095000
C	-4.863230000	-0.440165000	-0.110109000
C	-4.004719000	0.400244000	-0.818237000
C	-2.627082000	0.202498000	-0.801606000
H	-2.502568000	-2.543297000	1.175292000
H	-4.955456000	-2.180205000	1.152640000
H	-6.892391000	-1.147304000	-0.314018000
H	-4.420464000	1.214841000	-1.405866000
C	-6.353591000	-0.217131000	-0.109070000
H	-6.694845000	0.149200000	0.865456000
H	-6.645576000	0.518245000	-0.863093000
C	0.292007000	1.234382000	0.056224000
H	-0.722912000	1.547073000	0.267278000
C	1.282448000	2.278279000	-0.196125000
H	2.559198000	4.304090000	-0.802078000
H	2.252121000	5.139714000	0.742252000
N	0.978853000	3.530268000	0.286527000
H	-1.067006000	4.038624000	0.575232000
O	2.315680000	2.085276000	-0.847408000
C	1.784575000	4.661223000	-0.126586000
H	1.164340000	5.406329000	-0.640028000
C	-0.152469000	3.819558000	1.143613000
H	-0.347199000	2.987571000	1.822501000
H	0.087628000	4.697131000	1.750655000
H	4.216964000	-3.735354000	0.121797000
H	3.147582000	0.441962000	-0.118683000

C6

E = -975.073714152 Ha

C	4.266064000	-0.763073000	0.155431000
N	0.467741000	-2.307184000	-0.378202000
C	-0.227732000	-1.192067000	-0.004386000
C	0.616350000	-0.167088000	0.388923000
C	4.147517000	-2.122977000	-0.298616000
C	2.934984000	-2.715812000	-0.505926000
C	1.742604000	-1.987621000	-0.255558000
N	1.884736000	-0.670104000	0.210871000
C	3.103198000	-0.119478000	0.392260000
H	-1.818954000	0.907611000	-0.654334000
H	2.840942000	-3.733864000	-0.863992000
C	5.611091000	-0.112060000	0.334665000
H	6.174081000	-0.121519000	-0.603893000
H	5.500015000	0.925607000	0.654785000
H	6.205702000	-0.643037000	1.085250000
C	-1.696457000	-1.150131000	-0.031632000
C	-2.439503000	-2.302332000	0.248646000
C	-3.826494000	-2.264670000	0.235712000
C	-4.518145000	-1.083974000	-0.058780000
C	-3.773347000	0.055637000	-0.362118000
C	-2.381286000	0.024501000	-0.357005000
H	-1.908048000	-3.222321000	0.471226000
H	-4.389984000	-3.168091000	0.457490000
H	-6.439722000	-1.889194000	-0.625229000
H	-4.289223000	0.975545000	-0.627753000
C	-6.025266000	-1.055970000	-0.049382000
H	-6.414152000	-1.140110000	0.971373000
H	-6.407708000	-0.125376000	-0.476678000
C	0.367079000	1.167507000	1.000931000
H	-0.646277000	1.176990000	1.404684000
H	1.059594000	1.320259000	1.841581000
C	0.634374000	2.298409000	0.005869000
H	0.759296000	4.121610000	-1.647713000
H	0.250632000	5.327064000	-0.439621000
N	-0.268769000	3.321182000	-0.037629000
H	-2.140958000	2.710413000	0.771728000
O	1.625276000	2.252905000	-0.706823000
C	-0.040989000	4.413200000	-0.970382000
H	-0.953063000	4.612156000	-1.541478000
C	-1.362104000	3.468207000	0.913673000
H	-1.010453000	3.422594000	1.949142000
H	-1.814122000	4.449325000	0.759263000
H	5.062630000	-2.677416000	-0.490452000

C8

E = -975.109746577 Ha

C	4.353659000	-0.686687000	0.145938000
N	0.589285000	-2.291510000	-0.366990000
C	-0.137840000	-1.185371000	-0.023763000
C	0.681670000	-0.129804000	0.339041000
C	4.252818000	-2.071491000	-0.268530000
C	3.050949000	-2.666309000	-0.469353000
C	1.851740000	-1.929062000	-0.246822000
N	1.966433000	-0.603561000	0.173685000
C	3.171168000	0.020982000	0.346367000
H	-1.798829000	0.849939000	-0.708174000
H	2.954430000	-3.695528000	-0.794254000
C	5.603405000	-0.069865000	0.317660000
H	6.520649000	-0.620006000	0.150645000
H	5.678727000	0.970156000	0.609705000
C	-1.606230000	-1.189960000	-0.045814000
C	-2.311019000	-2.359987000	0.260680000
C	-3.698405000	-2.367047000	0.254920000
C	-4.429540000	-1.215090000	-0.058137000
C	-3.723267000	-0.058388000	-0.387715000
C	-2.330723000	-0.044862000	-0.390342000
H	-1.749111000	-3.257820000	0.498324000
H	-4.231262000	-3.283580000	0.497734000
H	-6.326343000	-2.081388000	-0.617638000
H	-4.269622000	0.839235000	-0.668437000
C	-5.936674000	-1.236170000	-0.041837000
H	-6.318085000	-1.335157000	0.980367000
H	-6.351204000	-0.317896000	-0.465811000
C	0.364572000	1.183535000	0.971330000
H	-0.638153000	1.115932000	1.396038000
H	1.054687000	1.368254000	1.807736000
C	0.526525000	2.355163000	0.002809000
H	0.476091000	4.203195000	-1.631892000
H	-0.075801000	5.335450000	-0.373998000
N	-0.468345000	3.288662000	-0.029431000
H	-2.244826000	2.487636000	0.825703000
O	1.522789000	2.421395000	-0.702888000
C	-0.324802000	4.423117000	-0.928817000
H	-1.260142000	4.584110000	-1.472848000
C	-1.559307000	3.334515000	0.936191000
H	-1.191954000	3.360469000	1.967394000
H	-2.125397000	4.250718000	0.761183000
H	5.173663000	-2.622681000	-0.432936000
H	3.136363000	1.079345000	0.570577000

C9

E = -975.077874836 Ha

C	4.316066000	-0.792597000	0.128821000
N	0.515858000	-2.332104000	-0.385248000
C	-0.175713000	-1.207605000	-0.034348000
C	0.671881000	-0.175459000	0.329522000
C	4.142738000	-2.135098000	-0.280231000
C	2.972733000	-2.766830000	-0.499522000
C	1.789417000	-2.005364000	-0.268624000
N	1.943640000	-0.682290000	0.158585000
C	3.167462000	-0.081167000	0.330726000
H	-1.781536000	0.869096000	-0.725186000
H	2.878188000	-3.794431000	-0.832086000
C	5.676669000	-0.172997000	0.297261000
H	6.245725000	-0.224738000	-0.635607000
H	5.592240000	0.876571000	0.588820000
H	6.252716000	-0.699121000	1.064556000
C	-1.644692000	-1.170521000	-0.049650000
C	-2.380657000	-2.317909000	0.267878000
C	-3.767779000	-2.285971000	0.267600000
C	-4.467337000	-1.116057000	-0.050988000
C	-3.730185000	0.017951000	-0.391403000
C	-2.337707000	-0.007957000	-0.399475000
H	-1.843069000	-3.229563000	0.509202000
H	-4.325314000	-3.185408000	0.518791000
H	-6.389762000	-1.931872000	-0.598677000
H	-4.252213000	0.928652000	-0.676323000
C	-5.974432000	-1.094668000	-0.029148000
H	-6.354648000	-1.177127000	0.994958000
H	-6.364598000	-0.167526000	-0.456936000
C	0.388219000	1.142821000	0.968364000

H	-0.617769000	1.100054000	1.388408000
H	1.078365000	1.304540000	1.809624000
C	0.586308000	2.316055000	0.008995000
H	0.597889000	4.175785000	-1.613836000
H	0.067875000	5.311135000	-0.349387000
N	-0.385745000	3.272990000	-0.028195000
H	-2.178022000	2.503205000	0.821707000
O	1.591438000	2.363843000	-0.686290000
C	-0.202255000	4.411546000	-0.915111000
H	-1.128087000	4.604290000	-1.464945000
C	-1.482807000	3.342196000	0.929242000
H	-1.122768000	3.373820000	1.963044000
H	-2.036235000	4.263396000	0.740555000
H	3.145697000	0.976104000	0.568185000

C10

E = -975.074271924 Ha

C	4.305587000	-0.780743000	0.121813000
N	0.512613000	-2.334416000	-0.396600000
C	-0.182834000	-1.217626000	-0.041752000
C	0.660105000	-0.178895000	0.326969000
C	4.213783000	-2.154409000	-0.301412000
C	2.991561000	-2.689277000	-0.487995000
C	1.785770000	-1.998869000	-0.279066000
N	1.931405000	-0.672857000	0.153499000
C	3.159348000	-0.074451000	0.327628000
H	-1.801228000	0.853899000	-0.720808000
C	5.654861000	-0.139046000	0.299211000
H	6.228293000	-0.171753000	-0.632768000
H	5.558254000	0.906926000	0.599920000
H	6.239297000	-0.661426000	1.063854000
C	-1.652259000	-1.188687000	-0.055848000
C	-2.381180000	-2.341918000	0.256509000
C	-3.768453000	-2.318094000	0.256239000
C	-4.474841000	-1.150813000	-0.056812000
C	-3.744459000	-0.010786000	-0.391659000
C	-2.351846000	-0.028386000	-0.399727000
H	-1.838242000	-3.251563000	0.493385000
H	-4.320619000	-3.222002000	0.503106000
H	-6.392274000	-1.975289000	-0.608631000
H	-4.271829000	0.898207000	-0.672093000
C	-5.982022000	-1.138447000	-0.034921000
H	-6.361696000	-1.228312000	0.988756000
H	-6.377691000	-0.211533000	-0.458109000
C	0.365929000	1.135747000	0.969045000
H	-0.637952000	1.083086000	1.392977000
H	1.058670000	1.302010000	1.807032000
C	0.550306000	2.311265000	0.009423000
H	0.540266000	4.175167000	-1.608249000
H	0.009229000	5.303994000	-0.338350000
N	-0.428210000	3.262025000	-0.019232000
H	-2.210820000	2.477991000	0.837716000
O	1.550218000	2.365853000	-0.692241000
C	-0.257663000	4.403794000	-0.904620000
H	-1.187816000	4.591209000	-1.448977000
C	-1.520372000	3.321077000	0.944411000
H	-1.154959000	3.351592000	1.976363000
H	-2.080751000	4.239299000	0.761842000
H	5.124604000	-2.721035000	-0.476667000
H	3.136948000	0.980842000	0.569349000

C14

E = -975.082836686 Ha

C	-4.266398000	-0.775728000	-0.163798000
N	-0.462822000	-2.208988000	0.425383000
C	0.218984000	-1.116914000	-0.020512000
C	-0.638810000	-0.110093000	-0.439701000
C	-4.132645000	-2.103606000	0.353950000
C	-2.906212000	-2.650857000	0.589914000
C	-1.741406000	-1.897158000	0.298587000
N	-1.903252000	-0.613225000	-0.220283000
C	-3.142795000	-0.054092000	-0.430528000
H	-2.775908000	-3.648645000	0.991710000
C	-5.632108000	-0.182520000	-0.381490000
H	-6.203641000	-0.163383000	0.552184000
H	-5.563846000	0.841632000	-0.755810000
H	-6.205277000	-0.772032000	-1.104916000
C	1.686141000	-1.107744000	-0.032779000
C	2.414868000	-2.280257000	0.231954000
C	3.804273000	-2.271431000	0.230220000
C	4.536005000	-1.107938000	-0.034272000
C	3.824914000	0.073496000	-0.290349000
C	2.452844000	0.015352000	-0.276193000
H	1.858468000	-3.187644000	0.445887000
H	4.340556000	-3.193091000	0.441488000
H	6.443870000	-1.810006000	0.689749000
H	4.355844000	1.002390000	-0.488109000
C	6.042851000	-1.127164000	-0.064517000
H	6.410533000	-1.462756000	-1.040738000
H	6.456803000	-0.132391000	0.121009000
C	-0.384424000	1.207554000	-1.098145000
H	0.610916000	1.175945000	-1.537971000
H	-1.100287000	1.351202000	-1.917930000
C	-0.620843000	2.369891000	-0.129744000
H	-0.853797000	4.128488000	1.570482000
H	0.291339000	5.234101000	0.762154000
N	0.399370000	3.215541000	0.187945000
H	2.452088000	2.792703000	0.426415000
O	-1.743214000	2.500751000	0.343731000
C	0.161397000	4.235994000	1.195911000
H	0.875483000	4.117822000	2.018887000
C	1.756595000	3.191075000	-0.322734000
H	1.842516000	2.593293000	-1.227080000
H	2.057769000	4.216126000	-0.565599000
H	-5.033481000	-2.670434000	0.571990000
H	-3.146689000	0.980212000	-0.749616000

C15

E = -975.079122347 Ha

C	4.268827000	-0.691557000	0.144332000
N	0.519073000	-2.294021000	-0.380297000
C	-0.199401000	-1.189779000	-0.031106000
C	0.622477000	-0.135923000	0.339078000
C	4.185062000	-2.058565000	-0.273789000
C	2.980950000	-2.664875000	-0.480542000
C	1.786767000	-1.934460000	-0.255981000
N	1.902444000	-0.612557000	0.172727000
C	3.117424000	0.005922000	0.348179000
H	-1.847795000	0.872679000	-0.728759000
H	2.891423000	-3.692583000	-0.812008000
C	5.611258000	-0.035791000	0.323050000
H	6.187047000	-0.063453000	-0.607736000
H	5.505281000	1.009605000	0.622683000
H	6.200554000	-0.551241000	1.088801000
C	-1.668535000	-1.182557000	-0.053949000
C	-2.389569000	-2.341736000	0.249175000
C	-3.780892000	-2.341462000	0.242818000
C	-4.514233000	-1.185005000	-0.063424000
C	-3.750993000	-0.077675000	-0.375515000
C	-2.379676000	-0.019254000	-0.402630000
H	-1.837362000	-3.245651000	0.485040000
H	-4.319242000	-3.256342000	0.481423000
H	-6.426938000	-2.174741000	-0.070475000
C	-6.021170000	-1.160199000	-0.046140000
H	-6.394523000	-0.670052000	0.859286000
H	-6.415420000	-0.609587000	-0.904224000
C	0.305213000	1.177670000	0.971544000
H	-0.700438000	1.112146000	1.389941000
H	0.990550000	1.361308000	1.812058000
C	0.471055000	2.347205000	0.000594000
H	0.404561000	4.170469000	-1.659143000
H	-0.170285000	5.327078000	-0.433503000
N	-0.519275000	3.284782000	-0.028978000
H	-2.355016000	2.544446000	0.761344000
O	1.463788000	2.405358000	-0.711015000
C	-0.400266000	4.394411000	-0.961783000
H	-1.339172000	4.520474000	-1.509313000
C	-1.614278000	3.333836000	0.932058000
H	-1.251970000	3.263245000	1.961878000
H	-2.115014000	4.297290000	0.823034000
H	5.107247000	-2.607574000	-0.442488000
H	3.080398000	1.060964000	0.590304000

C17

E = -975.111192774 Ha

C	4.254709000	-0.662304000	0.134969000
N	0.519331000	-2.305723000	-0.361261000
C	-0.211222000	-1.203362000	-0.025726000

C	0.604215000	-0.137289000	0.330480000
C	4.182680000	-2.034866000	-0.266888000
C	2.983840000	-2.654695000	-0.463992000
C	1.783137000	-1.932880000	-0.245497000
N	1.887630000	-0.604314000	0.166490000
C	3.097274000	0.027086000	0.332548000
H	-1.883232000	0.839942000	-0.668434000
H	2.903198000	-3.687150000	-0.782705000
C	5.591379000	0.007720000	0.303486000
H	6.166069000	-0.026152000	-0.627783000
H	5.476395000	1.055705000	0.590494000
H	6.186486000	-0.492927000	1.074554000
C	-1.675171000	-1.216172000	-0.046919000
C	-2.374223000	-2.403690000	0.232290000
C	-3.752532000	-2.426790000	0.236108000
C	-4.514460000	-1.259891000	-0.050450000
C	-3.793454000	-0.076352000	-0.363906000
C	-2.412464000	-0.062116000	-0.367566000
H	-1.800530000	-3.299874000	0.446338000
H	-4.279815000	-3.349878000	0.461973000
H	-6.462373000	-2.188838000	0.191378000
H	-4.347975000	0.820933000	-0.627557000
C	-5.918814000	-1.280777000	-0.040064000
H	-6.493407000	-0.390984000	-0.268131000
C	0.281763000	1.175091000	0.962560000
H	-0.717591000	1.103186000	1.394404000
H	0.975125000	1.364927000	1.795269000
C	0.431228000	2.347300000	-0.007339000
H	0.354631000	4.194428000	-1.642623000
H	-0.179418000	5.327276000	-0.377584000
N	-0.564583000	3.280364000	-0.025387000
H	-2.335259000	2.483169000	0.846685000
O	1.418389000	2.415022000	-0.725491000
C	-0.435810000	4.414157000	-0.927741000
H	-1.379377000	4.573760000	-1.457805000
C	-1.642393000	3.324498000	0.955020000
H	-1.260951000	3.338596000	1.981232000
H	-2.204527000	4.246078000	0.796218000
H	5.109568000	-2.577329000	-0.430940000
H	3.051137000	1.084657000	0.561833000

C18

E = -975.079088903 Ha

C	4.277882000	-0.642591000	0.136084000
N	0.554318000	-2.310566000	-0.368118000
C	-0.181989000	-1.217046000	-0.022954000
C	0.622963000	-0.147320000	0.338978000
C	4.215997000	-2.012788000	-0.275333000
C	3.021656000	-2.640207000	-0.475616000
C	1.816127000	-1.928791000	-0.250946000
N	1.910529000	-0.602883000	0.170333000
C	3.115549000	0.036594000	0.339716000
H	-1.878652000	0.792146000	-0.702168000
H	2.948302000	-3.670969000	-0.801502000
C	5.609609000	0.036359000	0.308232000
H	6.183494000	0.013743000	-0.623866000
H	5.486935000	1.081281000	0.603093000
H	6.209296000	-0.465457000	1.074953000
C	-1.651032000	-1.241484000	-0.037986000
C	-2.335495000	-2.428703000	0.278466000
C	-3.704942000	-2.390487000	0.264971000
C	-4.495616000	-1.296320000	-0.036796000
C	-3.791479000	-0.133399000	-0.372458000
C	-2.397487000	-0.108167000	-0.379763000
H	-1.769285000	-3.323764000	0.517943000
H	-6.371596000	-2.169979000	-0.642459000
H	-4.347256000	0.759042000	-0.654132000
C	-6.001484000	-1.351686000	-0.018211000
H	-6.375167000	-1.519941000	0.996742000
H	-6.430163000	-0.416741000	-0.387993000
C	0.286737000	1.162695000	0.968734000
H	-0.714458000	1.082041000	1.394596000
H	0.974093000	1.359943000	1.804539000
C	0.431660000	2.334477000	-0.002200000
H	0.356092000	4.180160000	-1.639628000
H	-0.203240000	5.304350000	-0.377908000
N	-0.577339000	3.253009000	-0.037855000
H	-2.331230000	2.422811000	0.834725000
O	1.427545000	2.414631000	-0.706992000
C	-0.445329000	4.391127000	-0.934438000
H	-1.383127000	4.545221000	-1.476153000
C	-1.666793000	3.287901000	0.929965000
H	-1.298412000	3.339774000	1.960014000
H	-2.256160000	4.186472000	0.740946000
H	5.146805000	-2.547049000	-0.443976000
H	3.061615000	1.091978000	0.576995000

C19

E = -975.076517092 Ha

C	4.292778000	-0.683428000	0.138164000
N	0.554051000	-2.316230000	-0.373973000
C	-0.170248000	-1.219024000	-0.018544000
C	0.642775000	-0.157173000	0.347452000
C	4.218169000	-2.050242000	-0.282721000
C	3.018077000	-2.665460000	-0.485800000
C	1.818836000	-1.945084000	-0.255201000
N	1.925967000	-0.622458000	0.175217000
C	3.136964000	0.004835000	0.347814000
H	-1.850418000	0.805616000	-0.747792000
H	2.934784000	-3.693475000	-0.817909000
C	5.630775000	-0.017885000	0.314062000
H	6.203369000	-0.038040000	-0.618915000
H	5.517882000	1.025690000	0.617568000
H	6.226926000	-0.531267000	1.075893000
C	-1.638899000	-1.217462000	-0.037313000
C	-2.388841000	-2.333385000	0.291116000
C	-3.757776000	-2.400826000	0.305789000
C	-4.485269000	-1.249288000	-0.043487000
C	-3.773044000	-0.103569000	-0.402622000
C	-2.378869000	-0.084935000	-0.410104000
H	-4.278952000	-3.315507000	0.579186000
H	-6.379045000	-2.080003000	-0.660226000
H	-4.319306000	0.786739000	-0.704219000
C	-5.992477000	-1.269814000	-0.033910000
H	-6.377045000	-1.428589000	0.979158000
H	-6.403620000	-0.328229000	-0.406573000
C	0.313098000	1.154360000	0.977272000
H	-0.691944000	1.080196000	1.395641000
H	0.995673000	1.346067000	1.818246000
C	0.471589000	2.325718000	0.007913000
H	0.412646000	4.167260000	-1.634811000
H	-0.150377000	5.298183000	-0.380828000
N	-0.532674000	3.249374000	-0.034860000
H	-2.307818000	2.436715000	0.812166000
O	1.472310000	2.401002000	-0.690416000
C	-0.392158000	4.383496000	-0.935065000
H	-1.326338000	4.538462000	-1.482837000
C	-1.629384000	3.289093000	0.924441000
H	-1.268314000	3.320190000	1.957724000
H	-2.201580000	4.200488000	0.744106000
H	5.144011000	-2.591716000	-0.455717000
H	3.093004000	1.058824000	0.593262000

Table S9. Coordinates and energies of the stationary points of the HAT from C4 site of zolpidem to between HO•. Level of theory: M06-2X/6-31G(d).

RC

E = -1051.46480906 Ha

C	4.112939000	-0.688318000	-0.199624000
N	0.343335000	-2.296966000	-0.558489000
C	-0.360405000	-1.188928000	-0.187784000
C	0.479271000	-0.127353000	0.118426000
C	4.015277000	-2.064040000	-0.575729000
C	2.802110000	-2.670203000	-0.748222000
C	1.614900000	-1.933334000	-0.510482000
N	1.746116000	-0.601236000	-0.119964000
C	2.962199000	0.026166000	0.001549000
H	-2.054419000	0.864006000	-0.724141000
H	2.704543000	-3.706475000	-1.049793000
C	5.454792000	-0.033908000	-0.026506000
H	6.064023000	-0.139896000	-0.929648000
H	5.346716000	1.029693000	0.195872000
H	6.001987000	-0.494002000	0.802800000
C	-1.827825000	-1.190014000	-0.116549000
C	-2.515694000	-2.363213000	0.213499000
C	-3.900868000	-2.366846000	0.295577000
C	-4.645788000	-1.207596000	0.050748000
C	-3.957394000	-0.046575000	-0.301793000
C	-2.568086000	-0.036296000	-0.392322000
H	-1.943013000	-3.266625000	0.398330000
H	-4.420660000	-3.286399000	0.554607000
H	-6.576088000	-2.092637000	-0.339951000
H	-4.517165000	0.857532000	-0.530195000
C	-6.148579000	-1.222329000	0.167124000
H	-6.461396000	-1.270032000	1.216111000
H	-6.589637000	-0.323448000	-0.271515000
C	0.220894000	1.180336000	0.787225000
H	-0.748205000	1.117329000	1.284489000
H	0.980567000	1.330990000	1.569037000
C	0.321040000	2.359259000	-0.179178000
H	-0.285416000	5.365501000	-0.463935000
H	-1.544525000	4.619699000	-1.479991000
N	-0.647186000	3.317261000	-0.104459000
H	-2.191124000	4.306971000	0.861595000
O	1.246105000	2.410637000	-0.977907000
C	-0.572117000	4.456442000	-1.005460000
H	0.175914000	4.241949000	-1.766076000
C	-1.658012000	3.358483000	0.944400000
H	-2.389510000	2.548600000	0.846394000
H	-1.211253000	3.312595000	1.942433000
H	2.932688000	1.092418000	0.182686000
O	3.210967000	-0.020958000	2.423893000
H	3.070216000	-0.985930000	2.347234000
H	4.931405000	-2.623093000	-0.743242000

TS

E = -1051.45624520 Ha

C	3.723656000	-1.674233000	-0.046000000
N	-0.305648000	-2.472016000	-0.269006000
C	-0.755982000	-1.205818000	-0.082392000
C	0.296407000	-0.302936000	0.076695000
C	3.329283000	-3.029303000	-0.268924000
C	2.012175000	-3.381345000	-0.367051000
C	1.019462000	-2.383319000	-0.238668000
N	1.435302000	-1.071203000	-0.034790000
C	2.758341000	-0.716190000	0.060713000
H	-2.020131000	1.014417000	-1.033155000
H	1.689117000	-4.401828000	-0.534476000
C	5.181225000	-1.312141000	0.047834000
H	5.703341000	-1.552401000	-0.883981000
H	5.312000000	-0.245011000	0.241944000
H	5.673098000	-1.868403000	0.852541000
C	-2.192954000	-0.899776000	-0.061926000
C	-3.093808000	-1.843408000	0.447036000
C	-4.453081000	-1.570813000	0.479943000
C	-4.960319000	-0.355838000	0.004028000
C	-4.061785000	0.570416000	-0.524506000
C	-2.695995000	0.303668000	-0.564692000
H	-2.705293000	-2.789938000	0.809442000
H	-5.140137000	-2.312481000	0.880730000
H	-7.021376000	-0.906440000	-0.327043000
H	-4.437181000	1.507201000	-0.928570000
C	-6.438383000	-0.066995000	0.064142000
H	-6.763814000	0.102832000	1.096404000
H	-6.692846000	0.823165000	-0.516811000
C	0.334347000	1.107884000	0.476805000
H	-0.664543000	1.446742000	0.765229000
H	0.982905000	1.216437000	1.422012000
C	0.992179000	2.050893000	-0.531456000
H	2.297270000	4.914578000	-0.711064000
H	0.693267000	5.035782000	-1.473865000
N	0.958649000	3.374850000	-0.215058000
H	0.843256000	4.855016000	1.231080000
O	1.520336000	1.614577000	-1.542964000
C	1.481776000	4.340138000	-1.164122000
H	1.854649000	3.801502000	-2.033253000
C	0.356113000	3.905337000	0.995874000
H	-0.718592000	4.093796000	0.872796000
H	0.518961000	3.237656000	1.842683000
H	2.965273000	0.336194000	0.210743000
O	2.188497000	1.490796000	2.371690000
H	2.243762000	0.596088000	2.763885000
H	4.102280000	-3.786642000	-0.365098000

Table S10. Coordinates and energies of the stationary points of the HAT from C4 site of zolpidem to HOO$^{\bullet}$ Level of theory: M06-2X/6-31G(d).

TS

E = -1126.58025454 Ha

C	3.728152000	-1.620687000	-0.230740000
N	-0.302151000	-2.404888000	-0.434559000
C	-0.752587000	-1.140103000	-0.308504000
C	0.303805000	-0.213385000	-0.213626000
C	3.327644000	-2.978090000	-0.407222000
C	2.007460000	-3.322551000	-0.501063000
C	1.028427000	-2.310298000	-0.421357000
N	1.446193000	-0.994014000	-0.295819000
C	2.767950000	-0.652673000	-0.176369000
H	-2.082293000	1.009583000	-1.357713000
H	1.673345000	-4.346070000	-0.620235000
C	5.185498000	-1.266507000	-0.110096000
H	5.738043000	-1.575280000	-1.003367000
H	5.321324000	-0.190002000	0.015797000
H	5.639856000	-1.769122000	0.749839000
C	-2.192823000	-0.848555000	-0.273789000
C	-3.063847000	-1.776558000	0.311356000
C	-4.427684000	-1.528450000	0.360745000
C	-4.969837000	-0.354518000	-0.174545000
C	-4.101636000	0.554643000	-0.779678000
C	-2.732196000	0.313390000	-0.835143000
H	-2.648855000	-2.694434000	0.715990000
H	-5.090172000	-2.258461000	0.819847000
H	-4.505074000	1.457513000	-1.231106000
C	-6.450385000	-0.085237000	-0.092629000
H	-6.749898000	0.701563000	-0.789737000
H	-7.029319000	-0.984236000	-0.323810000
C	0.291274000	1.177289000	0.180844000
H	-0.729417000	1.523178000	0.353535000
H	0.784804000	1.150396000	1.354222000
C	1.127236000	2.174843000	-0.583040000
H	2.262730000	4.040903000	-1.728307000
H	2.412768000	5.057634000	-0.269300000
N	1.046114000	3.469572000	-0.152299000
H	-0.781166000	4.217835000	0.626987000
O	1.842537000	1.834023000	-1.516410000
C	1.715745000	4.508416000	-0.911880000
H	0.984541000	5.217214000	-1.318817000
C	0.221241000	3.912739000	0.956426000
H	0.128616000	3.137415000	1.717939000
H	0.703529000	4.776673000	1.422410000
H	2.983920000	0.400849000	-0.069720000
O	1.116608000	0.843794000	2.568228000
O	0.828509000	-0.500546000	2.576118000
H	-0.089617000	-0.539193000	2.898143000
H	-6.735334000	0.236585000	0.915306000
H	4.094718000	-3.745649000	-0.460796000

Table S11. Coordinates and energies of the stationary points of the HAT from c4 site of zolpidem to $CH_3O^{\bullet}$. Level of theory: M06-2X/6-31G(d).

RC

E = -1090.76658061 Ha

C	4.143322000	-0.331524000	-0.365738000
N	0.448673000	-2.046093000	-0.923757000
C	-0.301025000	-1.028510000	-0.408260000
C	0.491692000	0.022112000	0.030176000
C	4.101317000	-1.635531000	-0.956555000
C	2.916170000	-2.266694000	-1.201489000
C	1.703776000	-1.625989000	-0.843998000
N	1.779004000	-0.358582000	-0.272213000
C	2.970795000	0.283030000	-0.044886000
H	-2.098236000	0.978779000	-0.750889000
H	2.857725000	-3.249834000	-1.653439000
C	5.463398000	0.353080000	-0.135435000
H	6.003239000	0.488971000	-1.078246000
H	5.324942000	1.337080000	0.318607000
H	6.102943000	-0.239945000	0.526713000
C	-1.767181000	-1.109060000	-0.340621000
C	-2.394800000	-2.341684000	-0.128078000
C	-3.777859000	-2.423819000	-0.052618000
C	-4.580873000	-1.285751000	-0.189221000
C	-3.952482000	-0.063341000	-0.426755000
C	-2.565428000	0.026182000	-0.509029000
H	-1.777761000	-3.229538000	-0.029820000
H	-4.249945000	-3.389179000	0.115033000
H	-6.465247000	-2.213744000	-0.689627000
H	-4.557531000	0.828956000	-0.570464000
C	-6.080988000	-1.388243000	-0.082645000
H	-6.390182000	-1.573009000	0.952071000
H	-6.566432000	-0.467406000	-0.416238000
C	0.155022000	1.252605000	0.801982000
H	-0.818268000	1.094903000	1.269218000
H	0.879375000	1.375733000	1.618412000
C	0.212536000	2.509867000	-0.061757000
H	-0.006064000	4.507204000	-1.491706000
H	-0.526002000	5.501493000	-0.108921000
N	-0.797646000	3.416725000	0.081178000
H	-2.528769000	2.513352000	0.930060000
O	1.143268000	2.669974000	-0.839044000
C	-0.768143000	4.626809000	-0.724064000
H	-1.743638000	4.785223000	-1.194103000
C	-1.817117000	3.325283000	1.118165000
H	-1.376474000	3.184195000	2.109717000
H	-2.371167000	4.265387000	1.130767000
H	2.899072000	1.289474000	0.347699000
C	1.851623000	-2.030835000	2.309053000
H	1.810306000	-2.705348000	3.177037000
H	2.843169000	-2.051481000	1.833173000
H	1.116817000	-2.420645000	1.576974000
O	1.427541000	-0.768376000	2.635917000
H	5.038906000	-2.115684000	-1.222836000

TS

E = -1090.75321899 Ha

C	3.638886000	-1.649668000	-0.306284000
N	-0.400848000	-2.413697000	-0.451387000
C	-0.839248000	-1.148546000	-0.255637000
C	0.225279000	-0.243454000	-0.132939000
C	3.228529000	-2.998894000	-0.528705000
C	1.906196000	-3.339613000	-0.605169000
C	0.927941000	-2.331829000	-0.460382000
N	1.357552000	-1.023782000	-0.275034000
C	2.683170000	-0.683103000	-0.185637000
H	-2.121734000	1.076951000	-1.172217000
H	1.570362000	-4.357478000	-0.762400000
C	5.100393000	-1.303543000	-0.216217000
H	5.617675000	-1.549099000	-1.149331000
H	5.242809000	-0.238333000	-0.020845000
H	5.586827000	-1.864842000	0.588043000
C	-2.273605000	-0.836665000	-0.196198000
C	-3.162143000	-1.778282000	0.337731000
C	-4.519568000	-1.503341000	0.405427000
C	-5.036691000	-0.288557000	-0.060191000
C	-4.150580000	0.635371000	-0.613664000
C	-2.786710000	0.367228000	-0.687678000
H	-2.765994000	-2.724830000	0.691725000
H	-5.197182000	-2.242842000	0.825663000
H	-7.106538000	-0.838066000	-0.331457000
H	-4.534806000	1.572012000	-1.009500000
C	-6.512035000	0.003190000	0.037795000
H	-6.808597000	0.180625000	1.077430000
H	-6.780824000	0.889812000	-0.542036000
C	0.285221000	1.155111000	0.273329000
H	-0.703321000	1.521470000	0.561861000

H	0.939515000	1.185980000	1.266352000
C	1.004200000	2.107170000	-0.671994000
H	1.971981000	3.899005000	-2.059143000
H	2.479202000	4.904772000	-0.675289000
N	1.069147000	3.405855000	-0.261254000
H	-0.542593000	4.186970000	0.880973000
O	1.500395000	1.709144000	-1.715869000
C	1.632880000	4.400554000	-1.154650000
H	0.878797000	5.153330000	-1.413065000
C	0.509623000	3.891769000	0.988776000
H	0.602039000	3.146516000	1.780316000
H	1.079224000	4.772010000	1.298330000
H	2.901731000	0.362894000	-0.015957000
C	1.410113000	-0.258042000	2.890086000
H	1.123997000	-0.207278000	3.950527000
H	2.218359000	-0.991931000	2.749231000
H	0.526105000	-0.650961000	2.347116000
O	1.751886000	0.993040000	2.407762000
H	3.992661000	-3.763926000	-0.634560000

Table S12. Coordinates and energies of the stationary points of the HAT from C4 site of zolpidem to $CH_3OO^{\bullet}$. Level of theory: M06-2X/6-31G(d).

RC

E = -1165.90399234 Ha

C	4.572357000	-0.705101000	0.290511000
N	0.917042000	-2.406081000	-0.507229000
C	0.154424000	-1.288301000	-0.333785000
C	0.923733000	-0.193573000	0.035971000
C	4.545852000	-2.103293000	-0.018984000
C	3.377065000	-2.744622000	-0.305519000
C	2.160048000	-2.017371000	-0.275713000
N	2.217098000	-0.663492000	0.050715000
C	3.400454000	-0.012705000	0.307495000
H	-1.510153000	0.704884000	-1.190034000
H	3.332516000	-3.797391000	-0.558018000
C	5.881725000	-0.014924000	0.561037000
H	6.557056000	-0.107981000	-0.295674000
H	5.735112000	1.049292000	0.760300000
H	6.386615000	-0.456880000	1.426539000
C	-1.304391000	-1.331384000	-0.512527000
C	-1.997972000	-2.522220000	-0.263728000
C	-3.379802000	-2.575643000	-0.393398000
C	-4.117033000	-1.449027000	-0.777999000
C	-3.419448000	-0.268623000	-1.042783000
C	-2.033425000	-0.210760000	-0.925602000
H	-1.430402000	-3.398657000	0.033147000
H	-3.901965000	-3.508328000	-0.192591000
H	-6.060636000	-2.212518000	-0.223710000
H	-3.967152000	0.614879000	-1.362525000
C	-5.613411000	-1.523383000	-0.945714000
H	-6.077620000	-0.542142000	-0.814966000
H	-5.876470000	-1.882349000	-1.947030000
C	0.540829000	1.172814000	0.495811000
H	-0.511767000	1.151397000	0.773871000
H	1.098827000	1.436360000	1.406755000
C	0.841764000	2.244921000	-0.553488000
H	0.987287000	3.906016000	-2.366809000
H	0.298819000	5.199602000	-1.352019000
N	-0.088470000	3.224470000	-0.730679000
H	-1.083222000	3.154883000	1.143260000
O	1.883387000	2.192327000	-1.193508000
C	0.121001000	4.206583000	-1.780696000
H	-0.762857000	4.256551000	-2.425452000
C	-1.276541000	3.392424000	0.096082000
H	-1.578146000	4.441306000	0.043319000
H	-2.116047000	2.775529000	-0.249850000
H	3.329268000	1.057385000	0.457316000
C	-2.492382000	-0.345901000	2.445409000
H	-2.836148000	-0.457666000	3.474874000
H	-1.495131000	-0.771715000	2.315407000
H	-3.192723000	-0.777281000	1.729930000
O	-2.433997000	1.060166000	2.135556000
O	-1.629280000	1.681222000	2.951579000
H	5.485292000	-2.648632000	-0.038986000

TS

E = -1165.87278457 Ha

C	3.818554000	-1.482797000	-0.402448000
N	-0.194098000	-2.347629000	-0.622569000
C	-0.673149000	-1.091789000	-0.501036000
C	0.362342000	-0.139929000	-0.400147000
C	3.444804000	-2.850433000	-0.567493000
C	2.132154000	-3.217544000	-0.673961000
C	1.132480000	-2.223478000	-0.609857000
N	1.522330000	-0.894223000	-0.483003000
C	2.842662000	-0.529478000	-0.366209000
H	-2.043685000	0.992866000	-1.613013000
H	1.816542000	-4.247333000	-0.790707000
C	5.269468000	-1.100332000	-0.287535000
H	5.823955000	-1.401940000	-1.181983000
H	5.385430000	-0.020970000	-0.166697000
H	5.737502000	-1.591927000	0.571539000
C	-2.118791000	-0.831900000	-0.471962000
C	-2.968375000	-1.758082000	0.144461000
C	-4.337418000	-1.539988000	0.181945000
C	-4.904347000	-0.399067000	-0.397125000
C	-4.055899000	0.508627000	-1.031399000
C	-2.681146000	0.297467000	-1.073886000
H	-2.534448000	-2.649257000	0.587058000
H	-4.984224000	-2.266266000	0.668352000
H	-6.685639000	0.180448000	0.671556000
H	-4.478428000	1.386674000	-1.513241000
C	-6.390820000	-0.160999000	-0.326957000
H	-6.705285000	0.600578000	-1.045218000
H	-6.948955000	-1.078435000	-0.536169000
C	0.286387000	1.228986000	0.057466000
H	-0.756648000	1.527828000	0.176497000
H	0.605353000	1.149030000	1.304706000
C	1.137729000	2.301370000	-0.565575000
H	2.280121000	4.280815000	-1.495427000
H	2.241397000	5.218233000	0.023201000
N	0.958036000	3.561516000	-0.070833000
H	-0.129451000	3.078855000	1.674472000
O	1.947570000	2.051818000	-1.452815000
C	1.636995000	4.672648000	-0.709888000
H	0.907931000	5.366865000	-1.145007000
C	0.010952000	3.904680000	0.976178000
H	0.413341000	4.751113000	1.540069000
H	-0.962306000	4.201701000	0.563107000
H	3.038901000	0.530932000	-0.293976000
C	0.596158000	-1.400617000	2.662919000
H	0.934587000	-1.488034000	3.700112000
H	1.463879000	-1.336147000	1.998769000
H	-0.027757000	-2.253715000	2.385820000
O	-0.229674000	-0.256468000	2.511996000
O	0.548806000	0.868491000	2.557549000
H	4.225980000	-3.604364000	-0.607771000

Table S13. Coordinates and energies of the zolpidem metabolites, their radical form at the C4 site and at the OH/COOH sites, and of the transition states for the HAT from the C4 site and from the OH/COOH site to the studied radicals. Level of theory: M06-2X/6-31G(d) .

MI

E = -1124.97812108 Ha

C	4.747559000	-0.962823000	0.124848000
N	0.886744000	-2.279550000	-0.380509000
C	0.254854000	-1.124993000	-0.026905000
C	1.154987000	-0.135364000	0.339941000
C	4.559368000	-2.318962000	-0.296629000
C	3.312831000	-2.833020000	-0.498541000
C	2.177977000	-2.015467000	-0.264759000
N	2.394002000	-0.706889000	0.165857000
C	3.653419000	-0.181442000	0.336749000
H	-1.240289000	1.046192000	-0.664621000
H	3.144591000	-3.849984000	-0.832352000
C	6.136476000	-0.410676000	0.297543000
H	6.703603000	-0.480957000	-0.636267000
H	6.111405000	0.639336000	0.598489000
H	6.688604000	-0.970374000	1.059849000
C	-1.209715000	-1.017284000	-0.041849000
C	-1.993939000	-2.141776000	0.245754000
C	-3.376840000	-2.047322000	0.250555000
C	-3.998481000	-0.829369000	-0.038201000
C	-3.227502000	0.290808000	-0.353511000
C	-1.841812000	0.191951000	-0.362104000
H	-1.494934000	-3.080475000	0.462484000
H	-3.999577000	-2.906423000	0.478203000
H	-3.716244000	1.224959000	-0.609363000
C	-5.482203000	-0.781085000	-0.013666000
C	0.944841000	1.197096000	0.977854000
H	-0.058163000	1.210847000	1.407088000
H	1.649484000	1.323142000	1.812925000
C	1.196937000	2.353692000	0.009773000
H	1.281757000	4.203360000	-1.621833000
H	0.844597000	5.378524000	-0.357892000
N	0.289384000	3.372108000	-0.002753000
H	-1.554465000	2.746224000	0.858773000
O	2.183465000	2.331948000	-0.711940000
C	0.512710000	4.489727000	-0.907221000
H	-0.414178000	4.727168000	-1.437510000
C	-0.778315000	3.509708000	0.980017000
H	-0.397412000	3.466693000	2.005369000
H	-1.242865000	4.486690000	0.838404000
H	5.437108000	-2.934618000	-0.471968000
H	3.697552000	0.872713000	0.581217000
O	-6.201118000	-1.717050000	0.243079000
O	-5.975717000	0.440518000	-0.310720000
H	-6.943436000	0.353585000	-0.270403000

MI radical (C4)

E = -1124.33945452 Ha

C	4.406567000	-1.617664000	-0.012051000
N	0.366572000	-2.365577000	0.013235000
C	-0.085938000	-1.105270000	-0.028719000
C	0.978990000	-0.147261000	-0.050820000
C	3.984992000	-2.979103000	0.026408000
C	2.656256000	-3.303690000	0.025539000
C	1.698628000	-2.271945000	-0.008568000
N	2.128073000	-0.950573000	-0.061546000
C	3.465927000	-0.628987000	-0.054468000
H	-1.434720000	0.880080000	-1.351528000
H	2.297174000	-4.325149000	0.058613000
C	5.872299000	-1.275860000	-0.018167000
H	6.373008000	-1.720496000	-0.884297000
H	6.024907000	-0.195116000	-0.057330000
H	6.367339000	-1.658779000	0.880292000
C	-1.529146000	-0.835439000	-0.047656000
C	-2.385139000	-1.711745000	0.636636000
C	-3.753854000	-1.500194000	0.633389000
C	-4.292842000	-0.415710000	-0.063914000
C	-3.454202000	0.446328000	-0.771390000
C	-2.081185000	0.235059000	-0.765328000
H	-1.951311000	-2.553751000	1.165301000
H	-4.427983000	-2.163071000	1.165925000
H	-3.880771000	1.269427000	-1.333970000
C	-5.766691000	-0.231178000	-0.032837000
C	0.849638000	1.235535000	0.078132000
H	-0.159544000	1.557779000	0.302124000
C	1.849551000	2.273321000	-0.173106000
H	3.131896000	4.296067000	-0.779201000
H	2.886576000	5.090953000	0.797170000
N	1.569004000	3.519096000	0.334050000
H	-0.460066000	4.058486000	0.676909000
O	2.867490000	2.075832000	-0.845776000
C	2.384507000	4.646796000	-0.070521000
H	1.762422000	5.416759000	-0.542770000
C	0.460441000	3.807393000	1.221525000
H	0.263391000	2.962521000	1.883483000
H	0.729489000	4.664329000	1.845544000
H	4.737583000	-3.762037000	0.055650000
H	3.696619000	0.424863000	-0.128789000
O	-6.539600000	-0.947616000	0.557036000
O	-6.178777000	0.840716000	-0.741542000
H	-7.147222000	0.862739000	-0.655552000

MI TS(C4) HO˙

E = -1200.67043700 Ha

C	4.244359000	-1.690369000	-0.043665000
N	0.213721000	-2.463169000	-0.306130000
C	-0.229811000	-1.196993000	-0.105005000
C	0.824975000	-0.301458000	0.075025000
C	3.844199000	-3.040121000	-0.291576000
C	2.526732000	-3.383852000	-0.404303000
C	1.538662000	-2.381735000	-0.266134000
N	1.959491000	-1.075405000	-0.038614000
C	3.284311000	-0.728911000	0.072486000
H	-1.470675000	1.052050000	-1.012560000
H	2.199174000	-4.399540000	-0.590763000
C	5.703277000	-1.338935000	0.066162000
H	6.230021000	-1.567973000	-0.865805000
H	5.839421000	-0.275980000	0.278189000
H	6.185470000	-1.911359000	0.865287000
C	-1.666181000	-0.888131000	-0.091894000
C	-2.568221000	-1.847322000	0.385498000
C	-3.928351000	-1.577666000	0.420195000
C	-4.404315000	-0.342577000	-0.029163000
C	-3.515968000	0.608963000	-0.530843000
C	-2.155990000	0.335302000	-0.569232000
H	-2.179274000	-2.801638000	0.724736000
H	-4.627462000	-2.316886000	0.795447000
H	-3.913106000	1.548616000	-0.900691000
C	-5.849392000	0.001730000	-0.008876000
C	0.869566000	1.105602000	0.488902000
H	-0.125756000	1.450052000	0.781898000
H	1.519768000	1.202076000	1.438260000
C	1.538676000	2.052050000	-0.509359000
H	2.850678000	4.912482000	-0.666011000
H	1.252790000	5.040677000	-1.440744000
N	1.504726000	3.373628000	-0.187658000
H	1.373812000	4.850623000	1.260402000
O	2.074565000	1.616197000	-1.517028000
C	2.037659000	4.342323000	-1.128530000
H	2.416196000	3.807107000	-1.997293000
C	0.891666000	3.899751000	1.020482000
H	-0.182631000	4.084755000	0.890116000
H	1.051545000	3.231084000	1.867206000
H	4.614113000	-3.799615000	-0.394660000
H	3.495718000	0.319460000	0.242329000
O	2.689757000	1.454305000	2.405663000
H	2.709615000	0.567928000	2.819705000
O	-6.621179000	-0.991605000	0.477941000
H	-7.535607000	-0.662355000	0.444313000
O	-6.313704000	1.053245000	-0.380774000

MI TS(C4) HOO˙

E = -1275.79397314 Ha

C	4.225713000	-1.604210000	-0.274314000
N	0.198501000	-2.404607000	-0.457764000

C	-0.255182000	-1.144495000	-0.302009000
C	0.796311000	-0.214570000	-0.197769000
C	3.830221000	-2.959850000	-0.477305000
C	2.511510000	-3.309638000	-0.566834000
C	1.528464000	-2.303782000	-0.456353000
N	1.940566000	-0.988460000	-0.306667000
C	3.261777000	-0.642445000	-0.190351000
H	-1.587890000	1.024517000	-1.289250000
H	2.181428000	-4.332012000	-0.705186000
C	5.682345000	-1.246202000	-0.158086000
H	6.227765000	-1.531158000	-1.063508000
H	5.814701000	-0.172516000	-0.007428000
H	6.146127000	-1.767607000	0.685377000
C	-1.697180000	-0.863681000	-0.255800000
C	-2.556156000	-1.816684000	0.309242000
C	-3.919572000	-1.578467000	0.375083000
C	-4.447024000	-0.387579000	-0.130955000
C	-3.604537000	0.556050000	-0.720178000
C	-2.237842000	0.315224000	-0.785949000
H	-2.130017000	-2.739971000	0.687634000
H	-4.598050000	-2.301782000	0.815607000
H	-4.024260000	1.464741000	-1.137344000
C	-5.914990000	-0.179173000	-0.031814000
C	0.788351000	1.171170000	0.214680000
H	-0.226451000	1.515004000	0.421937000
H	1.325759000	1.130770000	1.371727000
C	1.606503000	2.176019000	-0.560860000
H	2.709765000	4.051077000	-1.722169000
H	2.909599000	5.048269000	-0.255844000
N	1.537702000	3.466129000	-0.117042000
H	-0.269640000	4.200347000	0.720973000
O	2.296768000	1.839984000	-1.514282000
C	2.190341000	4.511109000	-0.883800000
H	1.450802000	5.228343000	-1.259209000
C	0.743874000	3.899361000	1.018280000
H	0.679226000	3.120062000	1.778741000
H	1.235368000	4.763601000	1.473585000
H	4.600842000	-3.721786000	-0.554212000
H	3.473572000	0.409081000	-0.058649000
O	1.743474000	0.818824000	2.549436000
O	1.449819000	-0.523949000	2.580464000
H	0.568997000	-0.558091000	2.993948000
O	-6.690673000	-0.960601000	0.464189000
O	-6.316921000	0.996171000	-0.558683000
H	-7.282330000	1.025302000	-0.444875000

MI TS(C4) $CH_3O^{\bullet}$

E = -1239.96697394 Ha

C	4.166299000	-1.612184000	-0.323127000
N	0.137006000	-2.421563000	-0.479280000
C	-0.314703000	-1.163744000	-0.268151000
C	0.737383000	-0.247370000	-0.133026000
C	3.771619000	-2.963621000	-0.564016000
C	2.454055000	-3.318818000	-0.645858000
C	1.464214000	-2.323775000	-0.487220000
N	1.877879000	-1.013393000	-0.283318000
C	3.200193000	-0.658366000	-0.189365000
H	-1.614499000	1.059241000	-1.150345000
H	2.129792000	-4.338051000	-0.817605000
C	5.623826000	-1.251115000	-0.229073000
H	6.142587000	-1.478287000	-1.165941000
H	5.754862000	-0.187289000	-0.019057000
H	6.116677000	-1.818546000	0.566863000
C	-1.753947000	-0.873799000	-0.208038000
C	-2.625344000	-1.841809000	0.308781000
C	-3.985668000	-1.588827000	0.382227000
C	-4.495688000	-0.367957000	-0.067363000
C	-3.639531000	0.592528000	-0.607379000
C	-2.276025000	0.336579000	-0.681807000
H	-2.212165000	-2.786546000	0.646137000
H	-4.675014000	-2.323061000	0.786160000
H	-4.046088000	1.526030000	-0.980395000
C	-5.961315000	-0.145783000	0.036767000
C	0.782119000	1.147089000	0.290671000
H	-0.207841000	1.500596000	0.589596000
H	1.441045000	1.172371000	1.285753000
C	1.490364000	2.117342000	-0.644602000
H	2.436308000	3.933228000	-2.015851000
H	2.933687000	4.929590000	-0.621699000
N	1.539634000	3.412006000	-0.222020000
H	-0.080573000	4.167435000	0.925309000
O	1.990563000	1.732871000	-1.691674000
C	2.092544000	4.421663000	-1.105997000
H	1.330122000	5.168708000	-1.355850000
C	0.973905000	3.880427000	1.032176000
H	1.071944000	3.128483000	1.816638000
H	1.535212000	4.762472000	1.351314000
H	4.544858000	-3.717879000	-0.679930000
H	3.406933000	0.387788000	-0.006627000
C	1.933295000	-0.275711000	2.893323000
H	1.671883000	-0.235293000	3.960228000
H	2.749121000	-0.995461000	2.728487000
H	1.041986000	-0.674980000	2.368989000
O	2.246444000	0.986760000	2.416750000
O	-6.749482000	-0.941443000	0.488522000
O	-6.345876000	1.060264000	-0.430483000
H	-7.311227000	1.095990000	-0.318298000

MI TS(C4) $CH_3OO^{\bullet}$

E = -1315.08653195 Ha

C	4.292575000	-1.483799000	-0.467266000
N	0.276250000	-2.337979000	-0.635630000
C	-0.196691000	-1.083016000	-0.488815000
C	0.840166000	-0.133475000	-0.391703000
C	3.913299000	-2.848303000	-0.648835000
C	2.598923000	-3.211354000	-0.740759000
C	1.602854000	-2.215830000	-0.644182000
N	1.996749000	-0.889359000	-0.502786000
C	3.320194000	-0.529044000	-0.400400000
H	-1.576939000	1.017171000	-1.545482000
H	2.278916000	-4.238302000	-0.869608000
C	5.746046000	-1.106860000	-0.368976000
H	6.285286000	-1.396310000	-1.276605000
H	5.867129000	-0.029885000	-0.233277000
H	6.225559000	-1.613332000	0.474908000
C	-1.642643000	-0.825790000	-0.431057000
C	-2.475161000	-1.766403000	0.188965000
C	-3.842301000	-1.551945000	0.258036000
C	-4.397879000	-0.397839000	-0.299890000
C	-3.580319000	0.534129000	-0.940397000
C	-2.209925000	0.316863000	-1.008627000
H	-2.028231000	-2.661032000	0.609784000
H	-4.501807000	-2.265079000	0.741658000
H	-4.021691000	1.415008000	-1.393245000
C	-5.868975000	-0.214574000	-0.197197000
C	0.773101000	1.229274000	0.086251000
H	-0.266668000	1.531060000	0.223893000
H	1.103178000	1.126476000	1.333228000
C	1.621951000	2.307858000	-0.530299000
H	2.761229000	4.295456000	-1.446576000
H	2.748784000	5.208015000	0.087538000
N	1.454400000	3.560462000	-0.014970000
H	0.383756000	3.057550000	1.735720000
O	2.418135000	2.066169000	-1.431950000
C	2.131328000	4.677984000	-0.645920000
H	1.400009000	5.382796000	-1.059326000
C	0.522630000	3.893443000	1.049273000
H	0.938592000	4.726987000	1.622285000
H	-0.452747000	4.205258000	0.652717000
H	4.692286000	-3.602729000	-0.713609000
H	3.520203000	0.529575000	-0.314862000
C	1.091335000	-1.441476000	2.653672000
H	1.445082000	-1.535734000	3.684851000
H	1.948574000	-1.377655000	1.975900000
H	0.458326000	-2.289590000	2.382407000
O	0.268695000	-0.291977000	2.521950000
O	1.052239000	0.828608000	2.574925000
O	-6.625468000	-0.990114000	0.336303000
O	-6.298647000	0.929641000	-0.769117000
H	-7.263291000	0.944762000	-0.646722000

MI TS(C4) $CH_2CHOO^{\bullet}$

E = -1353.16075641 Ha

C	4.217295000	-1.351643000	-0.682954000
N	0.213661000	-2.270537000	-0.786294000
C	-0.276497000	-1.032977000	-0.585936000
C	0.748714000	-0.067493000	-0.479627000
C	3.858150000	-2.713076000	-0.908712000

C	2.547201000	-3.096924000	-0.979027000
C	1.539897000	-2.123407000	-0.820361000
N	1.912437000	-0.796417000	-0.652802000
C	3.228450000	-0.418358000	-0.558130000
H	-1.713583000	1.089719000	-1.517542000
H	2.241400000	-4.124156000	-1.136754000
C	5.665175000	-0.951567000	-0.593619000
H	6.198546000	-1.208773000	-1.514291000
H	5.769342000	0.123733000	-0.432525000
H	6.163834000	-1.469858000	0.231901000
C	-1.724801000	-0.803119000	-0.487289000
C	-2.528923000	-1.786097000	0.104287000
C	-3.897803000	-1.599218000	0.210029000
C	-4.483733000	-0.430633000	-0.282710000
C	-3.695187000	0.544055000	-0.895388000
C	-2.322989000	0.354744000	-1.000173000
H	-2.058810000	-2.692157000	0.472196000
H	-4.535383000	-2.345718000	0.672192000
H	-4.160425000	1.436592000	-1.298763000
C	-5.955725000	-0.278950000	-0.143377000
C	0.672414000	1.275112000	0.051425000
H	-0.368584000	1.552798000	0.227123000
H	1.056993000	1.156681000	1.260943000
C	1.476834000	2.389428000	-0.568831000
H	2.542933000	4.422527000	-1.472244000
H	2.559508000	5.298906000	0.082805000
N	1.299693000	3.624692000	-0.017508000
H	0.306834000	3.060562000	1.760302000
O	2.245771000	2.185636000	-1.502114000
C	1.930820000	4.771947000	-0.643172000
H	1.170895000	5.468811000	-1.016342000
C	0.394713000	3.910851000	1.083206000
H	0.803852000	4.748322000	1.655134000
H	-0.603114000	4.197308000	0.725317000
H	4.648057000	-3.450330000	-1.022255000
H	3.413142000	0.639120000	-0.432111000
C	1.071760000	-1.412308000	2.420911000
O	0.327160000	-0.269898000	2.539615000
O	1.092706000	0.863814000	2.540400000
O	-6.687257000	-1.092271000	0.367943000
O	-6.416081000	0.882172000	-0.653346000
H	-7.378349000	0.874509000	-0.512694000
C	2.398148000	-1.496674000	2.420888000
H	2.865162000	-2.466075000	2.300710000
H	3.018835000	-0.618852000	2.541546000
H	0.396496000	-2.255632000	2.312969000

MI radical (COO˙)

E = -1124.29539623 Ha

C	4.703624000	-0.982191000	0.128892000
N	0.835760000	-2.279066000	-0.371484000
C	0.211087000	-1.119460000	-0.022060000
C	1.116496000	-0.133627000	0.342022000
C	4.507609000	-2.338987000	-0.287868000
C	3.258576000	-2.847053000	-0.487911000
C	2.128391000	-2.022038000	-0.256540000
N	2.351606000	-0.713480000	0.169862000
C	3.614202000	-0.194046000	0.338595000
H	-1.277404000	1.064319000	-0.642236000
H	3.084724000	-3.864108000	-0.818448000
C	6.095811000	-0.437610000	0.298579000
H	6.660781000	-0.512725000	-0.636106000
H	6.077340000	0.612932000	0.597988000
H	6.645668000	-0.999551000	1.060790000
C	-1.252443000	-1.006943000	-0.040043000
C	-2.037906000	-2.135458000	0.232367000
C	-3.420736000	-2.042841000	0.234157000
C	-4.033865000	-0.819180000	-0.044044000
C	-3.265375000	0.306085000	-0.345261000
C	-1.880448000	0.207808000	-0.350559000
H	-1.538214000	-3.075807000	0.439610000
H	-4.045312000	-2.903950000	0.450638000
H	-3.749648000	1.246747000	-0.594795000
C	-5.511016000	-0.755298000	-0.024861000
C	0.915835000	1.203091000	0.974004000
H	-0.085819000	1.226317000	1.406178000
H	1.622869000	1.328455000	1.807067000
C	1.172869000	2.352101000	-0.002412000
H	1.255826000	4.189246000	-1.649782000
H	0.856919000	5.378080000	-0.386114000
N	0.278821000	3.382231000	-0.008698000
H	-1.572288000	2.800473000	0.869378000
O	2.149595000	2.312238000	-0.736133000
C	0.503079000	4.491052000	-0.924247000
H	-0.429102000	4.738506000	-1.440379000
C	-0.772359000	3.539771000	0.988621000
H	-0.380550000	3.473911000	2.008371000
H	-1.209976000	4.531389000	0.864234000
H	5.381946000	-2.959965000	-0.461185000
H	3.664355000	0.860610000	0.579543000
O	-6.279919000	-1.666829000	0.202041000
O	-6.062925000	0.422875000	-0.277296000

MI TS(COOH) HO˙

E = -1200.67203139 Ha

C	5.114508000	-1.033902000	0.128151000
N	1.228780000	-2.275788000	-0.374324000
C	0.619846000	-1.107954000	-0.023975000
C	1.539288000	-0.135333000	0.340995000
C	4.899676000	-2.387356000	-0.289748000
C	3.643477000	-2.877471000	-0.490581000
C	2.524853000	-2.037046000	-0.258972000
N	2.766451000	-0.732023000	0.168547000
C	4.036037000	-0.230715000	0.338039000
H	-0.836182000	1.097350000	-0.643900000
H	3.455425000	-3.891721000	-0.822020000
C	6.514071000	-0.508729000	0.298660000
H	7.078403000	-0.590892000	-0.635850000
H	6.509907000	0.541815000	0.598688000
H	7.056078000	-1.078512000	1.060722000
C	-0.842103000	-0.973190000	-0.040290000
C	-1.645643000	-2.087580000	0.232644000
C	-3.027610000	-1.972365000	0.237031000
C	-3.623742000	-0.738233000	-0.036228000
C	-2.834804000	0.373030000	-0.337960000
C	-1.452271000	0.251220000	-0.348715000
H	-1.162296000	-3.036964000	0.437833000
H	-3.660721000	-2.826706000	0.451683000
H	-3.315123000	1.314924000	-0.583424000
C	-5.102492000	-0.617822000	-0.019123000
C	1.357256000	1.203531000	0.974309000
H	0.355639000	1.239970000	1.405526000
H	2.065962000	1.318173000	1.807526000
C	1.630930000	2.350017000	-0.000451000
H	1.345966000	5.378396000	-0.392199000
H	0.057962000	4.748026000	-1.449758000
N	0.747465000	3.389020000	-0.012101000
H	-0.737875000	4.552085000	0.847667000
O	2.611807000	2.300898000	-0.728349000
C	0.985804000	4.493262000	-0.929382000
H	1.738462000	4.182539000	-1.651230000
C	-0.309117000	3.557317000	0.977782000
H	-1.113966000	2.824154000	0.855057000
H	0.075986000	3.491389000	2.000148000
H	5.765225000	-3.020466000	-0.463452000
H	4.100780000	0.823011000	0.579590000
O	-7.616477000	-0.178772000	-0.150440000
H	-7.693877000	0.364877000	0.653505000
O	-5.812316000	-1.650506000	0.203244000
H	-6.882648000	-1.120705000	0.102231000
O	-5.629233000	0.515469000	-0.217744000

MI TS(COOH) HOO˙

E = -1275.77338009 Ha

C	5.443543000	-1.089180000	0.140892000
N	1.543283000	-2.237528000	-0.458052000
C	0.948774000	-1.078776000	-0.057594000
C	1.880089000	-0.136000000	0.354950000
C	5.210429000	-2.415752000	-0.346158000
C	3.947934000	-2.872170000	-0.584027000
C	2.842059000	-2.023778000	-0.323385000
N	3.100757000	-0.743633000	0.165062000
C	4.377507000	-0.276025000	0.376387000
H	-0.482379000	1.163735000	-0.580243000
H	3.745096000	-3.866077000	-0.964781000
C	6.849778000	-0.599634000	0.357290000
H	7.427317000	-0.647294000	-0.571570000
H	6.859866000	0.434990000	0.708069000

H	7.369243000	-1.215792000	1.098707000
C	-0.511930000	-0.927120000	-0.062304000
C	-1.327124000	-2.041081000	0.176499000
C	-2.707063000	-1.906794000	0.198896000
C	-3.291202000	-0.656108000	-0.020622000
C	-2.489915000	0.454410000	-0.287429000
C	-1.108785000	0.315499000	-0.315637000
H	-0.854272000	-3.002894000	0.345201000
H	-3.345651000	-2.762439000	0.392941000
H	-2.964327000	1.410343000	-0.484117000
C	-4.772658000	-0.493242000	0.008579000
C	1.711175000	1.173448000	1.055984000
H	0.715824000	1.182662000	1.497455000
H	2.430354000	1.240074000	1.883249000
C	2.011045000	2.356819000	0.134003000
H	0.512200000	4.644236000	-1.587618000
H	2.215690000	4.101321000	-1.616337000
N	1.062480000	3.318716000	-0.071575000
H	-0.030224000	4.441293000	1.329013000
O	3.097034000	2.389207000	-0.428860000
C	1.390049000	4.408579000	-0.978568000
H	1.680685000	5.306654000	-0.419540000
C	-0.140173000	3.541758000	0.710268000
H	-0.991759000	3.693196000	0.037516000
H	-0.370991000	2.701668000	1.360296000
H	6.066532000	-3.055743000	-0.540485000
H	4.457133000	0.763287000	0.669734000
O	-7.580579000	0.240372000	-0.426974000
H	-6.548788000	0.628342000	-0.244310000
O	-5.472708000	-1.548733000	0.092186000
H	-7.764822000	-1.577592000	-0.077082000
O	-5.254250000	0.675257000	-0.054014000
O	-7.496193000	-0.800599000	0.453626000

MI TS(COOH) $CH_3O^{\bullet}$

E = -1239.94753492 Ha

C	5.486240000	-0.965179000	0.193829000
N	1.637404000	-2.275131000	-0.410612000
C	0.998105000	-1.123287000	-0.061348000
C	1.890220000	-0.137396000	0.334615000
C	5.307122000	-2.317489000	-0.243654000
C	4.065357000	-2.829016000	-0.478571000
C	2.925759000	-2.012890000	-0.263464000
N	3.132459000	-0.708271000	0.183478000
C	4.387874000	-0.185024000	0.387545000
H	-0.485504000	1.058206000	-0.695643000
H	3.904465000	-3.842931000	-0.825041000
C	6.871097000	-0.415313000	0.402624000
H	7.458399000	-0.475778000	-0.519314000
H	6.839536000	0.631424000	0.714155000
H	7.406444000	-0.983300000	1.170731000
C	-0.465487000	-1.015736000	-0.107652000
C	-1.254613000	-2.145679000	0.146025000
C	-2.637500000	-2.053897000	0.124137000
C	-3.252744000	-0.830540000	-0.155449000
C	-2.477652000	0.295228000	-0.439623000
C	-1.091896000	0.197907000	-0.421512000
H	-0.758634000	-3.086722000	0.359936000
H	-3.263676000	-2.915929000	0.329851000
H	-2.962989000	1.234171000	-0.685376000
C	-4.747049000	-0.784460000	-0.153342000
C	1.667331000	1.189497000	0.979910000
H	0.655768000	1.200371000	1.388691000
H	2.354872000	1.307649000	1.830222000
C	1.939896000	2.353891000	0.026642000
H	2.052208000	4.211532000	-1.595273000
H	1.601933000	5.379528000	-0.329470000
N	1.033434000	3.372865000	0.003727000
H	-0.828717000	2.747044000	0.825670000
O	2.940680000	2.336537000	-0.675327000
C	1.274245000	4.495945000	-0.889601000
H	0.355834000	4.740669000	-1.431087000
C	-0.051469000	3.505719000	0.968251000
H	0.310676000	3.451066000	1.999782000
H	-0.509270000	4.486023000	0.827854000
H	6.188384000	-2.932128000	-0.404228000
H	4.426731000	0.866928000	0.642088000
O	-7.467701000	0.605921000	-0.189970000
O	-5.447189000	-1.688540000	0.262882000
O	-5.228327000	0.335551000	-0.670219000
H	-6.612943000	0.305120000	-0.704370000
C	-7.969967000	-0.382473000	0.668954000
H	-8.099113000	-1.344629000	0.168113000
H	-7.302567000	-0.526375000	1.528317000
H	-8.923838000	0.007209000	1.039428000

MII

E = -1124.97756556 Ha

C	3.769567000	-0.817868000	0.041745000
N	0.001302000	-2.324649000	-0.388782000
C	-0.691491000	-1.200272000	-0.031595000
C	0.155461000	-0.163538000	0.315155000
C	3.668612000	-2.181196000	-0.373629000
C	2.446545000	-2.756985000	-0.546972000
C	1.274036000	-1.996784000	-0.295150000
N	1.426314000	-0.666771000	0.126048000
C	2.646043000	-0.074644000	0.270971000
H	-2.318661000	0.868139000	-0.702501000
H	2.322711000	-3.782600000	-0.872841000
C	5.115831000	-0.222833000	0.190950000
C	-2.160570000	-1.170999000	-0.027403000
C	-2.884438000	-2.322956000	0.300898000
C	-4.271492000	-2.299245000	0.319151000
C	-4.981968000	-1.134018000	0.007587000
C	-4.256558000	0.004305000	-0.343837000
C	-2.864373000	-0.012515000	-0.369073000
H	-2.338525000	-3.231258000	0.535978000
H	-4.820203000	-3.201576000	0.578870000
H	-6.904819000	-1.953904000	-0.530633000
H	-4.788008000	0.911108000	-0.623223000
C	-6.488692000	-1.122721000	0.047072000
H	-6.855947000	-1.223898000	1.074120000
H	-6.889793000	-0.191814000	-0.361787000
C	-0.120211000	1.165816000	0.931668000
H	-1.122587000	1.133270000	1.361429000
H	0.578014000	1.345798000	1.762308000
C	0.069293000	2.311490000	-0.063433000
H	0.066854000	4.137800000	-1.719686000
H	-0.446080000	5.318033000	-0.488897000
N	-0.876805000	3.292806000	-0.079325000
H	-2.697030000	2.602950000	0.783224000
O	1.044274000	2.311750000	-0.801249000
C	-0.720684000	4.396194000	-1.014558000
H	-1.658585000	4.561799000	-1.553131000
C	-1.947583000	3.393129000	0.904141000
H	-1.563468000	3.362208000	1.928497000
H	-2.444446000	4.354465000	0.764643000
H	4.588313000	-2.725664000	-0.555387000
H	2.656043000	0.979367000	0.516961000
O	5.084166000	1.058808000	0.611229000
H	6.010605000	1.349842000	0.660931000
O	6.149806000	-0.806799000	-0.028305000

MII radical (C4)

E = -1124.33830637 Ha

C	3.465489000	-1.313723000	0.018345000
N	-0.485676000	-2.321223000	0.009807000
C	-1.029388000	-1.092285000	-0.035998000
C	-0.036691000	-0.063914000	-0.053438000
C	3.158242000	-2.704066000	0.047597000
C	1.855128000	-3.110278000	0.035698000
C	0.830623000	-2.140777000	-0.002909000
N	1.170479000	-0.783516000	-0.055605000
C	2.473873000	-0.372027000	-0.034762000
H	-2.521430000	0.788401000	-1.369844000
H	1.560331000	-4.152031000	0.063828000
C	4.891331000	-0.910899000	0.036470000
C	-2.486722000	-0.924817000	-0.061410000
C	-3.285390000	-1.856892000	0.616442000
C	-4.666815000	-1.744128000	0.600946000
C	-5.301077000	-0.709353000	-0.096503000
C	-4.504088000	0.199444000	-0.792818000
C	-3.116521000	0.096911000	-0.781255000
H	-2.799398000	-2.668070000	1.148909000
H	-5.270667000	-2.472761000	1.136464000
H	-7.280238000	-1.558730000	-0.235475000
H	-4.976497000	0.991877000	-1.367637000
C	-6.802691000	-0.585705000	-0.086891000

H	-7.156629000	-0.191387000	0.872178000
H	-7.150852000	0.088832000	-0.873209000
C	-0.264315000	1.306519000	0.066115000
H	-1.294624000	1.557368000	0.284785000
C	0.665746000	2.403041000	-0.202560000
H	1.840747000	4.483413000	-0.824507000
H	1.496525000	5.311252000	0.716244000
N	0.303133000	3.638807000	0.274123000
H	-1.763082000	4.048998000	0.570018000
O	1.698125000	2.252784000	-0.864857000
C	1.051304000	4.805988000	-0.148793000
H	0.392807000	5.515601000	-0.664428000
C	-0.837292000	3.876344000	1.135787000
H	-0.988547000	3.039188000	1.819280000
H	-0.636918000	4.766653000	1.738354000
H	3.980232000	-3.410336000	0.080258000
H	2.650801000	0.693337000	-0.102367000
O	5.063648000	0.423506000	0.038282000
H	6.023949000	0.576428000	0.038845000
O	5.814912000	-1.689141000	0.052781000

MII TS(C4) HO•

E = -1200.66902887 Ha

C	3.376549000	-1.379093000	-0.069072000
N	-0.561798000	-2.433329000	-0.269606000
C	-1.101078000	-1.198122000	-0.073347000
C	-0.117638000	-0.226999000	0.088104000
C	3.094439000	-2.756926000	-0.306322000
C	1.804003000	-3.190496000	-0.394388000
C	0.748287000	-2.258110000	-0.245824000
N	1.075621000	-0.913591000	-0.032214000
C	2.362146000	-0.469851000	0.057428000
H	-2.528509000	0.927257000	-1.013120000
H	1.543784000	-4.226972000	-0.570877000
C	4.792899000	-0.956350000	0.025139000
C	-2.556193000	-0.999317000	-0.049981000
C	-3.382404000	-2.011194000	0.454671000
C	-4.758106000	-1.841400000	0.490132000
C	-5.355480000	-0.665923000	0.019573000
C	-4.529863000	0.327990000	-0.505338000
C	-3.147988000	0.165495000	-0.546992000
H	-2.924047000	-2.928027000	0.811617000
H	-5.387017000	-2.634538000	0.887579000
H	-7.367623000	-1.364091000	-0.330024000
H	-4.975199000	1.235174000	-0.905583000
C	-6.851111000	-0.490731000	0.079825000
H	-7.190176000	-0.367098000	1.114167000
H	-7.171026000	0.388927000	-0.484344000
C	-0.179112000	1.186185000	0.475744000
H	-1.198068000	1.457036000	0.764549000
H	0.465557000	1.353774000	1.420262000
C	0.416734000	2.157181000	-0.544860000
H	1.509454000	5.102292000	-0.765265000
H	-0.086738000	5.091857000	-1.554463000
N	0.277933000	3.479417000	-0.258240000
H	0.029026000	4.978115000	1.151220000
O	0.989323000	1.737715000	-1.539406000
C	0.745292000	4.462120000	-1.219229000
H	1.170825000	3.935585000	-2.071376000
C	-0.375463000	3.985850000	0.936953000
H	-1.461137000	4.080719000	0.803926000
H	-0.162265000	3.354156000	1.800233000
H	3.933374000	-3.435309000	-0.413727000
H	2.516607000	0.588483000	0.226919000
O	1.620156000	1.737346000	2.349390000
H	1.707014000	0.887074000	2.825798000
O	5.735463000	-1.700648000	-0.099164000
O	4.933594000	0.359873000	0.274527000
H	5.890108000	0.531960000	0.306868000

MII TS(C4) HOO•

E = -1275.79304623 Ha

C	3.373864000	-1.349470000	-0.223614000
N	-0.571105000	-2.369267000	-0.418590000
C	-1.104154000	-1.131191000	-0.293388000
C	-0.113332000	-0.140874000	-0.199412000
C	3.079427000	-2.731340000	-0.402027000
C	1.783501000	-3.150136000	-0.492497000
C	0.744650000	-2.195398000	-0.407272000
N	1.080052000	-0.846803000	-0.282597000
C	2.368926000	-0.423222000	-0.163696000
H	-2.569996000	0.930023000	-1.337923000
H	1.507713000	-4.190474000	-0.612907000
C	4.792906000	-0.941311000	-0.105927000
C	-2.559801000	-0.936945000	-0.262387000
C	-3.368111000	-1.925330000	0.314186000
C	-4.745343000	-1.769288000	0.359373000
C	-5.362986000	-0.631675000	-0.173283000
C	-4.555841000	0.337183000	-0.770045000
C	-3.173029000	0.189350000	-0.820415000
H	-2.894399000	-2.815538000	0.716009000
H	-5.359015000	-2.544504000	0.811979000
H	-5.017390000	1.212768000	-1.219305000
C	-6.858998000	-0.466499000	-0.099730000
H	-7.372696000	-1.388851000	-0.386827000
H	-7.176229000	-0.219889000	0.919558000
C	-0.209310000	1.247883000	0.189366000
H	-1.246700000	1.534356000	0.369642000
H	0.300942000	1.250943000	1.362426000
C	0.569595000	2.281870000	-0.587254000
H	1.609820000	4.188372000	-1.754812000
H	1.712006000	5.223974000	-0.305292000
N	0.423003000	3.573973000	-0.171655000
H	-1.434353000	4.238041000	0.612553000
O	1.296523000	1.963720000	-1.519669000
C	1.041552000	4.636808000	-0.942270000
H	0.276412000	5.305400000	-1.354346000
C	-0.416262000	3.986119000	0.938316000
H	-0.465358000	3.214424000	1.707578000
H	0.025655000	4.876815000	1.393523000
H	3.910275000	-3.426022000	-0.454874000
H	2.538476000	0.637963000	-0.051811000
O	0.693245000	0.966336000	2.551658000
O	0.477033000	-0.390847000	2.580087000
H	-0.415693000	-0.475344000	2.959606000
H	-7.203075000	0.334414000	-0.758946000
O	5.726709000	-1.704383000	-0.165748000
O	4.946764000	0.383548000	0.079290000
H	5.904230000	0.541616000	0.140978000

MII TS(C4) CH_3O•

E = -1239.96570207 Ha

C	3.307350000	-1.374491000	-0.266545000
N	-0.644327000	-2.385763000	-0.422956000
C	-1.170000000	-1.145954000	-0.241474000
C	-0.173254000	-0.173395000	-0.118019000
C	3.007264000	-2.751250000	-0.481992000
C	1.710667000	-3.170127000	-0.560100000
C	0.669812000	-2.221237000	-0.424052000
N	1.013004000	-0.877834000	-0.244878000
C	2.304343000	-0.450966000	-0.153151000
H	-2.597341000	0.981156000	-1.179077000
H	1.436045000	-4.206499000	-0.713382000
C	4.729614000	-0.969883000	-0.173224000
C	-2.622456000	-0.935805000	-0.196636000
C	-3.446269000	-1.937676000	0.331040000
C	-4.820425000	-1.759508000	0.385171000
C	-5.417703000	-0.585792000	-0.089153000
C	-4.594267000	0.397722000	-0.637751000
C	-3.214436000	0.227744000	-0.697244000
H	-2.987958000	-2.853572000	0.690426000
H	-5.447756000	-2.544800000	0.800021000
H	-7.243841000	0.425899000	-0.640974000
H	-5.040565000	1.302730000	-1.041756000
C	-6.910264000	-0.396783000	-0.003442000
H	-7.441539000	-1.302846000	-0.309536000
H	-7.217378000	-0.169099000	1.023363000
C	-0.209625000	1.229159000	0.277600000
H	-1.222339000	1.533564000	0.553080000
H	0.431057000	1.307110000	1.283393000
C	0.465456000	2.213353000	-0.667059000
H	0.172186000	5.237418000	-1.456764000
H	1.350519000	4.041109000	-2.062446000
N	0.436577000	3.518248000	-0.277949000
H	-1.241202000	4.211023000	0.825394000
O	1.008245000	1.828703000	-1.692931000
C	0.962584000	4.533071000	-1.172501000
H	1.767632000	5.090147000	-0.681088000

C	-0.174664000	3.984795000	0.955287000
H	-0.049153000	3.257896000	1.759282000
H	0.332836000	4.903232000	1.261416000
H	3.837267000	-3.442507000	-0.576474000
H	2.473642000	0.604660000	0.010381000
C	0.971536000	-0.091163000	2.920370000
H	0.690937000	-0.037974000	3.981661000
H	1.823707000	-0.774327000	2.787402000
H	0.109195000	-0.544147000	2.391493000
O	1.234254000	1.172952000	2.417130000
O	5.660377000	-1.733190000	-0.266046000
O	4.888244000	0.351191000	0.031373000
H	5.846739000	0.509138000	0.075713000

MII TS(C4) $CH_3OO^{\bullet}$

E = -1315.08521306 Ha

C	3.474900000	-1.258459000	-0.342860000
N	-0.455132000	-2.320972000	-0.593183000
C	-1.006230000	-1.087741000	-0.486538000
C	-0.029840000	-0.082237000	-0.379923000
C	3.197100000	-2.646093000	-0.510189000
C	1.907018000	-3.075647000	-0.624175000
C	0.856432000	-2.130509000	-0.567123000
N	1.174475000	-0.772675000	-0.442810000
C	2.463227000	-0.338001000	-0.316738000
H	-2.480217000	0.910014000	-1.626352000
H	1.641714000	-4.119033000	-0.742872000
C	4.889322000	-0.835891000	-0.210176000
C	-2.464120000	-0.912898000	-0.478626000
C	-3.265883000	-1.886723000	0.128144000
C	-4.645689000	-1.748503000	0.146922000
C	-5.270071000	-0.643918000	-0.443211000
C	-4.467586000	0.310340000	-1.069489000
C	-3.082662000	0.180430000	-1.092220000
H	-2.787563000	-2.751425000	0.577509000
H	-5.255379000	-2.510644000	0.626055000
H	-7.119776000	0.226926000	-1.137871000
H	-4.934118000	1.160298000	-1.560815000
C	-6.768418000	-0.491915000	-0.393229000
H	-7.269426000	-1.446817000	-0.577003000
H	-7.092062000	-0.136721000	0.591481000
C	-0.184900000	1.284787000	0.062880000
H	-1.243322000	1.531683000	0.162597000
H	0.110683000	1.229047000	1.322718000
C	0.626980000	2.387550000	-0.560681000
H	1.704197000	4.399345000	-1.497356000
H	1.598302000	5.352220000	0.008222000
N	0.385530000	3.643880000	-0.087602000
H	-0.711565000	3.135781000	1.644680000
O	1.457688000	2.157517000	-1.433790000
C	1.030751000	4.774147000	-0.729153000
H	0.281894000	5.431949000	-1.186269000
C	-0.590347000	3.960322000	0.941357000
H	-0.228619000	4.825389000	1.504338000
H	-1.566678000	4.217778000	0.509778000
H	4.034935000	-3.333687000	-0.540172000
H	2.621417000	0.728388000	-0.240618000
C	0.141343000	-1.302751000	2.712053000
H	0.487392000	-1.343815000	3.749156000
H	1.003785000	-1.243452000	2.040430000
H	-0.464196000	-2.179143000	2.470257000
O	-0.713027000	-0.184846000	2.524484000
O	0.033157000	0.961519000	2.567086000
O	5.829700000	-1.591720000	-0.252833000
O	5.027906000	0.490721000	-0.028824000
H	5.983162000	0.661031000	0.036121000

MII TS(C4) $CH_2CHOO^{\bullet}$

E = -1353.15988827 Ha

C	3.411195000	-1.165418000	-0.524226000
N	-0.507620000	-2.273631000	-0.736326000
C	-1.072027000	-1.055770000	-0.574181000
C	-0.104371000	-0.039096000	-0.454759000
C	3.150183000	-2.547458000	-0.744187000
C	1.863074000	-2.991571000	-0.847186000
C	0.803718000	-2.063907000	-0.731893000
N	1.104192000	-0.708153000	-0.578064000
C	2.385551000	-0.262438000	-0.444156000
H	-2.597479000	0.973999000	-1.584639000
H	1.609388000	-4.033565000	-0.998841000
C	-2.530925000	-0.900620000	-0.524658000
C	-3.306375000	-1.913262000	0.052977000
C	-4.686729000	-1.794075000	0.111029000
C	-5.338391000	-0.670695000	-0.410484000
C	-4.562840000	0.322710000	-1.009262000
C	-3.177476000	0.212517000	-1.070688000
H	-2.806814000	-2.792441000	0.447837000
H	-5.275563000	-2.586231000	0.566969000
H	-5.051339000	1.188627000	-1.448526000
C	-0.261750000	1.309980000	0.039158000
H	-1.319422000	1.540055000	0.179894000
H	0.096576000	1.241261000	1.262815000
C	0.510686000	2.439897000	-0.593420000
H	1.524295000	4.485947000	-1.526062000
H	1.456350000	5.407536000	0.000994000
N	0.267170000	3.682236000	-0.086795000
H	-0.750923000	3.127043000	1.678974000
O	1.312387000	2.238308000	-1.499084000
C	0.872369000	4.835066000	-0.727773000
H	0.098046000	5.489401000	-1.145600000
C	-0.677497000	3.962070000	0.981426000
H	-0.316456000	4.829579000	1.540817000
H	-1.675513000	4.199498000	0.589848000
H	3.996632000	-3.221145000	-0.818588000
H	2.531088000	0.801309000	-0.320594000
C	0.209814000	-1.295052000	2.487993000
O	-0.591248000	-0.187110000	2.559119000
O	0.118939000	0.981834000	2.544869000
C	1.538454000	-1.315782000	2.519099000
H	2.053802000	-2.264712000	2.438887000
H	2.114772000	-0.406753000	2.631097000
H	-0.422346000	-2.172307000	2.389550000
C	4.820232000	-0.728045000	-0.387489000
H	-7.212599000	0.222879000	-1.002928000
C	-6.836843000	-0.541981000	-0.318587000
H	-7.330572000	-1.488077000	-0.559110000
H	-7.142840000	-0.261792000	0.695470000
O	5.771991000	-1.464872000	-0.480335000
O	4.940502000	0.589669000	-0.137811000
H	5.893850000	0.771688000	-0.076428000

MII radical ($COO^{\bullet}$)

E = -1124.28074695 Ha

C	3.798951000	-0.811121000	0.046262000
N	0.033521000	-2.319224000	-0.385868000
C	-0.663281000	-1.196099000	-0.024140000
C	0.181456000	-0.161127000	0.328759000
C	3.700049000	-2.172837000	-0.375696000
C	2.477986000	-2.749017000	-0.548114000
C	1.303955000	-1.991097000	-0.290358000
N	1.454529000	-0.662021000	0.137886000
C	2.670551000	-0.069992000	0.283847000
H	-2.289826000	0.871817000	-0.696329000
H	2.353872000	-3.773252000	-0.878431000
C	5.126724000	-0.185428000	0.208913000
C	-2.132173000	-1.169165000	-0.025265000
C	-2.855369000	-2.322951000	0.297678000
C	-4.242472000	-2.300727000	0.310840000
C	-4.952932000	-1.135570000	-0.001041000
C	-4.227660000	0.004549000	-0.347275000
C	-2.835534000	-0.010381000	-0.366989000
H	-2.309895000	-3.231439000	0.533084000
H	-4.791108000	-3.204156000	0.566559000
H	-6.872256000	-1.955707000	-0.550192000
H	-4.759154000	0.911201000	-0.626697000
C	-6.459712000	-1.126247000	0.032467000
H	-6.830476000	-1.232184000	1.057718000
H	-6.860425000	-0.194252000	-0.374120000
C	-0.095067000	1.169582000	0.940882000
H	-1.101663000	1.141837000	1.360874000
H	0.595594000	1.349289000	1.777801000
C	0.109825000	2.309759000	-0.058485000
H	0.142735000	4.139375000	-1.710149000
H	-0.375175000	5.324717000	-0.486309000
N	-0.821009000	3.303725000	-0.075994000
H	-2.656657000	2.637879000	0.772653000
O	1.085050000	2.291509000	-0.796086000
C	-0.649920000	4.403840000	-1.013104000

H	-1.581793000	4.573252000	-1.560840000
C	-1.895671000	3.415716000	0.902077000
H	-1.517628000	3.373746000	1.928170000
H	-2.376679000	4.385311000	0.764806000
H	4.618290000	-2.717954000	-0.562970000
H	2.684393000	0.981345000	0.539797000
O	5.124037000	1.093586000	0.622041000
O	6.178454000	-0.766132000	-0.000346000

MII TS(COOH) HO$^{\bullet}$

E = -1200.66267720 Ha

C	3.365883000	-1.050803000	-0.052349000
N	-0.477835000	-2.372149000	-0.396656000
C	-1.107808000	-1.212361000	-0.034194000
C	-0.204485000	-0.216756000	0.289205000
C	3.191773000	-2.412050000	-0.451135000
C	1.939025000	-2.926409000	-0.596977000
C	0.810354000	-2.107124000	-0.330934000
N	1.036300000	-0.782779000	0.077578000
C	2.284857000	-0.249736000	0.191301000
H	-2.640622000	0.929453000	-0.693622000
H	1.758881000	-3.948249000	-0.908172000
C	4.748318000	-0.520057000	0.067961000
C	-2.573198000	-1.109796000	-0.003502000
C	-3.347639000	-2.221215000	0.348104000
C	-4.731112000	-2.127176000	0.391420000
C	-5.387586000	-0.930047000	0.082244000
C	-4.612532000	0.167400000	-0.292511000
C	-3.223756000	0.080131000	-0.342686000
H	-2.844203000	-3.154137000	0.581585000
H	-5.319677000	-2.998438000	0.669159000
H	-5.102790000	1.097565000	-0.570203000
C	-6.890837000	-0.842569000	0.148439000
H	-7.251582000	0.107415000	-0.254029000
H	-7.358566000	-1.651654000	-0.421099000
C	-0.401715000	1.129368000	0.899072000
H	-1.397497000	1.151703000	1.344449000
H	0.317699000	1.279274000	1.717522000
C	-0.167878000	2.255276000	-0.109279000
H	-0.524606000	5.284909000	-0.541542000
H	-1.788697000	4.589232000	-1.586956000
N	-1.056822000	3.287784000	-0.115590000
H	-1.706961000	3.410317000	1.902038000
O	0.792032000	2.194148000	-0.864497000
C	-0.854179000	4.376742000	-1.059117000
H	-0.090427000	4.073593000	-1.772494000
C	-2.105201000	3.451834000	0.883465000
H	-2.554282000	4.436072000	0.742103000
H	-2.895970000	2.700263000	0.781267000
H	4.079071000	-3.005253000	-0.639339000
H	2.351040000	0.804196000	0.429610000
O	6.968851000	1.041417000	0.636706000
H	-7.244251000	-0.925229000	1.181935000
O	5.736327000	-1.219945000	-0.069099000
O	4.783317000	0.781172000	0.333432000
H	5.939830000	1.203548000	0.239539000
H	7.124192000	0.103187000	0.377432000

MII TS(COOH) HOO$^{\bullet}$

E = -1275.77204546 Ha

C	3.054752000	-1.039995000	-0.084012000
N	-0.790461000	-2.368940000	-0.401527000
C	-1.419565000	-1.209691000	-0.036666000
C	-0.515472000	-0.211619000	0.277191000
C	2.879578000	-2.399895000	-0.486029000
C	1.626325000	-2.917258000	-0.621838000
C	0.498242000	-2.100880000	-0.345302000
N	0.724381000	-0.775725000	0.058898000
C	1.973922000	-0.243746000	0.169087000
H	-2.966311000	0.931906000	-0.673203000
H	1.444925000	-3.937640000	-0.936999000
C	4.409414000	-0.445186000	0.056946000
C	-2.885011000	-1.110652000	0.006684000
C	-3.653166000	-2.225966000	0.360119000
C	-5.036507000	-2.136913000	0.415994000
C	-5.699672000	-0.940657000	0.118139000
C	-4.931396000	0.160863000	-0.258382000
C	-3.542811000	0.078558000	-0.321251000
H	-3.144372000	-3.158146000	0.584764000
H	-5.619696000	-3.011468000	0.694901000
H	-5.427053000	1.090761000	-0.527371000
C	-7.202564000	-0.858123000	0.198489000
H	-7.570117000	0.090747000	-0.200530000
H	-7.673165000	-1.668650000	-0.366645000
C	-0.710066000	1.138658000	0.877398000
H	-1.699244000	1.161007000	1.337538000
H	0.021185000	1.301187000	1.682784000
C	-0.499940000	2.254044000	-0.148246000
H	-2.160137000	4.561340000	-1.609538000
H	-0.460003000	4.061756000	-1.821298000
N	-1.380440000	3.294797000	-0.130863000
H	-1.987296000	3.388772000	1.900115000
O	0.431516000	2.178822000	-0.935710000
C	-1.212348000	4.368723000	-1.097396000
H	-0.883282000	5.289684000	-0.602697000
C	-2.404170000	3.465213000	0.891410000
H	-2.826842000	4.465303000	0.782494000
H	-3.218415000	2.738406000	0.789108000
H	3.760709000	-2.997183000	-0.690868000
H	2.054833000	0.808606000	0.411252000
O	6.837400000	0.958217000	0.910931000
H	-7.546173000	-0.941777000	1.235253000
O	5.397050000	-1.221919000	-0.131726000
O	4.510119000	0.776964000	0.362358000
H	5.756383000	1.073611000	0.684071000
O	7.111788000	0.128806000	-0.139122000
H	7.589445000	-0.619158000	0.273434000

MII TS(COOH) $CH_3O^{\bullet}$

E = -1239.94646239 Ha

C	3.021681000	-1.159065000	-0.211630000
N	-0.865128000	-2.367260000	-0.463945000
C	-1.454981000	-1.200942000	-0.058229000
C	-0.517434000	-0.232437000	0.251670000
C	2.798271000	-2.499346000	-0.647059000
C	1.526862000	-2.976826000	-0.760715000
C	0.431202000	-2.135104000	-0.432780000
N	0.703558000	-0.826312000	-0.006375000
C	1.971246000	-0.334402000	0.091613000
H	-2.968418000	0.982494000	-0.610756000
H	1.306044000	-3.980793000	-1.102744000
C	4.424399000	-0.666021000	-0.104999000
C	-2.915519000	-1.070204000	0.034282000
C	-3.696837000	-2.173038000	0.398336000
C	-5.074485000	-2.051399000	0.505960000
C	-5.718061000	-0.834241000	0.252120000
C	-4.937117000	0.254662000	-0.134622000
C	-3.554441000	0.139572000	-0.250731000
H	-3.203555000	-3.120646000	0.590708000
H	-5.668769000	-2.915951000	0.792328000
H	-5.418958000	1.201287000	-0.367964000
C	-7.214381000	-0.716816000	0.390000000
H	-7.725418000	-1.506239000	-0.169814000
H	-7.521058000	-0.809636000	1.437496000
C	-0.663349000	1.103834000	0.902310000
H	-1.632161000	1.120540000	1.399057000
H	0.100706000	1.220167000	1.682713000
C	-0.431158000	2.241790000	-0.093441000
H	-0.833893000	5.191592000	-0.699792000
H	-2.009538000	4.457621000	-1.816951000
N	-1.385896000	3.202557000	-0.266968000
H	-2.372061000	4.321669000	1.218718000
O	0.610937000	2.237759000	-0.734703000
C	-1.111856000	4.267227000	-1.220870000
H	-0.293296000	3.958955000	-1.867096000
C	-2.540249000	3.446476000	0.578298000
H	-3.411798000	3.649350000	-0.053727000
H	-2.778140000	2.592549000	1.207782000
H	3.662311000	-3.102367000	-0.902427000
H	2.074724000	0.711219000	0.351303000
O	6.619054000	1.308009000	0.429924000
H	-7.573020000	0.247147000	0.020161000
O	5.359372000	-1.183448000	-0.674605000
O	4.502527000	0.354946000	0.736428000
H	5.659332000	1.065980000	0.757419000
C	7.540425000	0.356643000	0.889610000
H	7.474293000	0.205435000	1.973048000
H	7.393181000	-0.594481000	0.364878000

H	8.531328000	0.740909000	0.625585000

MIII

E = -1050.94525007 Ha

C	4.591648000	-0.689805000	0.167628000
N	0.848595000	-2.298915000	-0.380593000
C	0.124890000	-1.194944000	-0.040972000
C	0.942634000	-0.138521000	0.331629000
C	4.513146000	-2.058097000	-0.247258000
C	3.311528000	-2.666549000	-0.461850000
C	2.114712000	-1.937030000	-0.248691000
N	2.224883000	-0.613721000	0.176474000
C	3.437733000	0.006775000	0.360054000
H	-1.528827000	0.849657000	-0.717631000
H	3.225922000	-3.695331000	-0.791000000
C	5.931735000	-0.031673000	0.355077000
H	6.514444000	-0.060232000	-0.571356000
H	5.821982000	1.014129000	0.651895000
H	6.516102000	-0.544784000	1.126152000
C	-1.344365000	-1.198009000	-0.074811000
C	-2.048681000	-2.370248000	0.218525000
C	-3.437848000	-2.376664000	0.207235000
C	-4.157342000	-1.222177000	-0.107977000
C	-3.456719000	-0.056667000	-0.422062000
C	-2.065878000	-0.046821000	-0.413712000
H	-1.486903000	-3.266946000	0.460142000
H	-3.974002000	-3.291042000	0.451707000
H	-6.050430000	-2.052564000	0.477117000
H	-4.014316000	0.836582000	-0.690248000
C	-5.669263000	-1.232199000	-0.149246000
H	-6.017484000	-1.419390000	-1.170454000
C	0.622285000	1.177077000	0.958464000
H	-0.384985000	1.114664000	1.373119000
H	1.303584000	1.362028000	1.802037000
C	0.797720000	2.345662000	-0.011788000
H	0.761564000	4.182928000	-1.659662000
H	0.210180000	5.327058000	-0.412360000
N	-0.191652000	3.284584000	-0.053241000
H	-1.987813000	2.505467000	0.781393000
O	1.799114000	2.404519000	-0.710772000
C	-0.040713000	4.411512000	-0.960947000
H	-0.973641000	4.571814000	-1.509227000
C	-1.288626000	3.339535000	0.904734000
H	-0.927915000	3.349467000	1.938445000
H	-1.838070000	4.266769000	0.734961000
H	5.437387000	-2.606297000	-0.407084000
H	3.397751000	1.062526000	0.598393000
O	-6.241074000	0.007843000	0.216928000
H	-5.913214000	0.224033000	1.101738000

MIII radical (C4)

E = -1050.30703901 Ha

C	4.267392000	-1.420840000	0.005391000
N	0.279154000	-2.409448000	0.028625000
C	-0.249112000	-1.179077000	-0.018207000
C	0.757301000	-0.159582000	-0.044338000
C	3.928483000	-2.804750000	0.049463000
C	2.621149000	-3.207976000	0.048933000
C	1.603405000	-2.236232000	0.008701000
N	1.952878000	-0.891513000	-0.050195000
C	3.268936000	-0.490612000	-0.042671000
H	-1.728140000	0.716160000	-1.346562000
H	2.324092000	-4.249034000	0.086591000
C	5.709836000	-0.990887000	-0.000110000
H	6.238716000	-1.409016000	-0.862731000
H	5.796598000	0.096928000	-0.045325000
H	6.225684000	-1.337590000	0.901414000
C	-1.706393000	-0.996346000	-0.037105000
C	-2.508606000	-1.916282000	0.651692000
C	-3.890081000	-1.787951000	0.647466000
C	-4.509564000	-0.753530000	-0.057796000
C	-3.715279000	0.150778000	-0.762792000
C	-2.329655000	0.031578000	-0.756427000
H	-2.025493000	-2.723936000	1.191895000
H	-4.498590000	-2.499058000	1.201673000
H	-6.444960000	-1.094524000	0.809675000
H	-4.196171000	0.943051000	-1.328812000
C	-6.017023000	-0.631443000	-0.092129000
H	-6.416737000	-1.177638000	-0.953100000
C	0.542544000	1.214125000	0.073770000
H	-0.485483000	1.471718000	0.294983000
C	1.473094000	2.310115000	-0.187431000
H	2.634024000	4.400215000	-0.807664000
H	2.287812000	5.225775000	0.733841000
N	1.104401000	3.545174000	0.292992000
H	-0.966693000	3.935933000	0.583955000
O	2.511319000	2.171051000	-0.844102000
C	1.843864000	4.717232000	-0.130183000
H	1.180419000	5.423385000	-0.644572000
C	-0.039269000	3.776072000	1.151303000
H	-0.182844000	2.940973000	1.839157000
H	0.150929000	4.672020000	1.748961000
H	4.726608000	-3.541070000	0.082950000
H	3.435493000	0.575004000	-0.120602000
O	-6.464122000	0.698512000	-0.254003000
H	-6.093975000	1.218357000	0.473990000

MIII TS(C4) HO•

E = -1126.63791528 Ha

C	3.926641000	-1.875798000	-0.055860000
N	-0.147325000	-2.407459000	-0.254648000
C	-0.512080000	-1.114386000	-0.066643000
C	0.597714000	-0.282211000	0.085534000
C	3.442763000	-3.202397000	-0.274403000
C	2.104995000	-3.467339000	-0.364691000
C	1.180869000	-2.405908000	-0.231761000
N	1.682965000	-1.123843000	-0.031612000
C	3.027244000	-0.856193000	0.055133000
H	-1.631349000	1.178267000	-1.023372000
H	1.714674000	-4.464550000	-0.529014000
C	5.405418000	-1.610520000	0.028797000
H	5.904894000	-1.885667000	-0.905754000
H	5.607618000	-0.554232000	0.220840000
H	5.864028000	-2.197417000	0.831353000
C	-1.926413000	-0.716213000	-0.040447000
C	-2.882545000	-1.599937000	0.473448000
C	-4.223706000	-1.243896000	0.510706000
C	-4.644270000	-0.002035000	0.026617000
C	-3.696705000	0.867383000	-0.512287000
C	-2.351124000	0.516848000	-0.548323000
H	-2.551571000	-2.566679000	0.839578000
H	-4.964677000	-1.927763000	0.914149000
H	-4.016490000	1.819715000	-0.929161000
C	-6.105493000	0.384549000	0.090653000
H	-6.330474000	0.843919000	1.059188000
H	-6.320579000	1.138781000	-0.681397000
C	0.731033000	1.123894000	0.481952000
H	-0.240781000	1.529300000	0.776939000
H	1.392510000	1.190947000	1.423508000
C	1.443717000	2.018401000	-0.533426000
H	2.941446000	4.784130000	-0.729621000
H	1.344650000	5.014922000	-1.482113000
N	1.502702000	3.342155000	-0.221040000
H	1.504844000	4.827298000	1.224741000
O	1.933011000	1.544121000	-1.547476000
C	2.085148000	4.266837000	-1.176143000
H	2.414015000	3.702129000	-2.046462000
C	0.946665000	3.916924000	0.991913000
H	-0.111160000	4.185927000	0.872502000
H	1.061995000	3.239485000	1.838589000
H	4.163885000	-4.008853000	-0.373780000
H	3.303747000	0.180717000	0.201206000
O	2.611387000	1.387336000	2.364511000
H	2.611881000	0.492542000	2.760468000
O	-6.977831000	-0.721460000	-0.007845000
H	-6.763252000	-1.186872000	-0.829402000

MIII TS(C4) HOO•

E = -1201.75902996 Ha

C	3.973184000	-1.751738000	-0.168315000
N	-0.079001000	-2.364397000	-0.489479000
C	-0.479160000	-1.082133000	-0.372862000
C	0.611809000	-0.200349000	-0.245672000
C	3.520685000	-3.090882000	-0.358433000
C	2.190397000	-3.378547000	-0.491515000
C	1.253300000	-2.325660000	-0.437671000
N	1.722527000	-1.028111000	-0.296421000
C	3.054081000	-0.743587000	-0.139715000

H	-1.689357000	1.113660000	-1.468668000
H	1.816473000	-4.386728000	-0.622544000
C	5.440317000	-1.459897000	-0.006221000
H	6.004393000	-1.792648000	-0.883529000
H	5.618336000	-0.390079000	0.124016000
H	5.848238000	-1.980872000	0.865988000
C	-1.906678000	-0.730260000	-0.372619000
C	-2.826764000	-1.608333000	0.210600000
C	-4.182365000	-1.304268000	0.234990000
C	-4.648832000	-0.116160000	-0.328153000
C	-3.736811000	0.754084000	-0.926197000
C	-2.381370000	0.450286000	-0.957766000
H	-2.458385000	-2.534789000	0.640205000
H	-4.892246000	-1.980380000	0.698304000
H	-4.091630000	1.674710000	-1.384555000
C	-6.121473000	0.212136000	-0.343697000
H	-6.522270000	0.004689000	-1.348311000
C	0.640994000	1.186970000	0.159679000
H	-0.371155000	1.572738000	0.294455000
H	1.079040000	1.129565000	1.354728000
C	1.545543000	2.156788000	-0.559281000
H	2.797542000	3.986985000	-1.639349000
H	2.935700000	4.979478000	-0.162539000
N	1.500531000	3.449269000	-0.116544000
H	-0.319052000	4.272566000	0.601876000
O	2.281675000	1.797237000	-1.469408000
C	2.240654000	4.467561000	-0.837322000
H	1.555168000	5.211323000	-1.261156000
C	0.653581000	3.914982000	0.966025000
H	0.493328000	3.133961000	1.710151000
H	1.156841000	4.747898000	1.465224000
H	4.255617000	-3.890384000	-0.390982000
H	3.311942000	0.300109000	-0.029070000
O	1.321525000	0.799047000	2.582581000
O	0.978385000	-0.531773000	2.557425000
H	0.039731000	-0.535014000	2.817147000
H	-6.254177000	1.288836000	-0.157993000
O	-6.785609000	-0.562930000	0.632020000
H	-7.736842000	-0.441554000	0.517651000

MIII TS(C4) $CH_3O^{\bullet}$

E = -1165.93481249 Ha

C	3.839022000	-1.835522000	-0.315756000
N	-0.240560000	-2.349456000	-0.437039000
C	-0.598706000	-1.059497000	-0.240575000
C	0.519579000	-0.221413000	-0.125181000
C	3.345025000	-3.157302000	-0.533701000
C	2.003970000	-3.416053000	-0.602329000
C	1.090596000	-2.349571000	-0.453185000
N	1.600791000	-1.070281000	-0.271904000
C	2.945640000	-0.811625000	-0.191201000
H	-1.746657000	1.234902000	-1.162827000
H	1.605245000	-4.411447000	-0.756467000
C	5.319623000	-1.580299000	-0.234819000
H	5.815045000	-1.857935000	-1.170775000
H	5.528921000	-0.525891000	-0.041147000
H	5.775013000	-2.170312000	0.567039000
C	-2.011674000	-0.661619000	-0.175111000
C	-2.951143000	-1.548147000	0.364241000
C	-4.291736000	-1.195723000	0.437089000
C	-4.727973000	0.044733000	-0.036434000
C	-3.797328000	0.916732000	-0.600440000
C	-2.452155000	0.570652000	-0.671347000
H	-2.608066000	-2.513924000	0.721702000
H	-5.019914000	-1.881152000	0.860542000
H	-4.130544000	1.868255000	-1.008421000
C	-6.187934000	0.427919000	0.066702000
H	-6.386095000	0.891257000	1.039171000
H	-6.426617000	1.178146000	-0.702232000
C	0.668376000	1.171864000	0.276592000
H	-0.293102000	1.600374000	0.570938000
H	1.330496000	1.164247000	1.266297000
C	1.439893000	2.074060000	-0.676330000
H	2.515028000	3.794839000	-2.074285000
H	3.091205000	4.772176000	-0.696974000
N	1.592117000	3.366520000	-0.269795000
H	0.044026000	4.259873000	0.877765000
O	1.900769000	1.641807000	-1.722838000
C	2.212621000	4.320285000	-1.170342000
H	1.506009000	5.117924000	-1.428276000
C	1.073364000	3.891793000	0.981896000
H	1.116806000	3.142976000	1.774142000
H	1.704461000	4.730328000	1.287962000
H	4.060077000	-3.967927000	-0.642762000
H	3.229335000	0.219384000	-0.025726000
C	1.720525000	-0.297939000	2.892752000
H	1.451174000	-0.223921000	3.956092000
H	2.479822000	-1.081200000	2.746489000
H	0.807104000	-0.636644000	2.362612000
O	2.134084000	0.927882000	2.400439000
O	-7.059721000	-0.680571000	-0.001827000
H	-6.873758000	-1.144731000	-0.831013000

MIII TS(C4) $CH_3OO^{\bullet}$

E = -1241.05433758 Ha

C	3.983710000	-1.733025000	-0.425033000
N	-0.085330000	-2.290598000	-0.593605000
C	-0.465352000	-1.001557000	-0.470694000
C	0.640225000	-0.130940000	-0.387222000
C	3.505090000	-3.068677000	-0.582088000
C	2.167248000	-3.335378000	-0.671417000
C	1.246878000	-2.267916000	-0.597907000
N	1.738140000	-0.971864000	-0.480640000
C	3.083702000	-0.708319000	-0.379753000
H	-1.686464000	1.178135000	-1.571544000
H	1.773088000	-4.338496000	-0.781142000
C	5.460716000	-1.461890000	-0.327890000
H	5.979819000	-1.805281000	-1.228466000
H	5.659887000	-0.394437000	-0.210000000
H	5.900124000	-1.987279000	0.526235000
C	-1.887467000	-0.634381000	-0.424588000
C	-2.795331000	-1.496440000	0.200887000
C	-4.145574000	-1.179737000	0.255509000
C	-4.623124000	-0.000842000	-0.323001000
C	-3.723724000	0.845016000	-0.971165000
C	-2.369081000	0.535036000	-1.023079000
H	-2.421466000	-2.415932000	0.640355000
H	-4.848879000	-1.845499000	0.746874000
H	-6.298683000	0.883821000	0.692542000
H	-4.088548000	1.746835000	-1.457426000
C	-6.093246000	0.346004000	-0.239145000
H	-6.359931000	1.020742000	-1.066612000
C	0.676236000	1.242612000	0.061510000
H	-0.338373000	1.621756000	0.196457000
H	1.007381000	1.145529000	1.305890000
C	1.597167000	2.241770000	-0.584266000
H	2.868328000	4.120519000	-1.554273000
H	2.933673000	5.067154000	-0.042322000
N	1.522473000	3.515791000	-0.098872000
H	0.433914000	3.131492000	1.670240000
O	2.370142000	1.923006000	-1.482110000
C	2.273779000	4.566357000	-0.759322000
H	1.592652000	5.312973000	-1.185146000
C	0.624680000	3.938868000	0.962362000
H	1.102027000	4.755498000	1.511477000
H	-0.330142000	4.307806000	0.564548000
H	4.226239000	-3.879795000	-0.629507000
H	3.360787000	0.334111000	-0.311822000
C	0.782263000	-1.381917000	2.684773000
H	1.135551000	-1.486725000	3.715245000
H	1.635879000	-1.408030000	1.999992000
H	0.074812000	-2.176154000	2.435185000
O	0.063181000	-0.167493000	2.534913000
O	0.943062000	0.880730000	2.558801000
O	-6.931052000	-0.790158000	-0.205726000
H	-6.734085000	-1.318574000	-0.992806000

MIII TS(C4) $CH_2CHOO^{\bullet}$

E = -1279.12871223 Ha

C	3.923606000	-1.591080000	-0.652105000
N	-0.136219000	-2.224804000	-0.747360000
C	-0.538130000	-0.952533000	-0.567077000
C	0.554726000	-0.061748000	-0.475659000
C	3.468957000	-2.926755000	-0.856301000
C	2.133706000	-3.217963000	-0.921543000
C	1.197454000	-2.173700000	-0.780414000
N	1.663790000	-0.874016000	-0.635109000
C	3.002637000	-0.588607000	-0.543947000

H	-1.824408000	1.254299000	-1.534786000
H	1.756533000	-4.223752000	-1.062176000
C	5.396037000	-1.292612000	-0.566012000
H	5.911024000	-1.599595000	-1.481935000
H	5.575271000	-0.225012000	-0.420127000
H	5.856634000	-1.832442000	0.267805000
C	-1.965254000	-0.615709000	-0.473537000
C	-2.843161000	-1.525723000	0.126848000
C	-4.197619000	-1.239040000	0.225360000
C	-4.709705000	-0.042856000	-0.283962000
C	-3.840766000	0.851566000	-0.908351000
C	-2.482023000	0.571960000	-1.003549000
H	-2.442625000	-2.458945000	0.510518000
H	-4.877598000	-1.942002000	0.697311000
H	-4.233235000	1.768414000	-1.342073000
C	0.577279000	1.292870000	0.028285000
H	-0.440735000	1.646371000	0.203240000
H	0.963996000	1.174503000	1.233870000
C	1.453123000	2.333943000	-0.621624000
H	2.653381000	4.267337000	-1.574442000
H	2.742473000	5.174063000	-0.039440000
N	1.367794000	3.590565000	-0.095878000
H	0.354841000	3.134278000	1.701089000
O	2.199140000	2.057675000	-1.554776000
C	2.073095000	4.676807000	-0.749955000
H	1.361552000	5.417432000	-1.134355000
C	0.495451000	3.962259000	1.005414000
H	0.967448000	4.780874000	1.555950000
H	-0.483365000	4.310483000	0.649491000
H	4.204620000	-3.719948000	-0.956861000
H	3.261494000	0.454858000	-0.432669000
C	0.771320000	-1.360686000	2.453543000
O	0.131373000	-0.155511000	2.555516000
O	0.993456000	0.906897000	2.524425000
C	2.085059000	-1.562452000	2.446502000
H	2.463522000	-2.571425000	2.341492000
H	2.781887000	-0.740806000	2.544833000
H	0.023544000	-2.143094000	2.366228000
H	-6.377786000	0.761133000	0.807398000
C	-6.183958000	0.270345000	-0.152308000
H	-6.482133000	0.976663000	-0.941739000
O	-6.998975000	-0.882519000	-0.152431000
H	-6.814841000	-1.367970000	-0.969721000

MIII radical (O˙)

E = -1050.27879450 Ha

C	4.560070000	-0.695852000	0.130719000
N	0.807844000	-2.298444000	-0.373600000
C	0.090770000	-1.193268000	-0.024047000
C	0.914487000	-0.138713000	0.339790000
C	4.474267000	-2.063544000	-0.284739000
C	3.269160000	-2.669900000	-0.485302000
C	2.076199000	-1.938751000	-0.256728000
N	2.193767000	-0.616056000	0.168483000
C	3.409730000	0.002355000	0.338003000
H	-1.561411000	0.851539000	-0.694814000
H	3.177982000	-3.698214000	-0.814429000
C	5.903397000	-0.040154000	0.302836000
H	6.475235000	-0.069362000	-0.630331000
H	5.798909000	1.005705000	0.601333000
H	6.495759000	-0.554617000	1.066867000
C	-1.378755000	-1.191440000	-0.039230000
C	-2.083601000	-2.358666000	0.274512000
C	-3.472144000	-2.358700000	0.280719000
C	-4.185823000	-1.200876000	-0.033867000
C	-3.490478000	-0.042237000	-0.369292000
C	-2.099008000	-0.040545000	-0.379324000
H	-1.522482000	-3.256032000	0.514924000
H	-4.009328000	-3.269439000	0.538128000
H	-6.104361000	-1.856730000	0.759527000
H	-4.048922000	0.851193000	-0.631989000
C	-5.699439000	-1.221431000	-0.048188000
H	-6.065527000	-1.704790000	-0.978339000
C	0.602318000	1.175954000	0.972603000
H	-0.400122000	1.113294000	1.398773000
H	1.293243000	1.358916000	1.808713000
C	0.767061000	2.346186000	0.002555000
H	0.714048000	4.188620000	-1.638685000
H	0.174577000	5.329048000	-0.382707000
N	-0.221928000	3.285550000	-0.024686000
H	-2.010121000	2.505015000	0.827477000
O	1.760102000	2.405200000	-0.708562000
C	-0.081149000	4.414745000	-0.931116000
H	-1.019877000	4.575925000	-1.469179000
C	-1.308843000	3.337971000	0.945457000
H	-0.936820000	3.344415000	1.975090000
H	-1.859492000	4.266046000	0.784708000
H	5.395600000	-2.613055000	-0.456410000
H	3.374077000	1.057868000	0.578165000
O	-6.313611000	-0.000386000	-0.036486000

MIII TS(OH) HO˙

E = -1126.63236783 Ha

C	-4.766167000	-1.267029000	0.031893000
N	-0.773916000	-2.217793000	0.254914000
C	-0.275532000	-1.009559000	-0.129737000
C	-1.286507000	-0.102495000	-0.414333000
C	-4.423806000	-2.599893000	0.426790000
C	-3.122965000	-2.993985000	0.537752000
C	-2.089135000	-2.072218000	0.235958000
N	-2.454875000	-0.786280000	-0.160129000
C	-3.767325000	-0.383415000	-0.243654000
H	1.087775000	1.269335000	0.430270000
H	-2.836531000	-3.992224000	0.846796000
C	-6.209340000	-0.848081000	-0.046220000
H	-6.706441000	-0.975257000	0.920953000
H	-6.302238000	0.200846000	-0.337588000
H	-6.754642000	-1.454112000	-0.777451000
C	1.171347000	-0.775042000	-0.236893000
C	2.021931000	-1.820699000	-0.615847000
C	3.386706000	-1.605735000	-0.743061000
C	3.936777000	-0.346006000	-0.487392000
C	3.096695000	0.687460000	-0.078632000
C	1.727347000	0.475779000	0.050716000
H	1.589188000	-2.797485000	-0.807195000
H	4.044247000	-2.418786000	-1.038501000
H	3.519675000	1.659138000	0.166925000
C	5.418046000	-0.118773000	-0.660955000
H	5.666449000	-0.007216000	-1.726488000
H	5.725928000	0.810262000	-0.162442000
C	-1.243946000	1.246430000	-1.056751000
H	-0.288194000	1.333365000	-1.571400000
H	-2.028691000	1.311797000	-1.822461000
C	-1.534107000	2.367796000	-0.058124000
H	-1.291981000	5.310428000	0.601778000
H	-0.043836000	4.644171000	1.682057000
N	-0.618604000	3.365462000	0.134238000
H	0.304518000	4.570023000	-1.323727000
O	-2.580290000	2.322462000	0.574663000
C	-0.940794000	4.400604000	1.104583000
H	-1.721970000	4.032784000	1.765812000
C	0.515688000	3.682387000	-0.713485000
H	1.386419000	3.900803000	-0.085168000
H	0.779538000	2.859615000	-1.373160000
H	-5.225525000	-3.296840000	0.654439000
H	-3.926310000	0.662571000	-0.474379000
O	6.036966000	-1.027431000	1.975339000
H	7.005607000	-0.983678000	2.081717000
O	6.210166000	-1.199050000	-0.232563000
H	5.924571000	-1.442258000	0.790903000

MIII TS(OH) HOO˙

E = -1201.74872777 Ha

C	-5.220747000	-0.514735000	0.093112000
N	-1.515984000	-2.261180000	0.438972000
C	-0.777122000	-1.216874000	-0.030230000
C	-1.576233000	-0.143464000	-0.397241000
C	-5.164481000	-1.855479000	0.592101000
C	-3.975013000	-2.503940000	0.749036000
C	-2.771686000	-1.845538000	0.391242000
N	-2.860951000	-0.546091000	-0.106678000
C	-4.059647000	0.115781000	-0.236511000
H	1.019610000	0.769865000	0.376081000
H	-3.903860000	-3.513282000	1.136621000
C	-6.543849000	0.190756000	-0.033492000
H	-7.051832000	0.246130000	0.934814000
H	-6.415287000	1.210018000	-0.405375000
H	-7.208077000	-0.341784000	-0.722362000

C	0.686459000	-1.294238000	-0.134410000
C	1.304270000	-2.513650000	-0.428675000
C	2.685974000	-2.585631000	-0.554713000
C	3.476948000	-1.447871000	-0.388996000
C	2.867572000	-0.235320000	-0.066198000
C	1.486665000	-0.162644000	0.067898000
H	0.682946000	-3.393448000	-0.561878000
H	3.156167000	-3.536501000	-0.796052000
H	3.482684000	0.644675000	0.102686000
C	4.978886000	-1.531924000	-0.498336000
H	5.403697000	-1.664018000	0.527522000
H	5.305042000	-2.432423000	-1.045432000
C	-1.253143000	1.111802000	-1.141932000
H	-0.302520000	0.955370000	-1.649512000
H	-2.009762000	1.279647000	-1.920155000
C	-1.297212000	2.343998000	-0.236897000
H	-1.128586000	4.151913000	1.445159000
H	-0.419549000	5.213227000	0.202367000
N	-0.192993000	3.139309000	-0.111945000
H	1.884480000	3.184926000	-0.327487000
O	-2.328241000	2.567530000	0.383780000
C	-0.282039000	4.288272000	0.776203000
H	0.644021000	4.369499000	1.353445000
C	0.988238000	3.136129000	-0.955902000
H	1.057629000	2.238989000	-1.565597000
H	0.987109000	4.011587000	-1.617730000
H	-6.093836000	-2.349266000	0.861992000
H	-3.995429000	1.151303000	-0.546939000
O	5.903357000	0.032728000	1.798029000
O	5.597491000	-0.438050000	-1.048415000
H	6.846323000	-0.123294000	1.986010000
O	5.946544000	0.984062000	0.795899000
H	5.772266000	0.419874000	-0.141314000

MIII TS(OH) $CH_3O^{\bullet}$

E = -1165.92690354 Ha

C	-4.898654000	-1.203550000	0.151932000
N	-0.924234000	-2.242705000	-0.003667000
C	-0.430087000	-1.018247000	-0.341810000
C	-1.439407000	-0.079030000	-0.491158000
C	-4.559648000	-2.568417000	0.422078000
C	-3.264528000	-2.995267000	0.401713000
C	-2.233989000	-2.074652000	0.084722000
N	-2.598999000	-0.758371000	-0.195294000
C	-3.902081000	-0.323524000	-0.141391000
H	0.998714000	1.202868000	0.285427000
H	-2.981165000	-4.018555000	0.617643000
C	-6.331995000	-0.751436000	0.224123000
H	-6.951177000	-1.294435000	-0.497695000
H	-6.750355000	-0.935334000	1.219021000
H	-6.422029000	0.316789000	0.012976000
C	1.010907000	-0.793709000	-0.522747000
C	1.821493000	-1.821698000	-1.021609000
C	3.181752000	-1.615836000	-1.203177000
C	3.765723000	-0.384311000	-0.893468000
C	2.967480000	0.630436000	-0.371281000
C	1.602816000	0.427299000	-0.181168000
H	1.362202000	-2.776946000	-1.255186000
H	3.810092000	-2.421413000	-1.575367000
H	3.425616000	1.568790000	-0.068345000
C	5.261704000	-0.210084000	-1.004179000
H	5.611032000	-0.530721000	-1.997685000
H	5.541716000	0.844987000	-0.880019000
C	-1.413023000	1.311283000	-1.031952000
H	-0.484710000	1.435425000	-1.591730000
H	-2.237460000	1.447335000	-1.747286000
C	-1.599358000	2.366141000	0.059001000
H	-1.395934000	5.368650000	0.641019000
H	0.041917000	4.735893000	1.481774000
N	-0.763406000	3.444388000	0.042230000
H	0.579289000	4.724984000	-0.881818000
O	-2.473876000	2.216059000	0.900257000
C	-0.932105000	4.468630000	1.061621000
H	-1.573178000	4.069424000	1.845038000
C	0.147518000	3.738398000	-1.056977000
H	0.968923000	3.016454000	-1.118090000
H	-0.370869000	3.766864000	-2.020914000
H	-5.358509000	-3.264007000	0.663390000
H	-4.052379000	0.739600000	-0.283788000
O	5.208390000	-0.172304000	1.843201000
O	5.958009000	-1.033263000	-0.108240000
H	5.829310000	-0.592292000	0.974548000
C	4.341206000	-1.164193000	2.317266000
H	4.853415000	-2.118158000	2.486165000
H	3.969072000	-0.792894000	3.281543000
H	3.478425000	-1.309819000	1.655520000

MIV

E = -1050.94414964 Ha

C	3.988052000	-0.941121000	-0.031402000
N	0.158604000	-2.357461000	-0.420897000
C	-0.495885000	-1.218700000	-0.054598000
C	0.387446000	-0.203272000	0.278476000
C	3.832568000	-2.301247000	-0.440642000
C	2.592878000	-2.846736000	-0.607621000
C	1.444733000	-2.057802000	-0.346478000
N	1.637530000	-0.738815000	0.070894000
C	2.883647000	-0.179183000	0.203892000
H	-2.077845000	0.898101000	-0.690464000
H	2.441207000	-3.871361000	-0.925608000
C	5.365159000	-0.329420000	0.094200000
H	6.076001000	-1.103606000	0.421130000
H	5.709331000	0.030563000	-0.880616000
C	-1.963687000	-1.147287000	-0.025114000
C	-2.714810000	-2.279227000	0.311885000
C	-4.100261000	-2.217494000	0.353087000
C	-4.783399000	-1.031951000	0.057795000
C	-4.032175000	0.086786000	-0.301751000
C	-2.641503000	0.031278000	-0.350793000
H	-2.190173000	-3.203032000	0.534773000
H	-4.669384000	-3.105469000	0.618660000
H	-6.738588000	-1.807570000	-0.428922000
H	-4.542580000	1.009325000	-0.568966000
C	-6.288345000	-0.977760000	0.124635000
H	-6.639346000	-1.048569000	1.160001000
H	-6.670985000	-0.043681000	-0.294773000
C	0.155812000	1.135937000	0.891210000
H	-0.834363000	1.127979000	1.349749000
H	0.881456000	1.309032000	1.699612000
C	0.337864000	2.271373000	-0.117278000
H	0.325508000	4.095987000	-1.773357000
H	-0.131603000	5.292516000	-0.536229000
N	-0.583918000	3.277498000	-0.101566000
H	-2.393781000	2.634530000	0.816863000
O	1.282401000	2.244944000	-0.891975000
C	-0.436958000	4.372270000	-1.047685000
H	-1.386918000	4.551360000	-1.560570000
C	-1.619487000	3.403894000	0.915264000
H	-1.204284000	3.359458000	1.926949000
H	-2.094173000	4.378926000	0.793989000
H	4.721110000	-2.898028000	-0.628227000
H	2.924957000	0.876635000	0.441265000
O	5.397345000	0.795458000	0.944973000
H	5.101090000	0.503110000	1.819252000

MIV radical (C4)

E = -1050.30520559 Ha

C	3.595576000	-1.627943000	-0.025487000
N	-0.435096000	-2.372064000	0.011013000
C	-0.890566000	-1.112829000	-0.044936000
C	0.173851000	-0.154887000	-0.081191000
C	3.181247000	-2.988183000	0.042295000
C	1.851833000	-3.310000000	0.039013000
C	0.895885000	-2.277525000	-0.014975000
N	1.325384000	-0.954641000	-0.088143000
C	2.663180000	-0.633280000	-0.094825000
H	-2.254235000	0.848053000	-1.398182000
H	1.489902000	-4.329519000	0.094193000
C	5.069729000	-1.287000000	-0.049401000
H	5.603955000	-1.966862000	0.632777000
H	5.475140000	-1.458484000	-1.051987000
C	-2.333212000	-0.840150000	-0.060713000
C	-3.191926000	-1.697762000	0.641554000
C	-4.561522000	-1.484663000	0.634758000
C	-5.125095000	-0.419234000	-0.077376000
C	-4.270231000	0.415792000	-0.796259000
C	-2.893496000	0.211442000	-0.794091000
H	-2.761240000	-2.531862000	1.186173000

H	-5.212198000	-2.156533000	1.189547000
H	-7.159325000	-1.116743000	-0.261740000
H	-4.688299000	1.231304000	-1.380902000
C	-6.614278000	-0.189299000	-0.061017000
H	-6.943903000	0.177183000	0.917420000
H	-6.910452000	0.548403000	-0.811082000
C	0.036249000	1.228592000	0.037074000
H	-0.975406000	1.543542000	0.259841000
C	1.030207000	2.267526000	-0.224031000
H	2.336793000	4.276790000	-0.816434000
H	2.006229000	5.139712000	0.708231000
N	0.742487000	3.520845000	0.264866000
H	-1.301306000	4.043132000	0.544902000
O	2.053295000	2.065224000	-0.886233000
C	1.552275000	4.645522000	-0.158739000
H	0.939141000	5.380743000	-0.694738000
C	-0.389565000	3.821489000	1.116888000
H	-0.591479000	2.994627000	1.800029000
H	-0.145856000	4.700901000	1.719692000
H	3.933531000	-3.770516000	0.098156000
H	2.908328000	0.415092000	-0.205173000
O	5.341659000	0.061541000	0.243962000
H	4.980778000	0.252271000	1.122054000

MIV TS(C4) HO˙

E = -1126.63799190 Ha

C	3.456997000	-1.727629000	-0.024899000
N	-0.571567000	-2.475194000	-0.252561000
C	-1.008292000	-1.203417000	-0.067299000
C	0.054155000	-0.314166000	0.103879000
C	3.056666000	-3.075237000	-0.269016000
C	1.734701000	-3.412206000	-0.353623000
C	0.753372000	-2.403861000	-0.209235000
N	1.183427000	-1.097471000	0.006210000
C	2.508301000	-0.759334000	0.114754000
H	-2.246317000	1.028997000	-1.034309000
H	1.398683000	-4.425881000	-0.536063000
C	4.922510000	-1.362626000	0.057773000
H	5.342845000	-1.701357000	1.010789000
H	5.468422000	-1.892579000	-0.737776000
C	-2.442423000	-0.882687000	-0.061057000
C	-3.355656000	-1.817513000	0.442074000
C	-4.712841000	-1.533540000	0.462708000
C	-5.205799000	-0.315572000	-0.020266000
C	-4.294939000	0.601807000	-0.543205000
C	-2.931147000	0.323752000	-0.570731000
H	-2.978493000	-2.766365000	0.810276000
H	-5.409327000	-2.268483000	0.859479000
H	-6.925140000	0.871336000	-0.566174000
H	-4.658888000	1.540841000	-0.952440000
C	-6.681617000	-0.013506000	0.027435000
H	-7.269485000	-0.852952000	-0.356240000
H	-7.011197000	0.172393000	1.055601000
C	0.105640000	1.100374000	0.486580000
H	-0.893817000	1.460689000	0.742794000
H	0.728936000	1.215651000	1.457051000
C	0.823064000	2.019243000	-0.502183000
H	2.163398000	4.835441000	-0.681401000
H	0.593689000	5.016811000	-1.502502000
N	0.744125000	3.350504000	-0.237163000
H	0.554507000	4.867265000	1.162817000
O	1.435660000	1.559007000	-1.455890000
C	1.343218000	4.292618000	-1.164489000
H	1.728028000	3.739223000	-2.018920000
C	0.083983000	3.908530000	0.931283000
H	-0.984845000	4.085399000	0.754085000
H	0.212526000	3.265081000	1.802277000
H	3.821639000	-3.836997000	-0.393871000
H	2.738657000	0.282681000	0.296393000
O	1.903813000	1.581875000	2.363042000
H	2.150732000	0.683028000	2.660246000
O	5.151793000	0.025166000	0.010045000
H	4.794079000	0.356322000	-0.828023000

MIV TS(C4) HOO˙

E = -1201.76202189 Ha

C	3.581118000	-1.185750000	-0.400668000
N	-0.349938000	-2.343646000	-0.515561000
C	-0.916519000	-1.131521000	-0.339251000
C	0.048119000	-0.110339000	-0.250212000
C	3.316495000	-2.573719000	-0.591689000
C	2.032535000	-3.037580000	-0.664903000
C	0.964149000	-2.122625000	-0.540587000
N	1.256748000	-0.773507000	-0.393706000
C	2.541174000	-0.310702000	-0.293332000
H	-2.474583000	0.913441000	-1.275816000
H	1.791048000	-4.085647000	-0.794415000
C	5.007880000	-0.707368000	-0.300759000
H	5.513630000	-0.820885000	-1.264575000
H	5.025520000	0.361171000	-0.043393000
C	-2.375893000	-0.981584000	-0.256048000
C	-3.137027000	-2.008310000	0.317636000
C	-4.515947000	-1.893957000	0.411334000
C	-5.182801000	-0.760180000	-0.067382000
C	-4.423293000	0.247863000	-0.661376000
C	-3.039203000	0.141260000	-0.760986000
H	-2.625009000	-2.894815000	0.678581000
H	-5.092336000	-2.699017000	0.861002000
H	-4.923700000	1.122316000	-1.069479000
C	-6.679584000	-0.639937000	0.060254000
H	-7.067808000	0.168025000	-0.565084000
H	-7.177216000	-1.568558000	-0.234907000
C	-0.076446000	1.264346000	0.178900000
H	-1.114447000	1.510193000	0.409340000
H	0.488998000	1.262797000	1.318181000
C	0.630375000	2.346565000	-0.601668000
H	1.533059000	4.325072000	-1.764976000
H	1.654171000	5.330711000	-0.295853000
N	0.444060000	3.622104000	-0.149154000
H	-1.415285000	4.161911000	0.723449000
O	1.338700000	2.083758000	-1.565080000
C	0.982270000	4.728947000	-0.917715000
H	0.172036000	5.372778000	-1.280121000
C	-0.370293000	3.969198000	1.001061000
H	-0.338492000	3.186649000	1.760397000
H	0.036208000	4.880013000	1.449249000
H	4.159731000	-3.254169000	-0.658582000
H	2.661794000	0.754989000	-0.154624000
O	0.979144000	0.969490000	2.483634000
O	0.809262000	-0.395472000	2.495473000
H	-0.058984000	-0.517076000	2.918803000
H	-6.969163000	-0.429385000	1.095771000
O	5.762996000	-1.481809000	0.609777000
H	5.321260000	-1.430552000	1.469913000

MIV TS(C4) CH_3O˙

E = -1165.93471432 Ha

C	3.382952000	-1.709691000	-0.241697000
N	-0.656887000	-2.413444000	-0.417421000
C	-1.078983000	-1.138982000	-0.238266000
C	-0.002735000	-0.251624000	-0.096034000
C	2.964668000	-3.051810000	-0.478470000
C	1.637316000	-3.375280000	-0.545684000
C	0.671873000	-2.354144000	-0.397951000
N	1.118340000	-1.051960000	-0.202994000
C	2.445577000	-0.730665000	-0.094808000
H	-2.313098000	1.095765000	-1.204327000
H	1.287395000	-4.386259000	-0.715941000
C	4.851580000	-1.354960000	-0.166673000
H	5.401109000	-1.950436000	-0.911901000
H	5.256421000	-1.619286000	0.815782000
C	-2.509877000	-0.806208000	-0.212954000
C	-3.421901000	-1.730534000	0.311455000
C	-4.776679000	-1.437089000	0.348257000
C	-5.267794000	-0.220412000	-0.139802000
C	-4.358059000	0.686009000	-0.683878000
C	-2.996692000	0.399212000	-0.726776000
H	-3.046124000	-2.678714000	0.682839000
H	-5.472549000	-2.163374000	0.761593000
H	-7.339369000	-0.747361000	-0.440773000
H	-4.721379000	1.623636000	-1.096726000
C	-6.740641000	0.092296000	-0.074827000
H	-7.054092000	0.291714000	0.955827000
H	-6.986537000	0.972223000	-0.674653000
C	0.075270000	1.152456000	0.289271000
H	-0.914610000	1.551138000	0.524086000
H	0.679766000	1.184777000	1.314662000
C	0.870944000	2.068155000	-0.630777000

H	1.940066000	3.814390000	-2.003915000
H	2.431740000	4.802059000	-0.602113000
N	0.933986000	3.373493000	-0.247040000
H	-0.712411000	4.218155000	0.795156000
O	1.427065000	1.636735000	-1.631993000
C	1.584688000	4.335570000	-1.117079000
H	0.878047000	5.120410000	-1.410522000
C	0.323676000	3.896528000	0.964124000
H	0.353505000	3.163619000	1.771704000
H	0.901221000	4.765891000	1.288936000
H	3.719334000	-3.823119000	-0.607271000
H	2.692091000	0.303339000	0.103891000
C	1.055248000	-0.248482000	2.970955000
H	0.734303000	-0.194613000	4.021126000
H	1.866747000	-0.983233000	2.859138000
H	0.187685000	-0.637931000	2.400369000
O	1.414377000	1.002865000	2.501333000
O	5.093857000	0.023199000	-0.320985000
H	4.717689000	0.296110000	-1.171925000

MIV TS(C4) $CH_3OO^{\bullet}$

E = -1241.05036994 Ha

C	3.645485000	-1.217818000	-0.608699000
N	-0.309466000	-2.307120000	-0.689290000
C	-0.856092000	-1.082085000	-0.531320000
C	0.124005000	-0.073184000	-0.448714000
C	3.349140000	-2.599791000	-0.793089000
C	2.055530000	-3.041777000	-0.849045000
C	1.005834000	-2.108107000	-0.718509000
N	1.323372000	-0.756646000	-0.580237000
C	2.621437000	-0.320366000	-0.504744000
H	-2.380940000	0.925612000	-1.580099000
H	1.792829000	-4.084067000	-0.983924000
C	5.074869000	-0.753859000	-0.468288000
H	5.715562000	-1.340349000	-1.142965000
H	5.161622000	0.295916000	-0.757762000
C	-2.312728000	-0.908248000	-0.453036000
C	-3.085993000	-1.887044000	0.182124000
C	-4.463480000	-1.750102000	0.264585000
C	-5.114599000	-0.641054000	-0.287448000
C	-4.341700000	0.319220000	-0.940427000
C	-2.958910000	0.189989000	-1.027424000
H	-2.586981000	-2.754017000	0.603712000
H	-5.050517000	-2.516167000	0.765488000
H	-6.894771000	-0.201042000	0.847016000
H	-4.830057000	1.173944000	-1.401411000
C	-6.609691000	-0.493199000	-0.169728000
H	-6.988442000	0.270089000	-0.854233000
H	-7.119176000	-1.435219000	-0.393564000
C	-0.018084000	1.284361000	0.027099000
H	-1.072860000	1.522447000	0.175394000
H	0.331692000	1.208665000	1.269910000
C	0.757639000	2.407534000	-0.605535000
H	1.767994000	4.452842000	-1.545856000
H	1.730703000	5.364611000	-0.011929000
N	0.523453000	3.651132000	-0.094989000
H	-0.494271000	3.093584000	1.670465000
O	1.555377000	2.207715000	-1.516432000
C	1.130836000	4.802255000	-0.735880000
H	0.356952000	5.467014000	-1.138039000
C	-0.409450000	3.935080000	0.982161000
H	-0.030397000	4.790004000	1.549337000
H	-1.405441000	4.194027000	0.598974000
H	4.170124000	-3.304543000	-0.900870000
H	2.765318000	0.746455000	-0.404542000
C	0.506555000	-1.346238000	2.594823000
H	0.876275000	-1.417175000	3.622354000
H	1.351446000	-1.221095000	1.910039000
H	-0.068390000	-2.235909000	2.326938000
O	-0.395137000	-0.256825000	2.472966000
O	0.310131000	0.915090000	2.514692000
O	5.542752000	-0.824105000	0.866490000
H	5.431593000	-1.735589000	1.172005000

MIV TS(C4) $CH_2CHOO^{\bullet}$

E = -1279.12754119 Ha

C	3.491797000	-1.411199000	-0.677884000
N	-0.511991000	-2.286663000	-0.795485000
C	-0.992560000	-1.044589000	-0.595205000
C	0.043252000	-0.089115000	-0.492060000
C	3.128763000	-2.767488000	-0.903951000
C	1.812674000	-3.136707000	-0.983575000
C	0.815499000	-2.152909000	-0.831111000
N	1.201157000	-0.827321000	-0.666072000
C	2.516721000	-0.460847000	-0.564652000
H	-2.413195000	1.093781000	-1.529285000
H	1.496521000	-4.161894000	-1.133846000
C	-2.436494000	-0.795616000	-0.495116000
C	-3.258121000	-1.762569000	0.096602000
C	-4.625325000	-1.555014000	0.200219000
C	-5.218329000	-0.384881000	-0.287337000
C	-4.398585000	0.563885000	-0.899129000
C	-3.025851000	0.364357000	-1.006785000
H	-2.804406000	-2.676834000	0.466350000
H	-5.250055000	-2.313042000	0.666476000
H	-4.842788000	1.466069000	-1.311708000
C	-0.009725000	1.260924000	0.018769000
H	-1.044550000	1.556275000	0.203146000
H	0.397222000	1.158890000	1.217592000
C	0.802412000	2.346357000	-0.644261000
H	1.921981000	4.329538000	-1.591531000
H	1.983179000	5.237521000	-0.056182000
N	0.683810000	3.592875000	-0.101268000
H	-0.292085000	3.076734000	1.699902000
O	1.526987000	2.107823000	-1.603079000
C	1.330876000	4.711340000	-0.761471000
H	0.582361000	5.418796000	-1.138406000
C	-0.178578000	3.922005000	1.020459000
H	0.283861000	4.738588000	1.582321000
H	-1.169768000	4.256670000	0.686339000
H	3.911477000	-3.515136000	-1.001070000
H	2.729960000	0.590868000	-0.433989000
C	0.444367000	-1.402780000	2.406749000
O	-0.301747000	-0.263346000	2.519111000
O	0.463255000	0.873046000	2.506424000
C	1.771115000	-1.485487000	2.427821000
H	2.243749000	-2.452527000	2.311459000
H	2.381898000	-0.603212000	2.567156000
H	-0.226395000	-2.248065000	2.284619000
C	4.945214000	-1.003752000	-0.573928000
H	5.522475000	-1.835032000	-0.141572000
H	5.355669000	-0.811254000	-1.570236000
H	-7.264057000	-1.066208000	-0.391242000
C	-6.701675000	-0.160511000	-0.145594000
H	-6.958514000	0.114841000	0.883340000
H	-7.046242000	0.643327000	-0.801127000
O	5.131904000	0.190847000	0.149746000
H	4.782996000	0.049697000	1.042292000

MIV radical (O$^{\bullet}$)

E = -1050.27770530 Ha

C	4.005991000	-0.952927000	0.036840000
N	0.183991000	-2.358763000	-0.400690000
C	-0.472249000	-1.219032000	-0.039558000
C	0.409551000	-0.207063000	0.307640000
C	3.857567000	-2.310548000	-0.380648000
C	2.618740000	-2.854339000	-0.559335000
C	1.469616000	-2.063391000	-0.308022000
N	1.660318000	-0.745499000	0.114914000
C	2.904888000	-0.188724000	0.266239000
H	-2.040451000	0.905318000	-0.686176000
H	2.468495000	-3.876717000	-0.884955000
C	5.385290000	-0.353585000	0.186167000
H	6.049551000	-1.022587000	0.764467000
H	5.885916000	-0.270733000	-0.799081000
C	-1.940089000	-1.143622000	-0.028846000
C	-2.698471000	-2.274995000	0.293446000
C	-4.084162000	-2.209654000	0.317155000
C	-4.760244000	-1.020948000	0.018419000
C	-4.001485000	0.097327000	-0.326447000
C	-2.610480000	0.038294000	-0.357880000
H	-2.179247000	-3.201122000	0.519322000
H	-4.659023000	-3.097166000	0.571641000
H	-6.711169000	-1.788464000	-0.497374000
H	-4.505954000	1.022490000	-0.595793000
C	-6.265759000	-0.962881000	0.066330000
H	-6.630092000	-1.038226000	1.096746000
H	-6.640447000	-0.025497000	-0.352886000

C	0.175773000	1.132198000	0.919174000
H	-0.820548000	1.128406000	1.364160000
H	0.891146000	1.300667000	1.737542000
C	0.376385000	2.267139000	-0.086241000
H	0.395102000	4.097236000	-1.736609000
H	-0.063840000	5.294020000	-0.500325000
N	-0.535974000	3.281649000	-0.075470000
H	-2.361662000	2.652171000	0.820449000
O	1.326893000	2.233530000	-0.853623000
C	-0.371727000	4.377650000	-1.017165000
H	-1.315463000	4.565747000	-1.538290000
C	-1.580536000	3.412921000	0.931517000
H	-1.176097000	3.358055000	1.946956000
H	-2.043827000	4.393552000	0.811322000
H	4.746970000	-2.907139000	-0.566753000
H	2.948844000	0.862197000	0.521629000
O	5.434590000	0.894365000	0.741125000

MIV TS(OH) HO˙

E = -1126.63321495 Ha

C	3.702577000	-0.171929000	-0.324226000
N	0.115863000	-2.143234000	-0.596204000
C	-0.684419000	-1.129847000	-0.155775000
C	0.049944000	-0.004420000	0.183024000
C	3.735139000	-1.526521000	-0.784573000
C	2.583967000	-2.249392000	-0.910905000
C	1.344543000	-1.656811000	-0.560942000
N	1.356195000	-0.337817000	-0.098023000
C	2.507915000	0.398798000	-0.002602000
H	-2.588366000	0.740945000	-0.650497000
H	2.570602000	-3.269143000	-1.277102000
C	4.974018000	0.625384000	-0.180685000
H	5.669826000	0.395128000	-0.995806000
H	4.745368000	1.697814000	-0.226209000
C	-2.143208000	-1.282587000	-0.063941000
C	-2.701257000	-2.524124000	0.260825000
C	-4.077394000	-2.671973000	0.359897000
C	-4.941554000	-1.593796000	0.136542000
C	-4.382044000	-0.364538000	-0.212311000
C	-3.002352000	-0.209649000	-0.319345000
H	-2.035872000	-3.365379000	0.427873000
H	-4.495842000	-3.642930000	0.614685000
H	-6.970457000	-0.908685000	-0.143409000
H	-5.035474000	0.478451000	-0.425348000
C	-6.433066000	-1.766166000	0.269849000
H	-6.775304000	-2.665082000	-0.251849000
H	-6.724722000	-1.868414000	1.320995000
C	-0.348005000	1.252495000	0.881253000
H	-1.308215000	1.074670000	1.367747000
H	0.375840000	1.481131000	1.677395000
C	-0.364862000	2.460493000	-0.055340000
H	-1.267617000	5.380454000	-0.283012000
H	-2.446622000	4.551153000	-1.330263000
N	-1.440553000	3.296286000	0.012162000
H	-3.069473000	2.302574000	0.954160000
O	0.569424000	2.639806000	-0.824210000
C	-1.465818000	4.465392000	-0.853444000
H	-0.696963000	4.344968000	-1.613981000
C	-2.462277000	3.209047000	1.048255000
H	-2.029288000	3.242617000	2.053416000
H	-3.124073000	4.069890000	0.941509000
H	4.694341000	-1.963288000	-1.043735000
H	2.386517000	1.437350000	0.281320000
O	6.400254000	-1.631627000	0.834045000
O	5.600270000	0.439589000	1.073533000
H	6.303352000	-0.370313000	1.016349000
H	5.691239000	-1.991830000	1.399940000

MIV TS(OH) HOO˙

E = -1201.75980285 Ha

C	3.412908000	-1.703633000	0.136039000
N	-0.558617000	-2.531475000	-0.439335000
C	-1.057087000	-1.324840000	-0.047715000
C	-0.049558000	-0.461351000	0.353482000
C	3.083761000	-3.004003000	-0.355314000
C	1.785685000	-3.358895000	-0.578692000
C	0.753642000	-2.424644000	-0.310451000
N	1.117818000	-1.164896000	0.169287000
C	2.424362000	-0.801601000	0.378893000
H	-2.308002000	1.017793000	-0.643335000
H	1.500346000	-4.334121000	-0.954593000
C	4.855694000	-1.315548000	0.350255000
H	5.347394000	-2.066100000	0.998606000
H	5.412592000	-1.351468000	-0.601641000
C	-2.500275000	-1.045714000	-0.055514000
C	-3.412740000	-2.071486000	0.216955000
C	-4.776377000	-1.815899000	0.226957000
C	-5.277501000	-0.535727000	-0.036439000
C	-4.366357000	0.477767000	-0.332965000
C	-2.996503000	0.227693000	-0.349904000
H	-3.029844000	-3.067691000	0.415042000
H	-5.471986000	-2.623670000	0.442310000
H	-7.141264000	-0.297794000	1.025596000
H	-4.734420000	1.471857000	-0.576507000
C	-6.760914000	-0.270691000	-0.001470000
H	-6.998997000	0.710710000	-0.419804000
H	-7.310664000	-1.025397000	-0.572103000
C	-0.108248000	0.886021000	0.986774000
H	-1.094449000	1.002859000	1.439301000
H	0.629501000	0.958475000	1.799688000
C	0.214392000	1.999050000	-0.006471000
H	0.442886000	3.833646000	-1.651406000
H	0.189163000	5.066219000	-0.390086000
N	-0.523397000	3.131958000	0.047696000
H	-1.147312000	3.201051000	2.072029000
O	1.121740000	1.837227000	-0.823990000
C	-0.252038000	4.203675000	-0.900744000
H	-1.184132000	4.513008000	-1.382546000
C	-1.536815000	3.382408000	1.067003000
H	-1.823867000	4.432987000	1.004963000
H	-2.432453000	2.769712000	0.914267000
H	3.885136000	-3.709875000	-0.557287000
H	2.615107000	0.211014000	0.713100000
O	4.607420000	1.430923000	-0.715085000
O	5.037916000	-0.108982000	0.988198000
H	5.018919000	0.940773000	0.110889000
O	3.720996000	2.335113000	-0.139144000
H	2.864949000	2.087163000	-0.553922000

MIV TS(OH) CH_3O˙

E = -1165.92566541 Ha

C	3.426965000	0.221432000	-0.478360000
N	-0.007618000	-2.005196000	-0.742462000
C	-0.868684000	-1.074758000	-0.238476000
C	-0.211343000	0.088948000	0.128447000
C	3.548134000	-1.106217000	-0.998084000
C	2.451730000	-1.909825000	-1.124445000
C	1.181561000	-1.427734000	-0.718646000
N	1.107358000	-0.132140000	-0.200365000
C	2.203475000	0.685619000	-0.101194000
H	-2.921696000	0.662902000	-0.604541000
H	2.504978000	-2.913238000	-1.530089000
C	4.643569000	1.102330000	-0.344908000
H	5.282818000	1.017745000	-1.234007000
H	4.334867000	2.155233000	-0.267605000
C	-2.308448000	-1.341922000	-0.113497000
C	-2.761810000	-2.633816000	0.175602000
C	-4.119409000	-2.889457000	0.307221000
C	-5.068225000	-1.872220000	0.152827000
C	-4.613272000	-0.591514000	-0.161620000
C	-3.253096000	-0.328341000	-0.300847000
H	-2.030484000	-3.427935000	0.289166000
H	-4.455982000	-3.898498000	0.533748000
H	-7.150722000	-1.343357000	-0.065168000
H	-5.334226000	0.206923000	-0.322042000
C	-6.537824000	-2.160963000	0.323222000
H	-6.823995000	-3.078396000	-0.199854000
H	-6.792166000	-2.295509000	1.380467000
C	-0.682333000	1.283221000	0.888328000
H	-1.611911000	1.013177000	1.391716000
H	0.045080000	1.535386000	1.674045000
C	-0.818873000	2.521751000	0.002454000
H	-1.958581000	5.368738000	-0.092302000
H	-3.097556000	4.479880000	-1.134929000
N	-1.952198000	3.268993000	0.134479000
H	-3.486012000	2.126825000	1.069176000
O	0.074328000	2.801652000	-0.784857000
C	-2.098899000	4.459571000	-0.688686000

H	-1.346417000	4.427695000	-1.474056000
C	-2.931906000	3.063325000	1.194053000
H	-2.468057000	3.070541000	2.185668000
H	-3.647344000	3.886201000	1.155333000
H	4.532146000	-1.457276000	-1.294576000
H	2.012144000	1.698854000	0.231329000
O	6.391553000	-1.099355000	0.352303000
O	5.385792000	0.856993000	0.821596000
H	6.144283000	0.000063000	0.624807000
C	5.857308000	-1.934862000	1.340437000
H	4.770719000	-2.046791000	1.234638000
H	6.316274000	-2.919468000	1.180501000
H	6.103932000	-1.593022000	2.351724000

MX

E = -1050.95844213 Ha

C	4.075125000	-0.083809000	0.214163000
N	0.542897000	-2.123586000	-0.320669000
C	-0.307451000	-1.101851000	0.003446000
C	0.377342000	0.043907000	0.362915000
C	4.151307000	-1.460832000	-0.184186000
C	3.027391000	-2.208719000	-0.393700000
C	1.755757000	-1.616086000	-0.189805000
N	1.712514000	-0.284522000	0.217795000
C	2.845388000	0.468688000	0.392509000
H	-2.180798000	0.718236000	-0.733169000
H	3.064775000	-3.245390000	-0.711222000
C	5.338870000	0.709027000	0.387074000
H	5.921847000	0.718239000	-0.538706000
H	5.111839000	1.740391000	0.666174000
H	5.974262000	0.267344000	1.160854000
C	-1.766106000	-1.274265000	-0.032619000
C	-2.337124000	-2.511589000	0.287270000
C	-3.714655000	-2.676483000	0.269179000
C	-4.568411000	-1.620302000	-0.070172000
C	-3.994349000	-0.396506000	-0.413454000
C	-2.612171000	-0.225255000	-0.404128000
H	-1.679022000	-3.335600000	0.544623000
H	-4.142886000	-3.643652000	0.522681000
H	-6.348997000	-2.699659000	-0.641928000
H	-4.635929000	0.428575000	-0.714669000
C	-6.063578000	-1.812595000	-0.067841000
H	-6.441880000	-1.948957000	0.951212000
H	-6.575415000	-0.949654000	-0.501735000
C	-0.093673000	1.318052000	0.979682000
H	-1.091746000	1.144131000	1.384662000
H	0.553649000	1.581691000	1.829288000
C	-0.038791000	2.496939000	0.008671000
H	-0.251377000	4.318659000	-1.644743000
H	-0.952498000	5.384775000	-0.403750000
N	-1.135030000	3.306944000	-0.065985000
H	-2.816812000	2.306081000	0.768480000
O	0.966184000	2.678455000	-0.664353000
C	-1.088947000	4.451364000	-0.962911000
H	-2.021745000	4.512810000	-1.531026000
C	-2.250494000	3.237523000	0.869884000
H	-1.920671000	3.340143000	1.909260000
H	-2.925518000	4.066272000	0.650591000
H	2.688753000	1.516371000	0.618360000
O	5.414631000	-1.937725000	-0.348837000
H	5.368412000	-2.861759000	-0.633582000

MX radical (C4)

E = -1050.32231668 Ha

C	3.855503000	-0.760130000	0.005761000
N	0.007828000	-2.211452000	0.009265000
C	-0.662370000	-1.047095000	-0.041624000
C	0.215171000	0.082186000	-0.060182000
C	3.674269000	-2.178091000	0.048283000
C	2.419982000	-2.733161000	0.040827000
C	1.300204000	-1.883631000	-0.003528000
N	1.491624000	-0.508082000	-0.061368000
C	2.752560000	0.037734000	-0.047789000
H	-2.346573000	0.666196000	-1.373125000
H	2.248329000	-3.803434000	0.077858000
C	5.244525000	-0.187948000	0.007402000
H	5.818631000	-0.557998000	-0.847413000
H	5.209601000	0.902265000	-0.040905000
H	5.787437000	-0.483387000	0.910479000
C	-2.129668000	-1.035310000	-0.067936000
C	-2.826545000	-2.047105000	0.608151000
C	-4.212303000	-2.082113000	0.591839000
C	-4.952952000	-1.119552000	-0.103927000
C	-4.256092000	-0.130650000	-0.798334000
C	-2.865316000	-0.085948000	-0.786765000
H	-2.256972000	-2.802376000	1.140056000
H	-4.735716000	-2.871424000	1.126328000
H	-6.832718000	-2.173159000	-0.234028000
H	-4.809584000	0.608777000	-1.371707000
C	-6.459446000	-1.154306000	-0.093764000
H	-6.853661000	-0.790933000	0.861915000
H	-6.876346000	-0.526602000	-0.885591000
C	-0.157353000	1.420580000	0.060804000
H	-1.210169000	1.554952000	0.273283000
C	0.642746000	2.616797000	-0.178787000
H	1.569439000	4.829414000	-0.767869000
H	1.079032000	5.610738000	0.757365000
N	0.118212000	3.800707000	0.288455000
H	-1.993717000	3.929799000	0.517695000
O	1.709868000	2.605241000	-0.805209000
C	0.726040000	5.051470000	-0.117316000
H	0.000664000	5.673791000	-0.656128000
C	-1.069784000	3.894494000	1.111648000
H	-1.127288000	3.055079000	1.806912000
H	-1.010898000	4.813594000	1.701426000
H	2.797746000	1.116119000	-0.124023000
O	4.814109000	-2.907601000	0.094054000
H	4.592279000	-3.850077000	0.113646000

MX TS(C4) HO˙

E = -1126.65168166 Ha

C	3.729024000	-0.893608000	0.019156000
N	-0.114840000	-2.345443000	-0.217488000
C	-0.769875000	-1.163473000	-0.053870000
C	0.114594000	-0.099548000	0.098115000
C	3.558366000	-2.301259000	-0.188289000
C	2.314880000	-2.867032000	-0.288063000
C	1.175356000	-2.039361000	-0.179056000
N	1.369534000	-0.675498000	0.007195000
C	2.616111000	-0.113241000	0.103622000
H	-2.380190000	0.805516000	-1.038163000
H	2.165886000	-3.930298000	-0.442825000
C	5.113286000	-0.318917000	0.114288000
H	5.677185000	-0.512275000	-0.803145000
H	5.071520000	0.760214000	0.276957000
H	5.671411000	-0.778209000	0.935807000
C	-2.237615000	-1.101874000	-0.048596000
C	-2.972647000	-2.179353000	0.461359000
C	-4.358753000	-2.139067000	0.479988000
C	-5.058230000	-1.030626000	-0.011558000
C	-4.322632000	0.029207000	-0.541313000
C	-2.931211000	-0.004430000	-0.567489000
H	-2.434072000	-3.044372000	0.835229000
H	-4.915419000	-2.982800000	0.881290000
H	-6.994828000	-1.933512000	-0.321137000
H	-4.846008000	0.886038000	-0.958149000
C	-6.564288000	-0.992436000	0.034389000
H	-6.922327000	-0.836198000	1.058064000
H	-6.959834000	-0.182611000	-0.584088000
C	-0.078631000	1.303525000	0.479706000
H	-1.123854000	1.481349000	0.747419000
H	0.527954000	1.525528000	1.426947000
C	0.435195000	2.326454000	-0.534671000
H	1.260149000	5.356795000	-0.743036000
H	-0.328685000	5.214109000	-1.533729000
N	0.171229000	3.630799000	-0.246962000
H	-0.231765000	5.100216000	1.157567000
O	1.054658000	1.969168000	-1.525514000
C	0.553627000	4.655501000	-1.200729000
H	1.023159000	4.172092000	-2.055392000
C	-0.530416000	4.070314000	0.947041000
H	-1.620381000	4.050794000	0.816129000
H	-0.251696000	3.466797000	1.811879000
H	2.652941000	0.960553000	0.240555000
O	1.713795000	2.047706000	2.350922000
H	1.906650000	1.196827000	2.793612000
O	4.712858000	-3.010375000	-0.276631000
H	4.503405000	-3.942204000	-0.435402000

MX TS(C4) HOO˙

E = -1201.77436055 Ha

C	3.729046000	-0.854238000	-0.158746000
N	-0.114179000	-2.289410000	-0.382873000
C	-0.766812000	-1.111849000	-0.278232000
C	0.118261000	-0.022714000	-0.189898000
C	3.556792000	-2.266871000	-0.317596000
C	2.306806000	-2.823033000	-0.418756000
C	1.183353000	-1.980418000	-0.362321000
N	1.377239000	-0.609360000	-0.256332000
C	2.620309000	-0.061269000	-0.129417000
H	-2.427313000	0.779255000	-1.356179000
H	2.170899000	-3.891667000	-0.521148000
C	5.107836000	-0.266313000	-0.029873000
H	5.719535000	-0.466822000	-0.918449000
H	5.053107000	0.817604000	0.086151000
H	5.636606000	-0.661455000	0.846447000
C	-2.235521000	-1.063649000	-0.257659000
C	-2.944506000	-2.120964000	0.326976000
C	-4.330977000	-2.104557000	0.362627000
C	-5.056861000	-1.041650000	-0.186907000
C	-4.347358000	-0.003757000	-0.791665000
C	-2.956342000	-0.012239000	-0.833040000
H	-2.385169000	-2.953782000	0.741574000
H	-4.866228000	-2.932555000	0.821435000
H	-4.891880000	0.815521000	-1.254312000
C	-6.562386000	-1.024507000	-0.120808000
H	-6.982655000	-0.303079000	-0.826269000
H	-6.979520000	-2.009324000	-0.351013000
C	-0.119627000	1.352067000	0.186974000
H	-1.184248000	1.530800000	0.347268000
H	0.369818000	1.426537000	1.348325000
C	0.550209000	2.459523000	-0.589083000
H	1.357363000	4.467331000	-1.773447000
H	1.333654000	5.516059000	-0.329944000
N	0.237891000	3.730256000	-0.194693000
H	-1.704869000	4.143978000	0.557178000
O	1.338763000	2.227012000	-1.497342000
C	0.737336000	4.852501000	-0.966221000
H	-0.095777000	5.428588000	-1.386223000
C	-0.665006000	4.046373000	0.896988000
H	-0.613437000	3.293526000	1.684781000
H	-0.358397000	5.001431000	1.332503000
H	2.666529000	1.014532000	-0.035754000
O	0.793410000	1.189858000	2.571125000
O	0.709191000	-0.183051000	2.594169000
H	-0.182222000	-0.355243000	2.945613000
H	-6.907930000	-0.749770000	0.882104000
O	4.630235000	-3.092259000	-0.366112000
H	5.445389000	-2.578966000	-0.278135000

MX TS(C4) CH_3O˙

E = -1165.94909175 Ha

C	3.652203000	-0.918525000	-0.195985000
N	-0.217675000	-2.310592000	-0.370480000
C	-0.852939000	-1.121868000	-0.214983000
C	0.051009000	-0.058963000	-0.103918000
C	3.455898000	-2.323815000	-0.389839000
C	2.200820000	-2.870070000	-0.472332000
C	1.080374000	-2.020603000	-0.365258000
N	1.297462000	-0.658462000	-0.211557000
C	2.552732000	-0.118801000	-0.114738000
H	-2.458509000	0.850654000	-1.201328000
H	2.031438000	-3.933044000	-0.605833000
C	5.046339000	-0.369150000	-0.098507000
H	5.611201000	-0.580331000	-1.011398000
H	5.023658000	0.711422000	0.056771000
H	5.590029000	-0.831881000	0.730512000
C	-2.319067000	-1.041178000	-0.181888000
C	-3.055307000	-2.101298000	0.361682000
C	-4.440195000	-2.045276000	0.405335000
C	-5.136456000	-0.938563000	-0.094629000
C	-4.399649000	0.103152000	-0.657968000
C	-3.009568000	0.054703000	-0.708131000
H	-2.519187000	-2.965014000	0.742038000
H	-4.998283000	-2.874826000	0.833161000
H	-7.088134000	-1.825715000	-0.348837000
H	-4.921555000	0.957821000	-1.080842000
C	-6.640740000	-0.882430000	-0.021187000
H	-6.976868000	-0.701309000	1.005776000
H	-7.039172000	-0.080901000	-0.648456000
C	-0.110152000	1.340907000	0.267774000
H	-1.150020000	1.559802000	0.523856000
H	0.506470000	1.492084000	1.265837000
C	0.478096000	2.367903000	-0.689794000
H	1.194582000	4.253924000	-2.105293000
H	1.517804000	5.353736000	-0.738059000
N	0.337489000	3.670680000	-0.312158000
H	-1.395294000	4.215048000	0.790264000
O	1.053179000	2.026087000	-1.713203000
C	0.765829000	4.718788000	-1.219435000
H	-0.086055000	5.345148000	-1.509304000
C	-0.311375000	4.093348000	0.917527000
H	-0.114285000	3.392168000	1.730045000
H	0.106945000	5.060332000	1.209001000
H	2.609373000	0.951809000	0.030579000
C	1.162815000	0.157363000	2.931017000
H	0.838380000	0.186385000	3.981575000
H	2.065157000	-0.466016000	2.830290000
H	0.357327000	-0.363021000	2.370712000
O	1.349473000	1.429738000	2.426540000
O	4.594983000	-3.054306000	-0.476442000
H	4.368979000	-3.985544000	-0.615305000

MX TS(C4) CH_3OO˙

E = -1241.06887491 Ha

C	3.826583000	-0.698695000	-0.292010000
N	0.018393000	-2.234090000	-0.537127000
C	-0.668367000	-1.070358000	-0.461479000
C	0.186331000	0.043556000	-0.372907000
C	3.685233000	-2.117463000	-0.424787000
C	2.451349000	-2.704393000	-0.534374000
C	1.302956000	-1.887423000	-0.508381000
N	1.462321000	-0.509687000	-0.415887000
C	2.701450000	0.068717000	-0.295077000
H	-2.350876000	0.723683000	-1.648885000
H	2.316237000	-3.776744000	-0.625413000
C	5.197718000	-0.097016000	-0.175107000
H	5.805218000	-0.344157000	-1.050799000
H	5.134782000	0.989686000	-0.089414000
H	5.722440000	-0.489535000	0.701100000
C	-2.137161000	-1.061254000	-0.463743000
C	-2.829083000	-2.105971000	0.160164000
C	-4.215833000	-2.124840000	0.168921000
C	-4.957001000	-1.110652000	-0.447566000
C	-4.262736000	-0.085007000	-1.089706000
C	-2.871642000	-0.058442000	-1.103382000
H	-2.258718000	-2.900522000	0.631038000
H	-4.739031000	-2.940792000	0.661799000
H	-6.832734000	-0.799843000	0.570106000
H	-4.818695000	0.696947000	-1.600764000
C	-6.463431000	-1.128198000	-0.407881000
H	-6.888387000	-0.462864000	-1.163915000
H	-6.852507000	-2.135711000	-0.582392000
C	-0.124980000	1.389550000	0.051229000
H	-1.206005000	1.513431000	0.137851000
H	0.167188000	1.393556000	1.299581000
C	0.551472000	2.574393000	-0.582519000
H	1.365802000	4.695232000	-1.545823000
H	1.142729000	5.643965000	-0.050382000
N	0.149097000	3.797731000	-0.128608000
H	-0.882785000	3.180021000	1.607788000
O	1.417479000	2.444327000	-1.442473000
C	0.650932000	4.992020000	-0.780890000
H	-0.172634000	5.548611000	-1.244240000
C	-0.866653000	4.001223000	0.890329000
H	-0.625085000	4.916429000	1.438463000
H	-1.865843000	4.120688000	0.450526000
H	2.721395000	1.148594000	-0.250215000
C	0.484183000	-1.098235000	2.726529000
H	0.817278000	-1.101504000	3.769174000
H	1.343233000	-0.931744000	2.068473000
H	-0.005632000	-2.041404000	2.473073000
O	-0.495008000	-0.091629000	2.528109000
O	0.110360000	1.135882000	2.570522000
O	4.848185000	-2.813090000	-0.430367000
H	4.657916000	-3.756693000	-0.535880000

MX TS(C4) $CH_2CHOO^{\bullet}$

E = -1279.14356303 Ha

C	3.753705000	-0.620447000	-0.465739000
N	-0.038483000	-2.201531000	-0.657826000
C	-0.737156000	-1.052712000	-0.540456000
C	0.107741000	0.072958000	-0.447565000
C	3.628609000	-2.035130000	-0.635022000
C	2.399150000	-2.637088000	-0.728650000
C	1.244399000	-1.836474000	-0.650832000
N	1.386150000	-0.460597000	-0.541350000
C	2.617111000	0.129843000	-0.422777000
H	-2.476170000	0.758244000	-1.621730000
H	2.275844000	-3.708692000	-0.842427000
C	5.118097000	-0.002780000	-0.354140000
H	5.716244000	-0.218881000	-1.244340000
H	5.041831000	1.080469000	-0.239694000
H	5.660859000	-0.409794000	0.504395000
C	-2.205236000	-1.063097000	-0.504510000
C	-2.866108000	-2.139402000	0.099798000
C	-4.251659000	-2.178389000	0.145298000
C	-5.022828000	-1.153708000	-0.414535000
C	-4.360047000	-0.096556000	-1.038907000
C	-2.970505000	-0.049195000	-1.088832000
H	-2.272346000	-2.942757000	0.524704000
H	-4.750153000	-3.018861000	0.622244000
H	-4.940200000	0.694408000	-1.507318000
C	-0.207055000	1.406527000	0.012174000
H	-1.286960000	1.515846000	0.129601000
H	0.136278000	1.416338000	1.225284000
C	0.430300000	2.606505000	-0.641618000
H	1.184915000	4.742784000	-1.618555000
H	0.992207000	5.683056000	-0.113545000
N	0.027025000	3.821154000	-0.167501000
H	-0.932083000	3.184729000	1.603761000
O	1.266187000	2.490559000	-1.531828000
C	0.489083000	5.025572000	-0.831117000
H	-0.357218000	5.569827000	-1.267244000
C	-0.957904000	4.004763000	0.885235000
H	-0.716800000	4.925554000	1.423892000
H	-1.973636000	4.102961000	0.479412000
H	2.624691000	1.207900000	-0.343143000
C	0.472034000	-1.064733000	2.524218000
O	-0.435809000	-0.043459000	2.560190000
O	0.155302000	1.191826000	2.544848000
C	1.795542000	-0.952550000	2.580313000
H	2.403899000	-1.846576000	2.526085000
H	2.275132000	0.011647000	2.683180000
H	-0.065477000	-2.003343000	2.427634000
H	-6.873584000	-0.901905000	0.662770000
C	-6.527143000	-1.193860000	-0.334899000
H	-6.981519000	-0.510948000	-1.057374000
H	-6.907279000	-2.200780000	-0.530919000
O	4.799232000	-2.714799000	-0.689268000
H	4.618606000	-3.657700000	-0.816101000

MX radical ($O^{\bullet}$)

E = -1050.32818821 Ha

C	4.115181000	-0.111796000	0.215843000
N	0.537016000	-2.140800000	-0.337547000
C	-0.285037000	-1.133959000	-0.005243000
C	0.437288000	0.014685000	0.372996000
C	4.239155000	-1.529653000	-0.200047000
C	3.009274000	-2.260660000	-0.416346000
C	1.787977000	-1.649336000	-0.207359000
N	1.747669000	-0.319403000	0.214886000
C	2.900212000	0.439062000	0.397566000
H	-2.124264000	0.743182000	-0.705030000
H	3.053198000	-3.294061000	-0.736286000
C	5.387784000	0.657920000	0.388088000
H	5.960309000	0.653978000	-0.543998000
H	5.192404000	1.691524000	0.682949000
H	6.019027000	0.180591000	1.143425000
C	-1.748221000	-1.269690000	-0.030313000
C	-2.341796000	-2.498125000	0.280818000
C	-3.722331000	-2.634082000	0.263147000
C	-4.553659000	-1.557283000	-0.066699000
C	-3.955555000	-0.341608000	-0.399475000
C	-2.570896000	-0.197373000	-0.387746000
H	-1.701371000	-3.338138000	0.530921000
H	-4.169889000	-3.594081000	0.508892000
H	-6.354620000	-2.625991000	-0.587994000
H	-4.580578000	0.498631000	-0.692494000
C	-6.052248000	-1.716572000	-0.060143000
H	-6.434098000	-1.791523000	0.963929000
H	-6.544345000	-0.866130000	-0.538819000
C	-0.033799000	1.291304000	0.978646000
H	-1.029003000	1.118523000	1.390913000
H	0.621360000	1.570342000	1.815737000
C	0.006486000	2.447503000	-0.027048000
H	-0.239397000	4.252019000	-1.687796000
H	-0.911736000	5.361138000	-0.467322000
N	-1.054527000	3.301151000	-0.034946000
H	-2.792828000	2.399791000	0.801896000
O	0.968214000	2.562483000	-0.771056000
C	-1.054622000	4.405109000	-0.983460000
H	-2.006821000	4.431687000	-1.521698000
C	-2.129940000	3.260529000	0.947813000
H	-1.743590000	3.241009000	1.971131000
H	-2.723653000	4.168966000	0.835451000
H	2.735091000	1.483423000	0.634120000
O	5.350809000	-2.045904000	-0.361558000

MX TS(OH) $HO^{\bullet}$

E = -1126.65647609 Ha

C	-3.837193000	0.420589000	-0.559319000
N	-0.516324000	-1.960143000	0.032592000
C	0.434483000	-1.001658000	-0.177800000
C	-0.136706000	0.223146000	-0.479609000
C	-4.069626000	-0.949312000	-0.205624000
C	-2.997227000	-1.839255000	0.000325000
C	-1.675983000	-1.337311000	-0.097975000
N	-1.498577000	0.007737000	-0.403779000
C	-2.551462000	0.861976000	-0.629202000
H	2.402258000	0.580881000	0.805839000
H	-3.140371000	-2.908835000	-0.036089000
C	-5.014131000	1.333639000	-0.742361000
H	-4.686977000	2.353158000	-0.958255000
H	-5.652259000	0.988018000	-1.561000000
H	-5.629522000	1.342382000	0.161643000
C	1.869993000	-1.301983000	-0.091489000
C	2.355227000	-2.550693000	-0.495704000
C	3.712022000	-2.832855000	-0.426147000
C	4.627326000	-1.886345000	0.048815000
C	4.135664000	-0.652171000	0.474247000
C	2.774716000	-0.363788000	0.413749000
H	1.649692000	-3.291435000	-0.858934000
H	4.074354000	-3.807266000	-0.745417000
H	6.648810000	-1.449799000	0.670683000
H	4.823676000	0.085680000	0.880452000
C	6.100271000	-2.202459000	0.098542000
H	6.279625000	-3.177828000	0.561013000
H	6.529521000	-2.235508000	-0.908892000
C	0.475090000	1.486454000	-0.984196000
H	1.480053000	1.251717000	-1.337324000
H	-0.091659000	1.854066000	-1.851917000
C	0.445932000	2.603603000	0.060086000
H	1.547233000	5.368974000	0.724276000
H	2.462959000	4.349316000	1.863132000
N	1.595617000	3.306285000	0.267983000
H	3.233037000	2.215056000	-0.540437000
O	-0.591260000	2.827364000	0.667794000
C	1.571476000	4.397219000	1.231436000
H	0.679430000	4.293094000	1.845726000
C	2.767368000	3.204084000	-0.593715000
H	2.529114000	3.428979000	-1.638990000
H	3.499805000	3.937270000	-0.252750000
H	-2.287073000	1.899922000	-0.792769000
O	-4.150699000	-2.346932000	1.904716000
H	-5.126256000	-2.008874000	0.817767000
O	-5.301440000	-1.349741000	0.025958000
H	-3.866712000	-3.268934000	2.022584000

MX TS(OH) $OOH^{\bullet}$

E = -1201.78355968 Ha

C	3.521615000	0.621529000	-0.226804000
N	0.253339000	-1.863429000	-0.658136000
C	-0.683846000	-1.007049000	-0.193296000

C	-0.117150000	0.207698000	0.206343000
C	3.765325000	-0.707541000	-0.752785000
C	2.708036000	-1.599390000	-0.916383000
C	1.408265000	-1.198312000	-0.584145000
N	1.216632000	0.084293000	-0.069265000
C	2.254771000	0.982499000	0.088859000
H	-2.834953000	0.598399000	-0.619343000
H	2.879937000	-2.588438000	-1.323133000
C	4.690034000	1.545130000	-0.054657000
H	5.213347000	1.680911000	-1.005645000
H	4.367925000	2.520829000	0.315370000
H	5.407561000	1.116694000	0.653534000
C	-2.106388000	-1.368543000	-0.125551000
C	-2.481831000	-2.691741000	0.133382000
C	-3.822784000	-3.039711000	0.206007000
C	-4.831198000	-2.086692000	0.020394000
C	-4.451935000	-0.774301000	-0.261883000
C	-3.108328000	-0.417675000	-0.340958000
H	-1.703856000	-3.436067000	0.271304000
H	-4.099028000	-4.071511000	0.410086000
H	-6.553598000	-2.722822000	1.153635000
H	-5.218215000	-0.024394000	-0.443791000
C	-6.282991000	-2.478875000	0.120538000
H	-6.937078000	-1.669936000	-0.214643000
H	-6.495913000	-3.362375000	-0.489059000
C	-0.710002000	1.361891000	0.939209000
H	-1.635163000	1.021795000	1.406881000
H	-0.034929000	1.674465000	1.749035000
C	-0.908554000	2.579433000	0.032307000
H	-1.530123000	4.434128000	-1.469498000
H	-2.247714000	5.345431000	-0.118597000
N	-2.085444000	3.257421000	0.144682000
H	-3.590147000	2.039151000	1.030833000
O	-0.023730000	2.898317000	-0.747749000
C	-2.302609000	4.419952000	-0.703229000
H	-3.288118000	4.356257000	-1.174009000
C	-3.071383000	2.992077000	1.184740000
H	-2.620833000	2.992869000	2.182030000
H	-3.814613000	3.790304000	1.155919000
H	1.973627000	1.974095000	0.420709000
O	6.002584000	-1.363840000	0.997432000
O	4.981661000	-1.048153000	-1.130064000
H	5.619366000	-1.115794000	-0.242549000
O	4.801810000	-1.321977000	1.641692000
H	4.537928000	-2.259027000	1.706958000

MX TS(OH) $CH_3O^{\bullet}$

E = -1165.94963209 Ha

C	3.377243000	1.469360000	0.140164000
N	0.631595000	-1.564579000	-0.374534000
C	-0.479517000	-0.866715000	-0.019844000
C	-0.166004000	0.432283000	0.364599000
C	3.892711000	0.179742000	-0.253151000
C	3.017377000	-0.889555000	-0.482325000
C	1.643982000	-0.711331000	-0.238322000
N	1.197795000	0.530425000	0.200989000
C	2.043311000	1.607093000	0.348612000
H	-2.825757000	0.312610000	-0.711846000
H	3.356540000	-1.825846000	-0.900293000
C	4.339534000	2.608346000	0.306818000
H	4.875962000	2.800543000	-0.626914000
H	3.817675000	3.520208000	0.605884000
H	5.092714000	2.363568000	1.061376000
C	-1.818645000	-1.471375000	-0.046057000
C	-1.983482000	-2.827176000	0.258469000
C	-3.246542000	-3.401751000	0.244287000
C	-4.382975000	-2.649696000	-0.074619000
C	-4.210503000	-1.304571000	-0.402090000
C	-2.945945000	-0.722024000	-0.395873000
H	-1.104807000	-3.416773000	0.500665000
H	-3.358637000	-4.456395000	0.484604000
H	-6.485766000	-2.650799000	-0.566704000
H	-5.074772000	-0.709532000	-0.688189000
C	-5.750789000	-3.282762000	-0.061445000
H	-5.740323000	-4.256922000	-0.559362000
H	-6.098925000	-3.444648000	0.964750000
C	-1.004254000	1.494453000	0.989571000
H	-1.894911000	1.016754000	1.400637000
H	-0.464472000	1.948226000	1.833202000
C	-1.329206000	2.626372000	0.011886000
H	-2.123331000	4.290329000	-1.627311000
H	-3.110618000	5.099106000	-0.385828000
N	-2.613802000	3.080809000	-0.016205000
H	-3.294484000	2.817730000	1.978310000
O	-0.444572000	3.079547000	-0.700013000
C	-2.949361000	4.161776000	-0.930751000
H	-3.860810000	3.910924000	-1.481364000
C	-3.631496000	2.677508000	0.946414000
H	-4.507877000	3.309286000	0.794169000
H	-3.937858000	1.634317000	0.812113000
H	1.568470000	2.549875000	0.591724000
O	5.160298000	-2.170292000	0.561408000
O	5.193573000	0.052603000	-0.383017000
H	5.370981000	-0.954730000	-0.087828000
C	5.465267000	-3.296282000	-0.171325000
H	6.542795000	-3.520813000	-0.061247000
H	4.924226000	-4.173618000	0.211303000
H	5.266252000	-3.187032000	-1.250721000

MXI

E = -1050.95249333 Ha

C	4.430969000	-0.542107000	0.174112000
N	0.822990000	-2.437847000	-0.361372000
C	0.014336000	-1.389439000	-0.042185000
C	0.746175000	-0.263054000	0.306456000
C	4.457729000	-1.916955000	-0.223041000
C	3.305690000	-2.616113000	-0.433942000
C	2.057130000	-1.975162000	-0.236565000
N	2.064123000	-0.639413000	0.163262000
C	3.227244000	0.070742000	0.349086000
H	-1.800174000	0.467744000	-0.820886000
H	3.297957000	-3.653604000	-0.746305000
C	5.716757000	0.216042000	0.364877000
H	6.311478000	0.214883000	-0.554335000
H	5.526500000	1.255674000	0.641853000
H	6.327718000	-0.239497000	1.151318000
C	-1.450419000	-1.511845000	-0.058398000
C	-2.059445000	-2.716771000	0.310896000
C	-3.442042000	-2.832116000	0.315562000
C	-4.262119000	-1.757187000	-0.047827000
C	-3.650059000	-0.566838000	-0.439626000
C	-2.262754000	-0.445948000	-0.453805000
H	-1.427993000	-3.554888000	0.588686000
H	-3.901115000	-3.774052000	0.606870000
H	-6.087545000	-2.804805000	-0.528589000
H	-4.266596000	0.270688000	-0.758172000
C	-5.762957000	-1.893787000	-0.016445000
H	-6.131398000	-1.950213000	1.013729000
H	-6.249355000	-1.041942000	-0.498653000
C	0.321337000	1.029266000	0.926796000
H	-0.671692000	0.875879000	1.348727000
H	0.995909000	1.271019000	1.759375000
C	0.421180000	2.201541000	-0.050405000
H	0.135006000	3.662741000	-2.161523000
H	0.011493000	4.861180000	-0.859965000
N	-0.697730000	2.917942000	-0.394094000
H	-2.072541000	2.050658000	0.919940000
O	1.506737000	2.459734000	-0.547859000
C	-0.486723000	4.013092000	-1.338504000
H	-1.459249000	4.338781000	-1.711432000
C	-1.946848000	2.964845000	0.336945000
H	-2.766641000	3.023907000	-0.383988000
H	3.107189000	1.123355000	0.573755000
H	5.421067000	-2.397174000	-0.370177000
O	-2.065617000	4.119503000	1.127443000
H	-1.405740000	4.071733000	1.834606000

MXI radical (C4)

E = -1050.31547040 Ha

C	-3.760774000	-1.885240000	-0.017239000
N	0.301618000	-2.500884000	-0.127802000
C	0.717660000	-1.241630000	0.051342000
C	-0.377412000	-0.324289000	0.180914000
C	-3.297910000	-3.219519000	-0.206953000
C	-1.958939000	-3.500103000	-0.243751000
C	-1.033864000	-2.450380000	-0.095692000
N	-1.502911000	-1.156605000	0.104567000
C	-2.850260000	-0.878686000	0.134280000

H	2.024254000	0.609086000	1.603964000
H	-1.568694000	-4.499799000	-0.391169000
C	-5.236142000	-1.590563000	0.027120000
H	-5.720218000	-2.143256000	0.838738000
H	-5.421100000	-0.525916000	0.185769000
H	-5.722757000	-1.886198000	-0.908115000
C	2.150903000	-0.924818000	0.094011000
C	3.032879000	-1.675373000	-0.695837000
C	4.395072000	-1.419237000	-0.668719000
C	4.927023000	-0.416390000	0.150124000
C	4.049198000	0.309657000	0.955255000
C	2.680155000	0.061716000	0.933777000
H	2.627002000	-2.461592000	-1.324308000
H	5.064282000	-2.007728000	-1.291762000
H	6.988058000	-1.057454000	0.155816000
H	4.443632000	1.071932000	1.622243000
C	6.406507000	-0.130860000	0.151613000
H	6.696781000	0.433135000	-0.741831000
H	6.696397000	0.458120000	1.025479000
C	-0.277868000	1.068089000	0.206259000
H	0.728155000	1.424106000	0.024904000
C	-1.293251000	2.052541000	0.568141000
H	-2.583565000	4.076710000	1.435513000
H	-2.846097000	4.285844000	-0.308721000
N	-1.015085000	3.377092000	0.254574000
H	0.861336000	3.258500000	-0.659598000
O	-2.333360000	1.763170000	1.162981000
C	-2.098508000	4.322205000	0.492945000
H	-1.680198000	5.329904000	0.545919000
C	-0.120222000	3.708859000	-0.834839000
H	0.005245000	4.792701000	-0.838148000
H	-3.113726000	0.152776000	0.322356000
H	-4.025900000	-4.017603000	-0.322303000
O	-0.621372000	3.370704000	-2.104022000
H	-0.625866000	2.402660000	-2.162298000

MXI TS(C4) HO˙

E = -1126.65359266 Ha

C	3.274646000	-2.306953000	-0.100008000
N	-0.833426000	-2.559732000	-0.129295000
C	-1.101931000	-1.231669000	-0.069295000
C	0.069033000	-0.470752000	-0.034162000
C	2.692591000	-3.610766000	-0.133587000
C	1.336220000	-3.784709000	-0.167100000
C	0.491079000	-2.653136000	-0.141309000
N	1.086584000	-1.394912000	-0.098660000
C	2.448887000	-1.219297000	-0.094973000
H	-2.073375000	1.046250000	-1.196782000
H	0.873640000	-4.763838000	-0.202376000
C	4.770181000	-2.141015000	-0.111225000
H	5.202902000	-2.583319000	-1.014034000
H	5.054559000	-1.086206000	-0.085048000
H	5.226618000	-2.639858000	0.749859000
C	-2.479772000	-0.725069000	-0.041160000
C	-3.483364000	-1.478322000	0.580090000
C	-4.787906000	-1.010014000	0.620229000
C	-5.135833000	0.216315000	0.041224000
C	-4.136773000	0.950852000	-0.597268000
C	-2.825233000	0.487273000	-0.645518000
H	-3.218668000	-2.432488000	1.024623000
H	-5.556921000	-1.603597000	1.108929000
H	-7.266022000	-0.060999000	-0.171090000
H	-4.391147000	1.890965000	-1.079903000
C	-6.554274000	0.720650000	0.111486000
H	-6.806822000	1.039564000	1.128723000
H	-6.705453000	1.574827000	-0.553357000
C	0.326089000	0.940091000	0.288844000
H	-0.612483000	1.443114000	0.538697000
H	0.945522000	0.965702000	1.241142000
C	1.107502000	1.709010000	-0.781894000
H	1.962604000	3.361373000	-2.506446000
H	3.265956000	3.565223000	-1.310623000
N	1.373845000	3.026535000	-0.534320000
H	1.069258000	4.671031000	0.678787000
O	1.452726000	1.149974000	-1.810784000
C	2.201679000	3.726154000	-1.509146000
H	1.989587000	4.795876000	-1.441264000
C	1.348853000	3.620648000	0.794529000
H	0.582277000	3.122781000	1.395317000
H	3.351558000	-4.474060000	-0.148604000
H	2.803672000	-0.197248000	-0.155632000
O	2.224020000	0.952012000	2.322182000
O	2.597916000	3.605152000	1.415255000
H	2.745345000	2.698085000	1.740250000
H	2.601023000	0.070731000	2.122986000

MXI TS(C4) HOO˙

E = -1201.77625346 Ha

C	3.261522000	-2.289907000	-0.237313000
N	-0.844860000	-2.491305000	-0.180013000
C	-1.110325000	-1.171358000	-0.213752000
C	0.069230000	-0.399163000	-0.266357000
C	2.664009000	-3.584261000	-0.214678000
C	1.304875000	-3.737364000	-0.205252000
C	0.486677000	-2.589161000	-0.221998000
N	1.089892000	-1.342763000	-0.279919000
C	2.452179000	-1.191780000	-0.266245000
H	-2.184638000	0.935304000	-1.590335000
H	0.821219000	-4.706189000	-0.176656000
C	4.758808000	-2.142059000	-0.230875000
H	5.202414000	-2.631236000	-1.103919000
H	5.052962000	-1.090291000	-0.247495000
H	5.192754000	-2.602447000	0.662440000
C	-2.495226000	-0.677240000	-0.195136000
C	-3.455910000	-1.364136000	0.557254000
C	-4.770984000	-0.924193000	0.589128000
C	-5.173303000	0.206369000	-0.130745000
C	-4.218479000	0.870360000	-0.901611000
C	-2.897255000	0.435912000	-0.939996000
H	-3.152108000	-2.249720000	1.106706000
H	-5.504767000	-1.466893000	1.180193000
H	-7.302951000	-0.145696000	-0.117056000
H	-4.516338000	1.730824000	-1.495130000
C	-6.599006000	0.690137000	-0.067037000
H	-6.789568000	1.222722000	0.871362000
H	-6.822960000	1.374739000	-0.889056000
C	0.254820000	1.024826000	-0.099694000
H	-0.703307000	1.548595000	-0.081117000
H	0.631557000	1.153927000	1.084700000
C	1.275621000	1.726412000	-0.978299000
H	2.401013000	4.729371000	-1.526684000
H	2.716932000	3.198640000	-2.389901000
N	1.588030000	3.018308000	-0.649211000
H	1.268586000	4.680552000	0.523148000
O	1.764773000	1.153935000	-1.940909000
C	2.645175000	3.669678000	-1.411941000
H	3.603787000	3.581731000	-0.890009000
C	1.336646000	3.598572000	0.662520000
H	0.374344000	3.240813000	1.040464000
H	3.309978000	-4.457579000	-0.199366000
H	2.827865000	-0.179330000	-0.299053000
O	1.106244000	-0.256016000	2.522860000
H	0.224225000	-0.548927000	2.813298000
O	0.946786000	1.103262000	2.368765000
O	2.375216000	3.372339000	1.568418000
H	2.238987000	2.493396000	1.966556000

MXI TS(C4) CH_3O˙

E = -1165.95147294 Ha

C	3.235828000	-2.246509000	-0.306643000
N	-0.870174000	-2.513927000	-0.252731000
C	-1.147767000	-1.194862000	-0.189173000
C	0.022994000	-0.415572000	-0.190206000
C	2.657286000	-3.548507000	-0.361477000
C	1.300000000	-3.727614000	-0.360551000
C	0.460239000	-2.596903000	-0.302769000
N	1.049791000	-1.339650000	-0.273479000
C	2.409517000	-1.159640000	-0.267084000
H	-2.194042000	1.028117000	-1.372196000
H	0.836593000	-4.706190000	-0.393280000
C	4.730820000	-2.075771000	-0.303628000
H	5.171139000	-2.479948000	-1.220735000
H	5.008012000	-1.021796000	-0.231193000
H	5.183119000	-2.605326000	0.540946000
C	-2.531356000	-0.704113000	-0.136477000
C	-3.502052000	-1.451494000	0.541298000
C	-4.814232000	-1.006571000	0.601612000
C	-5.202449000	0.188893000	-0.014356000

C	-4.236516000	0.915757000	-0.711005000
C	-2.917714000	0.476945000	-0.777829000
H	-3.207033000	-2.383912000	1.012231000
H	-5.557197000	-1.595412000	1.134145000
H	-6.838611000	1.432579000	-0.676490000
H	-4.523571000	1.829893000	-1.224222000
C	-6.625945000	0.674040000	0.081118000
H	-7.334142000	-0.149105000	-0.051345000
H	-6.822090000	1.119487000	1.062817000
C	0.248246000	1.004227000	0.054302000
H	-0.699118000	1.510554000	0.253136000
H	0.882068000	1.073632000	1.024510000
C	1.101565000	1.741055000	-0.978385000
H	2.581690000	3.116501000	-2.402712000
H	3.314736000	3.906347000	-0.975512000
N	1.439821000	3.027812000	-0.667382000
H	1.044542000	4.715968000	0.445168000
O	1.462953000	1.180036000	-2.000518000
C	2.385319000	3.728617000	-1.524900000
H	1.964379000	4.690746000	-1.834239000
C	1.211931000	3.651066000	0.629851000
H	0.303163000	3.234496000	1.073168000
H	3.317558000	-4.410261000	-0.402636000
H	2.762050000	-0.138538000	-0.222527000
C	1.458695000	-0.239173000	2.786922000
H	1.199192000	0.037022000	3.818210000
H	2.163643000	-1.085228000	2.778928000
H	0.529063000	-0.616318000	2.307400000
O	1.955792000	0.825037000	2.063991000
O	2.305808000	3.561286000	1.488790000
H	2.315917000	2.662936000	1.869753000

MXI TS(C4) $CH_3OO^{\bullet}$

E = -1241.06951075 Ha

C	3.280127000	-2.233637000	-0.374989000
N	-0.827018000	-2.429397000	-0.420919000
C	-1.087726000	-1.108651000	-0.442777000
C	0.093410000	-0.337915000	-0.461307000
C	2.680984000	-3.526814000	-0.385117000
C	1.321510000	-3.677995000	-0.415305000
C	0.505397000	-2.529176000	-0.437694000
N	1.111656000	-1.282940000	-0.469251000
C	2.472728000	-1.133711000	-0.414599000
H	-2.144233000	1.042999000	-1.760761000
H	0.836733000	-4.646707000	-0.410790000
C	4.776794000	-2.087683000	-0.325023000
H	5.244264000	-2.567239000	-1.190938000
H	5.072380000	-1.036156000	-0.321122000
H	5.185161000	-2.559027000	0.574610000
C	-2.467098000	-0.603762000	-0.409670000
C	-3.430091000	-1.296369000	0.335811000
C	-4.739364000	-0.840938000	0.389421000
C	-5.132925000	0.311472000	-0.300111000
C	-4.175577000	0.983471000	-1.061371000
C	-2.860168000	0.534524000	-1.121159000
H	-3.131183000	-2.198141000	0.861755000
H	-5.475229000	-1.388226000	0.973635000
H	-6.729495000	1.321037000	0.739730000
H	-4.467308000	1.862893000	-1.629604000
C	-6.552026000	0.810846000	-0.213566000
H	-6.773045000	1.519346000	-1.015857000
H	-7.266643000	-0.014689000	-0.280287000
C	0.283712000	1.073315000	-0.222217000
H	-0.665951000	1.611835000	-0.194931000
H	0.639587000	1.108190000	0.992698000
C	1.338102000	1.805140000	-1.029928000
H	2.740778000	3.420389000	-2.365754000
H	3.745938000	3.439284000	-0.895666000
N	1.688444000	3.059660000	-0.602726000
H	1.482734000	4.607508000	0.740180000
O	1.825711000	1.293500000	-2.027058000
C	2.774670000	3.716496000	-1.319197000
H	2.647976000	4.798665000	-1.234356000
C	1.491183000	3.515055000	0.765914000
H	0.517957000	3.171760000	1.127948000
H	3.325171000	-4.401289000	-0.362850000
H	2.851628000	-0.121738000	-0.431704000
O	0.765954000	-0.430883000	2.329760000
O	0.947423000	0.926830000	2.249513000
O	2.531800000	3.139802000	1.620956000
H	2.353815000	2.236683000	1.938466000
C	-0.539260000	-0.675736000	2.834639000
H	-1.287640000	-0.161736000	2.222430000
H	-0.678096000	-1.757049000	2.763674000
H	-0.610257000	-0.341439000	3.873846000

MXI TS(C4) $CH_2CHOO^{\bullet}$

E = -1279.14231888 Ha

C	3.521230000	-1.919225000	-0.571518000
N	-0.551589000	-2.496511000	-0.550208000
C	-0.931938000	-1.207878000	-0.559843000
C	0.178167000	-0.331545000	-0.608739000
C	3.043886000	-3.262877000	-0.569124000
C	1.703834000	-3.541271000	-0.583627000
C	0.784179000	-2.473954000	-0.592532000
N	1.271978000	-1.175514000	-0.646272000
C	2.615714000	-0.897640000	-0.610173000
H	-2.180827000	0.902398000	-1.769670000
H	1.312261000	-4.551266000	-0.569635000
C	4.998955000	-1.635728000	-0.547309000
H	5.493752000	-2.073899000	-1.419903000
H	5.195773000	-0.561414000	-0.551533000
H	5.464784000	-2.064034000	0.345961000
C	-2.348817000	-0.829765000	-0.498614000
C	-3.240963000	-1.640108000	0.215040000
C	-4.584522000	-1.306174000	0.292430000
C	-5.083465000	-0.162265000	-0.341622000
C	-4.194928000	0.627476000	-1.072067000
C	-2.845078000	0.300695000	-1.155473000
H	-2.858851000	-2.533739000	0.698772000
H	-5.265032000	-1.942553000	0.852967000
H	-4.567217000	1.503342000	-1.596973000
C	0.239891000	1.070812000	-0.269266000
H	-0.764052000	1.455869000	-0.087747000
H	0.745098000	1.074040000	0.865990000
H	3.766948000	-4.073565000	-0.553491000
H	2.889841000	0.146815000	-0.663080000
C	0.122340000	-1.027512000	2.676727000
O	-0.040188000	0.330730000	2.636163000
O	1.077916000	0.980668000	2.181241000
C	1.245298000	-1.706908000	2.465477000
H	1.224562000	-2.786872000	2.532398000
H	2.177836000	-1.207443000	2.235807000
H	-0.834323000	-1.477025000	2.923653000
H	-6.762892000	0.622887000	0.758442000
C	-6.541123000	0.202215000	-0.228619000
H	-6.824145000	0.945264000	-0.978420000
H	-7.179644000	-0.676331000	-0.360153000
C	1.122884000	2.018526000	-1.049608000
H	1.557332000	5.159992000	-1.538520000
H	2.527746000	3.768885000	-2.091348000
N	1.110364000	3.322150000	-0.635494000
H	0.231124000	4.834667000	0.441996000
O	1.815565000	1.619899000	-1.976835000
C	2.069807000	4.244564000	-1.226810000
H	2.838780000	4.500079000	-0.490665000
C	0.504304000	3.788704000	0.607042000
H	-0.410886000	3.224187000	0.801602000
O	1.374694000	3.758534000	1.696211000
H	1.304932000	2.879354000	2.112484000

MXI radical ($O^{\bullet}$)

E = -1050.28579828 Ha

C	-4.383989000	-0.627649000	-0.157490000
N	-0.719664000	-2.430350000	0.321742000
C	0.054716000	-1.344815000	0.042294000
C	-0.712004000	-0.233387000	-0.274618000
C	-4.369152000	-2.016638000	0.189388000
C	-3.197116000	-2.688581000	0.377289000
C	-1.967784000	-2.004036000	0.205995000
N	-2.016026000	-0.656391000	-0.149045000
C	-3.198926000	0.025654000	-0.309339000
H	1.785357000	0.553507000	0.909658000
H	-3.159414000	-3.735767000	0.653037000
C	-5.692035000	0.097823000	-0.321461000
H	-6.284819000	0.047748000	0.597653000
H	-5.533538000	1.151403000	-0.563534000
H	-6.290296000	-0.348969000	-1.122509000

C	1.522691000	-1.410736000	0.070634000
C	2.184620000	-2.576232000	-0.331213000
C	3.571085000	-2.635802000	-0.322781000
C	4.343316000	-1.542914000	0.087644000
C	3.678972000	-0.392667000	0.513451000
C	2.287507000	-0.327459000	0.513630000
H	1.591006000	-3.428989000	-0.645442000
H	4.070724000	-3.547980000	-0.640771000
H	6.203902000	-2.533700000	0.553704000
H	4.257810000	0.455116000	0.873494000
C	5.848650000	-1.618329000	0.070578000
H	6.230673000	-1.622375000	-0.956159000
H	6.294976000	-0.766079000	0.589523000
C	-0.322982000	1.093327000	-0.837614000
H	0.673945000	0.994627000	-1.269043000
H	-0.994931000	1.365418000	-1.662967000
C	-0.435903000	2.216309000	0.190788000
H	-0.169360000	3.825624000	2.140917000
H	0.002188000	4.994660000	0.817182000
N	0.660883000	3.018689000	0.411980000
H	2.286238000	2.136379000	-0.619894000
O	-1.475910000	2.371124000	0.807341000
C	0.473554000	4.143538000	1.322125000
H	1.444599000	4.449527000	1.717813000
C	1.747837000	3.100075000	-0.543497000
H	2.489590000	3.817851000	-0.158926000
H	-3.110697000	1.088321000	-0.499511000
H	-5.317848000	-2.530338000	0.317326000
O	1.407810000	3.449562000	-1.812232000

MXI TS(OH) HO˙

E = -1126.64453183 Ha

C	4.638074000	-0.277809000	0.127747000
N	1.167610000	-2.428590000	-0.339840000
C	0.290291000	-1.444793000	0.009306000
C	0.950614000	-0.276708000	0.366860000
C	4.757368000	-1.646120000	-0.276456000
C	3.655851000	-2.428945000	-0.461574000
C	2.367744000	-1.884237000	-0.229608000
N	2.286417000	-0.557490000	0.189108000
C	3.396178000	0.237759000	0.341319000
H	-1.699152000	0.363228000	-0.388772000
H	3.718484000	-3.461946000	-0.782564000
C	5.867269000	0.576005000	0.282644000
H	6.427605000	0.628935000	-0.656428000
H	5.608043000	1.595709000	0.577785000
H	6.538733000	0.162654000	1.042559000
C	-1.160182000	-1.682125000	-0.016354000
C	-1.658812000	-2.980193000	0.149158000
C	-3.025632000	-3.215716000	0.133952000
C	-3.942061000	-2.171904000	-0.041349000
C	-3.441722000	-0.882962000	-0.220092000
C	-2.070460000	-0.643619000	-0.222465000
H	-0.952610000	-3.792916000	0.285406000
H	-3.396346000	-4.229728000	0.265646000
H	-5.752424000	-2.813728000	0.942509000
H	-4.134043000	-0.056218000	-0.366591000
C	-5.424423000	-2.444581000	-0.035095000
H	-5.995323000	-1.540224000	-0.260564000
H	-5.689198000	-3.206050000	-0.775791000
C	0.468876000	1.010078000	0.949149000
H	-0.515673000	0.847267000	1.392552000
H	1.142697000	1.326861000	1.759761000
C	0.454223000	2.130119000	-0.094965000
H	-0.143016000	3.698521000	-1.966589000
H	-0.120109000	4.980026000	-0.743100000
N	-0.586568000	3.027773000	-0.050848000
O	1.328419000	2.199497000	-0.940383000
C	-0.637274000	4.071041000	-1.070485000
H	-1.682610000	4.296939000	-1.289227000
C	-1.479886000	3.149976000	1.080815000
H	-1.915681000	4.153672000	1.044698000
H	5.749884000	-2.051465000	-0.451977000
H	3.209278000	1.276883000	0.583095000
O	-3.522556000	2.527389000	-0.792722000
H	-3.032605000	1.824530000	-1.264399000
O	-2.468482000	2.166400000	1.159332000
H	-3.244244000	2.338385000	0.392805000
H	-0.929167000	3.048931000	2.025388000

MXI TS(OH) HOO˙

E = -1201.76242210 Ha

C	4.874919000	-0.067933000	0.286482000
N	1.521612000	-2.334571000	-0.454936000
C	0.597103000	-1.374046000	-0.179707000
C	1.185898000	-0.189690000	0.230641000
C	5.069117000	-1.431603000	-0.105269000
C	4.012623000	-2.250492000	-0.377718000
C	2.692946000	-1.749545000	-0.249309000
N	2.538333000	-0.425050000	0.161098000
C	3.604467000	0.408309000	0.400397000
H	-1.218157000	0.305709000	-1.280864000
H	4.135578000	-3.279965000	-0.692553000
C	6.060507000	0.824816000	0.534205000
H	5.746515000	1.832156000	0.817933000
H	6.690039000	0.426101000	1.336544000
H	6.683448000	0.905158000	-0.362509000
C	-0.851374000	-1.591691000	-0.314856000
C	-1.449065000	-2.767410000	0.146852000
C	-2.830964000	-2.930759000	0.071264000
C	-3.649702000	-1.942307000	-0.484742000
C	-3.041092000	-0.785574000	-0.983405000
C	-1.665637000	-0.605672000	-0.892275000
H	-0.820859000	-3.539888000	0.579607000
H	-3.285032000	-3.838564000	0.460208000
H	-5.464285000	-3.082265000	-0.194365000
H	-3.653306000	-0.001185000	-1.420819000
C	-5.148126000	-2.088808000	-0.522658000
H	-5.616961000	-1.344789000	0.129649000
H	-5.531194000	-1.927623000	-1.535084000
C	0.565695000	1.028388000	0.829303000
H	-0.403378000	0.725593000	1.225223000
C	0.479404000	2.171180000	-0.178794000
H	-0.720826000	4.818594000	-0.978587000
H	-1.837720000	3.739359000	-1.857554000
N	-0.730814000	2.792533000	-0.367027000
O	1.474447000	2.471699000	-0.817350000
C	-0.847904000	3.813372000	-1.401248000
H	-0.071211000	3.638502000	-2.141871000
C	-1.868959000	2.745659000	0.522252000
H	-2.046902000	3.764817000	0.912936000
H	6.085059000	-1.804190000	-0.201148000
H	3.357853000	1.440488000	0.619329000
O	-3.902111000	0.702886000	1.445336000
O	-3.017748000	2.303059000	-0.087411000
H	-3.608755000	1.440295000	0.718117000
H	-1.672258000	2.105869000	1.399473000
O	-2.726492000	0.194765000	1.960105000
H	-2.585290000	-0.613392000	1.422807000
H	1.169826000	1.382390000	1.675660000

MXI TS(OH) CH_3O˙

E = -1165.93318516 Ha

C	4.744205000	-0.289859000	0.358683000
N	1.337379000	-2.504264000	-0.277395000
C	0.435944000	-1.490540000	-0.149955000
C	1.057022000	-0.284127000	0.138187000
C	4.901053000	-1.692422000	0.118296000
C	3.824220000	-2.497962000	-0.111382000
C	2.521266000	-1.940483000	-0.093651000
N	2.401569000	-0.574220000	0.158445000
C	3.489372000	0.238860000	0.363552000
H	-1.395321000	0.148094000	-1.312644000
H	3.918305000	-3.559304000	-0.308279000
C	5.951798000	0.581520000	0.574106000
H	6.623120000	0.539756000	-0.289736000
H	5.666239000	1.624955000	0.728219000
H	6.522194000	0.252421000	1.449048000
C	-1.011656000	-1.711901000	-0.291650000
C	-1.596193000	-2.889710000	0.187063000
C	-2.966867000	-3.087370000	0.081949000
C	-3.795423000	-2.126361000	-0.509249000
C	-3.204814000	-0.960696000	-1.000668000
C	-1.831157000	-0.757967000	-0.902329000
H	-0.958468000	-3.640060000	0.644267000
H	-3.408082000	-4.003857000	0.466704000
H	-5.665542000	-2.943941000	0.198351000
H	-3.823650000	-0.200060000	-1.471316000

C	-5.278505000	-2.361691000	-0.642748000
H	-5.827739000	-1.417254000	-0.686904000
H	-5.505100000	-2.918679000	-1.558863000
C	0.481164000	1.017986000	0.571879000
H	-0.576681000	0.848640000	0.782333000
H	0.952843000	1.350383000	1.510586000
C	0.660370000	2.141746000	-0.448846000
H	-1.131080000	4.108113000	-2.066032000
H	0.649563000	4.016484000	-2.066322000
N	-0.248273000	3.178178000	-0.397427000
O	1.589517000	2.134083000	-1.234887000
C	-0.230574000	4.187374000	-1.449573000
H	-0.181268000	5.187679000	-1.009541000
C	-1.413495000	3.135987000	0.450807000
H	-1.815296000	4.152844000	0.523881000
H	5.904575000	-2.108436000	0.107278000
H	3.279250000	1.295730000	0.474633000
O	-3.732466000	1.896985000	1.586138000
O	-2.324088000	2.255710000	-0.150977000
H	-3.280841000	2.056285000	0.583391000
H	-1.145504000	2.793463000	1.457539000
C	-3.148390000	0.780573000	2.199213000
H	-3.779318000	0.558509000	3.069338000
H	-3.116182000	-0.096438000	1.544144000
H	-2.140502000	1.004841000	2.580276000