Supplementary Information for "A Computational Study of Hydrogen Shifts and Ring-Opening Mechanisms in α-pinene Ozonolysis Products" by Theo Kurtén, Matti P. Rissanen, Kasper Mackeprang, Joel A. Thornton, Noora Hyttinen, Solvejg Jørgensen, Mikael Ehn and Henrik G. Kjaergaard

Section S1 describes the formation mechanisms of the first-generation peroxy radicals encountered in α-pinene ozonolysis. Section S2 contains the parameters used in the MESMER calculations. Section S3 describes the background for the estimates of experimental HO_2 and RO_2 concentrations. Section S4 contains the kinetic parameters for the studied H-shifts. Section S5 contains absolute energetics for all the studied species, and Section S6 contains their Cartesian co-ordinates.

S1. Formation of peroxy radicals in α-pinene ozonolysis

The attack of ozone on the C=C double bond of α-pinene leads to a primary ozonide, which rapidly decomposes, yielding a mixture of four possible carbonyl-substituted Criegee intermediates: carbonyl oxides with mixed zwitterionic and biradical character. Especially for endocyclic alkenes such as α-pinene, the Criegee intermediates are formed with a large excess of energy (76-78 kcal/mol compared to the α-pinene and O_3 reactants at the F12 level).

The fourfold branching of the decomposition channel is caused by the asymmetric position of the double bond, leading to two different positions for the carbonyl oxide moiety (carbon atoms 2 and 3 in Figure 1), and two possible orientations of the terminal oxygen atom for each structural isomer, giving the syn and anti Criegee intermediates. Three of the four Criegee intermediates can undergo a 1,4 H-shift (see Figure S1) to form a vinyl hydroperoxide ($R_1R_2C=CR_3$-OOH, where R_1, R_2 and R_3 are arbitrary functional groups), which will rapidly decompose, forming OH and vinoxy radicals (with the dominant resonance structure $R_1R_2C\bullet$-CR_3=O). The fourth Criegee intermediate decomposes via a dioxirane channel that is not believed to lead to peroxy radical formation, and is thus not discussed further here. In atmospheric conditions, the vinoxy radicals behave like alkyl radicals, and rapidly combine with O_2, yielding the initial peroxy radicals (RO_2). In the case of the vinoxy radical with the planar C• radical center located on the cyclobutyl ring (carbon atom number 1 in Figure 1), O_2 addition can occur from two directions, leading to two different RO_2 isomers as shown in Figure S1.

To verify that all four possible peroxy radicals can form in α-pinene ozonolysis, we computed the transition states for the three Criegee intermediate 1,4 H-shift reactions possible in the α-pinene + O_3 system. The results are summarized in Figure S1 (with energetic and structural data given in sections S5 and S6). The zero-point corrected barriers for the three Criegee intermediate H-shifts are all remarkably similar; between 15.4 and 17.3 kcal/mol. Given that the Criegee intermediates are formed with several tens of kcal/mol of excess energy, it is thus clear that all three 1,4 H-shifts can and will happen, and all three vinylhydroperoxides will form in appreciable amounts. We did not explicitly study the vinylhydroperoxide dissociation reaction, or the O_2 addition to the vinoxy radical, as these likely require a multi-reference configuration interaction (MRCI) level treatment, which is impossible for systems of this size. On the other hand, the sole reaction channels for vinylhydroperoxides and vinoxy radicals in atmospheric conditions are expected to be dissociation and O_2 addition, respectively. Thus, the exact energetic details of these processes are of lesser importance to this study.

Given the large excess energy of the Criegee intermediates, an interesting question is whether they could undergo other types of H-shifts in addition to the 1,4 H-shift forming the vinylhydroperoxides. We attempted to search for transition states for 1,5 and 1,6 H-shifts of the α-pinene - derived Criegee Intermediates, but did not find any. This is unsurprising given the exotic electronic structure that products of such reactions would need to have.

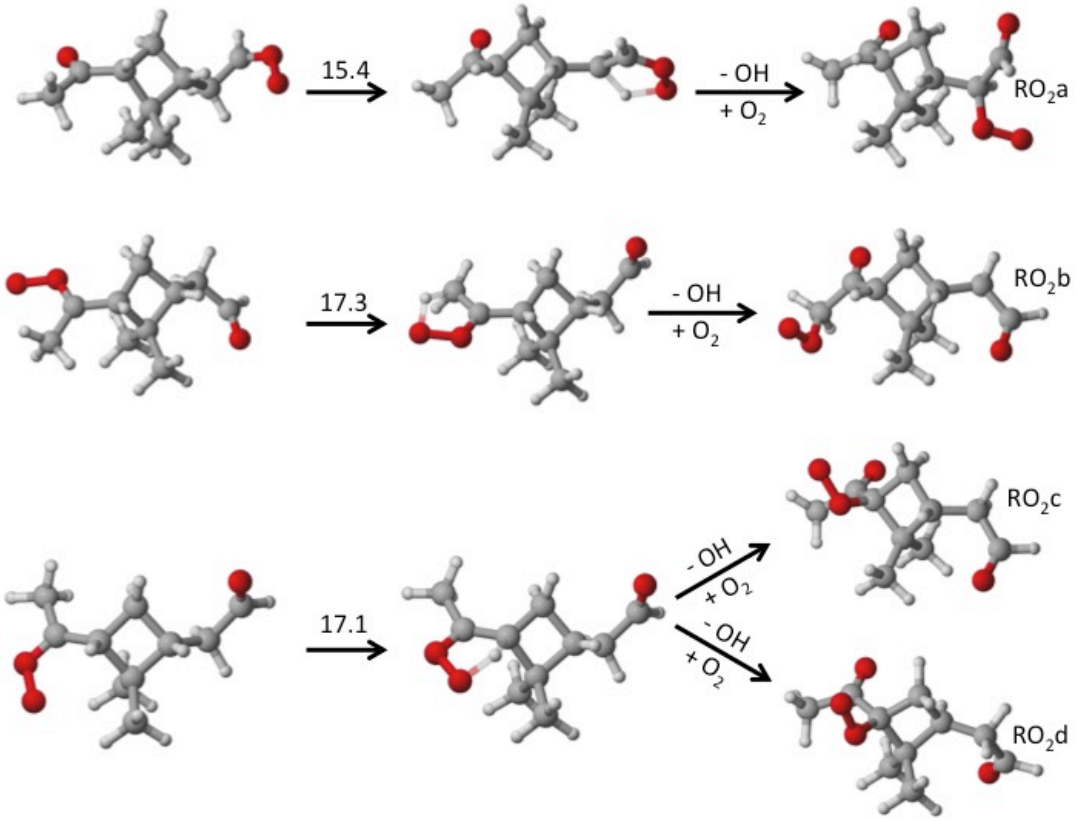

Figure S1: α-pinene ozonolysis yields four different Criegee intermediates. Three of these (shown in the left column) can undergo 1,4 H-shifts, followed by O_2 addition and OH loss to form four different peroxy radicals shown in the right column, and labeled RO_2a through RO_2d. The transition states for these H-shifts are shown in the middle column, along with their relative zero-point corrected barriers in kcal/mol at the F12 level. The vinylhydroperoxides formed by the H-shifts will dissociate to form OH and vinoxy radicals. The latter will subsequently add O_2, yielding the peroxy radicals. Color coding: gray = carbon, red = oxygen, white = hydrogen.

S2. Parameters used in the MESMER simulations.

The effect of chemical activation on the rates of the H-shifts of peroxy radical RO_2a was qualitatively estimated with the MESMER program by comparing the formation rate of H-shift products (more precisely, the time at which half of the RO_2a intermediates were converted into "QOOH" products, if the reverse reaction is ignored) with the transition state theory prediction (equation 1). Peroxy radicals were formed from the reaction of vinoxy radicals with O_2, which liberates 21.3 kcal/mol of energy at the F12 level. The vinoxy radicals were assumed to be thermalized. The Lennard-Jones (L-J) parameters of the bath gas (assumed to be nitrogen) was set to the default values of the program; ε/k_b = 48 K and σ = 3.9 Å. The L-J parameters of RO_2a were set to ε/k_b = 600 K and σ = 6.5 Å, where k_b is the Boltzmann constant (test calculations indicate that the relative effect of chemical activation is not particularly sensitive to the precise L-J parameter values used). The average collisional activation/deactivation energy transfer of all the molecules (using the exponential down energy transfer – model) was set to 225 cm^{-1} per collision, and the energy grain size was 50 cm^{-1}. The span of the energy grains is set to 25 k_bT above the highest stationary point. The vinoxy radical + O_2 reaction was modeled with an Arrhenius pre-exponential factor of 6.0×10^{-12} cm^3 $molecule^{-1}$ s^{-1}, an activation energy of 0, and a modified Arrhehius parameter of -0.5. The O_2 partial pressure was set to 0.2 atm, the total pressure was to 1 atm (or 10^{-20} torr for the low-pressure simulation), and the temperature to 298 K.

S3. Estimating the HO_2 and RO_2 concentrations in the experiments of Ehn et al. and Rissanen et al. (references 12, 13 and 17 in the main article).

In order to test the likelihood of bimolecular reaction steps forming alkoxy radicals, a simplified kinetic simulation was set up. As the complete reaction mechanism of the α-pinene + O_3 system contains a high number of intermediate species with multiple unknown or at best poorly known kinetic parameters, a simplified mechanism had to be used, with

rate coefficients lumped together for each reaction class. The peroxy radical rate coefficients used were $k(RO_2 + RO_2) = 4 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} [1] and $k(RO_2 + HO_2) = 1.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} [2]. For the unimolecular dissociation channels, reaction rates on the order of 0.01 to 0.3 s^{-1} were applied. For all the reactive species, a diffusion-limited wall loss rate was estimated, resulting in a wall loss of around 0.03 s^{-1}. All the rate coefficients in the simulation were varied by over a factor of 50 to assess the sensitivity of the simulation toward the parameters used. With these assumptions, the calculated peroxy radical concentrations were seen to vary between $[RO_2] = 2\text{-}50 \times 10^{10}$ cm^{-3}, and $[HO_2] = 1\text{-}20 \times 10^{10}$ cm^{-3}, and were generally at the lower end of the range. The most sensitive parameters in the simulation were observed to be the rate coefficients of the $RO_2 + HO_2$ and $RO_2 + RO_2$ reactions, which is not surprising but slightly disappointing, as these are the rate coefficients that likely vary the most between isomeric reactants, and thus are difficult to account for reliably. It should be emphasized that this was a highly simplified presentation of the true complexity of the system investigated, and should be taken only as a first estimate of these reactant concentrations.

References for section S3:

[1] Shallcross, D. E.; Raventos-Duran, M. T.; Bardwell, M. W.; Bacak, A.; Solman, Z.; Percival, C. J. A semi-empirical correlation for the rate coefficients for cross- and self-reactions of peroxy radicals in the gas-phase. Atmos. Environ. 2005, 39, 763.

[2] Le Crane, J-.P.; Rayez, M. T.; Rayez, J. C.; Villenave, E. A reinvestigation of the kinetics and the mechanism of the $CH_3C(O)O_2 + HO_2$ reaction using both experimental and theoretical approaches. Phys. Chem. Chem. Phys. 2006, 8, 2163.

S4. Kinetic data for the H-shift reactions.

Forward energy barriers (E_F), reverse energy barriers (E_R), wavenumbers of the imaginary vibrational modes (ν_i), Eckart tunneling corrections (κ), forward rate constants (k_F) and reverse rate constants (k_R) are given in Table S1. The energy barriers are computed using the ROHF-ROCCSD(T)-F12a/VDZ-F12 method at the ωB97XD/aug-cc-pVTZ geometries, and include zero-point vibrational energies computed at the latter level. The forward and reverse rate constants include the tunneling corrections.

Reaction	E_F kcal mol^{-1}	E_R kcal mol^{-1}	ν_i cm^{-1}	κ	k_F s^{-1}	k_R s^{-1}
ROOa → Tsa3 →Pa3	20.78	19.84	1871i	3.76×10^2	2.88×10^{-1}	2.26
ROOa → Tsa4 →Pa4	25.33	14.03	1869i	1.83×10^2	4.17×10^{-5}	8.08×10^4
ROOa → Tsa5 →Pa5	30.70	18.82	2158i	4.42×10^3	3.02×10^{-7}	4.12×10^1
ROOb → Tsb1 →Pb1	22.24	19.15	2002i	1.01×10^3	2.06×10^{-2}	8.44
ROOb → Tsb2 →Pb2	22.76	22.06	1821i	3.63×10^2	1.45×10^{-3}	4.81×10^{-3}
ROOb → Tsb3 →Pb3	28.33	15.77	1967i	5.03×10^2	3.94×10^{-7}	7.86×10^2
ROOc → Tsc1 →Pc1	31.61	20.52	1972i	1.58×10^3	7.68×10^{-8}	1.87
ROOc → Tsc3 →Pc3	63.09	60.96	2328i	7.26×10^8	5.68×10^{-26}	7.35×10^{-25}
ROOc → Tsc4 →Pc4	34.69	20.88	2372i	4.92×10^4	9.26×10^{-9}	1.21×10^2
ROOd → Tsd1 →Pd1	27.90	24.38	2295i	5.11×10^4	2.32×10^{-4}	4.09×10^{-2}
ROOd → Tsd2 →Pd2	21.17	18.49	1856i	2.99×10^2	1.37×10^{-1}	1.21×10^1
ROOd → Tsd4 →Pd4	35.57	21.02	2266i	2.28×10^4	1.63×10^{-9}	1.07×10^2

Table S1. Reaction rate data.

S5. Absolute energetic data

Absolute energetic data for all studied species are given in Table S2.

	E_{elec}(DFT)	ZPE	H_{therm}	G_{therm}	E_{elec} (F12)
reactant molecules					
alpha-pinene	-390.680241	0.237267	0.247945	0.203615	-390.067896
O_3	-225.426363	0.007812	0.011693	-0.015256	-225.209218
O_2	-150.334300	0.003882	0.007188	-0.016068	-150.177367
Criegee Intermediate (CI) to vinylhydroperoxide (VHP) reactions: see Figure S1					
primary CI1	-616.241006	0.247382	0.262530	0.205867	-615.400760
CI1 to VHP TS	-616.212953	0.242741	0.257448	0.201728	-615.371498
secondary CI2	-616.244416	0.246696	0.261773	0.205852	-615.403358
CI2 to VHP TS	-616.213439	0.242769	0.257278	0.201722	-615.371854
seondary CI3	-616.242456	0.246578	0.261696	0.205815	-615.401758
CI3 to VHP TS	-616.210748	0.242083	0.256991	0.201451	-615.370049
RO_2a reactions: see Figure 4					
RO_2a reactant	-690.869729	0.238799	0.255273	0.194699	-689.951946
TSa3	-690.831486	0.234396	0.250060	0.191746	-689.914424
TSa4	-690.823077	0.232914	0.248322	0.190688	-689.905699
TSa5	-690.813231	0.232587	0.248623	0.189449	-689.896807
Pa2	-690.852251	0.238459	0.254516	0.195698	-689.939283
Pa3	-690.863176	0.238750	0.255453	0.195099	-689.950403
Pa4	-690.846973	0.237683	0.253845	0.195760	-689.932825
Pa5	-690.845996	0.236460	0.253796	0.191094	-689.930665
RO_2b reactions: see Figure 5					
RO_2b reactant	-690.866544	0.239969	0.255952	0.195935	-689.947601
TSb1	-690.823406	0.234146	0.249346	0.192667	-689.906340
TSb2	-690.829344	0.235323	0.250118	0.194547	-689.906685
TSb3	-690.814207	0.233815	0.248996	0.192219	-689.896299
Pb1	-690.859913	0.239318	0.255421	0.196035	-689.942025
Pb2	-690.860440	0.240350	0.256431	0.196326	-689.946863
Pb3	-690.839752	0.237679	0.253905	0.193840	-689.925297
RO_2c reactions: see Figure 6					
RO_2c reactant	-690.873910	0.238720	0.254888	0.196108	-689.956838
TSc1	-690.813894	0.231989	0.248018	0.189207	-689.899728
TSc3	-690.764134	0.233793	0.249229	0.192553	-689.851371
TSc4	-690.809872	0.232148	0.248024	0.189703	-689.894982
Pc1	-690.849774	0.235997	0.253146	0.191760	-689.936440
Pc3	-690.864484	0.238353	0.255110	0.194764	-689.953078
Pc4	-690.844359	0.236489	0.253238	0.193846	-689.932597
RO_2d reactions: see Figure 7					
RO_2d reactant	-690.874480	0.238695	0.254890	0.196114	-689.957478
TSd1	-690.822721	0.232502	0.247896	0.191390	-689.906828

TSd2	-690.838229	0.233583	0.248939	0.192320	-689.918627
TSd4	-690.809704	0.232178	0.248156	0.189280	-689.894279
Pd1	-690.864676	0.237606	0.254276	0.194304	-689.950790
Pd2	-690.864094	0.238464	0.255131	0.195830	-689.952966
Pd4	-690.843286	0.235961	0.251488	0.193706	-689.931563
Criegee Intermediate ring opening: see Figure 9					
CI2 ring-opening TS	-616.188331	0.241904	0.257828	0.199762	-615.351847
CI3 ring-opening TS	-616.186137	0.242054	0.258145	0.199211	-615.350305
CI2 ring-opening prod.	-616.195074	0.242065	0.259019	0.197641	-
CI3 ring-opening prod.	-616.192842	0.242032	0.259301	0.196332	-
Vinoxy radical ring opening: see Figure 10					
reactant	-540.504244	0.229903	0.244187	0.188842	-539.735682
TS	-540.478606	0.227338	0.242083	0.185763	-539.710451
product	-540.494924	0.227346	0.243323	0.182866	-539.728760

Table S2. Absolute energetics of all species, in Hartree. E_{elec}(DFT) denotest the electronic energy, ZPE the vibrational zero-point energy, H_{therm} the thermal contribution to the enthalpy and G_{herm} the thermal contribution to the Gibbs free energy (at 298.15 K and 1 atm reference pressure), all computed at the ωB97XD/aug-cc-pVTZ level, using tight optimization criteria and the ultrafine integration grid. E_{elec} (F12) denotes the ROHF-ROCCSD(T)-F12a/VDZ-F12 electronic energy computed at the ωB97XD/aug-cc-pVTZ geometry. CI2 denotes the secondary Criegee Intermediate with the OO group pointing toward CH3 (middle row in Figure S1), while CI3 denotes the secondary Criegee Intermediate with the OO group pointing toward the cyclobutyl ring (bottom row in Figure S1).

S6. Cartesian co-ordinates of all studied species, at the ωB97XD/aug-cc-pVTZ level, using tight optimization criteria and the ultrafine integration grid.

α-pinene

C	1.43460	-0.27927	-0.09036
C	1.50416	0.90639	0.50670
H	2.41188	1.23800	0.99712
C	0.29123	1.80080	0.53629
H	0.52720	2.77547	0.09907
H	-0.00412	1.99672	1.57204
C	-0.86368	1.15695	-0.23498
H	-1.74392	1.80053	-0.25666
C	-0.31659	0.61223	-1.57465
H	0.47845	1.18004	-2.05489
H	-1.09837	0.40074	-2.29792
C	0.12312	-0.63042	-0.75881
H	0.14691	-1.60398	-1.24888
C	-1.07541	-0.32675	0.20469
C	2.55142	-1.26958	-0.14449
H	3.44569	-0.89602	0.35287
H	2.80633	-1.51293	-1.17902
H	2.25581	-2.20650	0.33507
C	-2.39145	-0.89832	-0.31804
H	-2.56839	-0.68734	-1.37077
H	-3.22980	-0.48549	0.24699
H	-2.40857	-1.98255	-0.19010
C	-0.95664	-0.68323	1.67770
H	-0.02293	-0.34795	2.12195
H	-1.01999	-1.76542	1.81072
H	-1.78075	-0.23615	2.23810

O_2

O	0.00000	0.00000	0.59800
O	0.00000	0.00000	-0.59800

O_3

O	0.00000	0.00000	0.42509
O	0.00000	1.06284	-0.21255
O	0.00000	-1.06284	-0.21255

Criegee Intermediate 1 (primary)

C	-0.52167	0.79039	0.19673
C	0.74115	-0.03723	-0.17917
C	-1.32229	-0.19616	-0.73568
C	-0.16292	-1.19459	-0.63717
H	0.11617	-1.72398	-1.54524
H	-0.35536	-1.92021	0.15340
C	-0.49325	2.24657	-0.22606
H	0.24714	2.79843	0.35619
H	-1.46256	2.72429	-0.06787
H	-0.23039	2.34659	-1.27939
C	-0.91710	0.65978	1.66229
H	-0.19307	1.17172	2.29795
H	-0.98440	-0.37925	1.98490
H	-1.89022	1.12045	1.84047
C	1.80182	-0.28806	0.90025
C	-2.69052	-0.61765	-0.26774
O	-2.88057	-1.66700	0.29822
C	-3.80503	0.36677	-0.51934
H	-3.51103	1.36456	-0.18911
H	-4.71105	0.05315	-0.00870
H	-3.99382	0.43167	-1.59272
C	2.94372	-1.02615	0.34379
H	3.12221	-2.08405	0.49734
O	3.81406	-0.49068	-0.38143
O	3.69314	0.82912	-0.65330
H	2.18086	0.67664	1.24913
H	1.22910	0.43402	-1.03137
H	-1.40027	0.24471	-1.73110
H	1.38024	-0.85232	1.73069

Criegee Intermediate 2 (secondary, OO toward CH_3)

C	-0.02118	-1.24195	-1.10451
C	-0.77540	0.07966	-0.90873
C	1.28294	-0.52043	-0.71296
C	0.44138	0.62407	-0.06254
H	1.77774	-0.12220	-1.59988
H	-0.83061	0.65091	-1.83776
H	-0.07200	-1.69387	-2.09197
H	-0.31521	-1.98459	-0.36434
C	0.86849	2.04322	-0.38350
H	0.11520	2.75963	-0.04823
H	1.01250	2.17691	-1.45657
H	1.81076	2.27786	0.10967
C	0.23514	0.44502	1.43500
H	-0.48868	1.16885	1.81243
H	1.17311	0.61550	1.96523
H	-0.13003	-0.54953	1.69414
C	2.28451	-1.30715	0.10379

H	1.83919	-1.69929	1.02435
H	2.60575	-2.19817	-0.44799
C	3.53084	-0.56855	0.49648
H	4.25639	-1.16338	1.08668
O	3.77248	0.57483	0.21766
C	-2.10960	0.10366	-0.27423
C	-2.88068	1.33861	-0.06692
H	-3.86709	1.21921	-0.52148
H	-2.35988	2.20294	-0.46921
H	-3.07738	1.45197	1.00204
O	-2.56754	-0.99060	0.13887
O	-3.77848	-0.97044	0.76992

Ciregee Intermediate 3 (secondary, OO toward ring)

C	0.60111	-1.02350	-0.56803
C	-0.74476	-0.27941	-0.63468
C	1.29214	0.31951	-0.28080
C	-0.08104	0.94288	0.11321
H	1.61565	0.76302	-1.22334
H	-1.01236	0.04511	-1.64384
H	0.92120	-1.56365	-1.45449
H	0.66414	-1.69523	0.28946
C	-0.33896	2.32163	-0.46121
H	-1.35281	2.64970	-0.24597
H	-0.20594	2.32493	-1.54349
H	0.36934	3.03572	-0.03225
C	-0.37486	0.91761	1.60699
H	-1.42147	1.17219	1.77919
H	0.23792	1.65136	2.13278
H	-0.18047	-0.05837	2.05769
C	2.44162	0.36216	0.69848
H	2.70909	1.39361	0.95522
H	2.18447	-0.11033	1.65299
C	3.69532	-0.30642	0.20696
H	4.54592	-0.28235	0.91773
O	3.81550	-0.83976	-0.86215
C	-1.94478	-0.91340	-0.06408
C	-1.95817	-2.25910	0.56248
H	-1.33910	-2.25583	1.46183
H	-1.52794	-2.99406	-0.11893
H	-2.97193	-2.54691	0.82603
O	-3.05714	-0.32989	-0.09915
O	-3.10355	0.91706	-0.64950

CI-to-VHP TS 1 (primary)

C	-0.55662	0.74949	-0.16235
C	0.55422	-0.18317	-0.74228
C	-1.59603	-0.30056	-0.70416
C	-0.46936	-1.33677	-0.77592
H	-0.45136	-1.99992	-1.63789
H	-0.44406	-1.93813	0.13203
C	-0.62036	2.14103	-0.76120
H	0.26342	2.71646	-0.47792
H	-1.49667	2.68737	-0.40614
H	-0.66457	2.10200	-1.85066
C	-0.53417	0.81718	1.35942
H	0.33771	1.37606	1.70055
H	-0.50678	-0.17113	1.81838

H	-1.42211	1.32852	1.73513
C	1.84008	-0.33095	0.01677
C	-2.79880	-0.58528	0.15687
O	-2.85936	-1.55336	0.87513
C	-3.91331	0.42924	0.08972
H	-3.51596	1.43742	0.21909
H	-4.66190	0.22076	0.84874
H	-4.37510	0.39486	-0.89901
C	3.03095	-0.55548	-0.68191
H	3.15781	-0.78391	-1.73452
O	4.13303	-0.23911	-0.09583
O	3.85221	0.26555	1.16254
H	2.55388	0.50980	0.75446
H	0.76487	0.14730	-1.76255
H	-1.93075	0.01193	-1.69565
H	1.76474	-0.89236	0.95140

CI-to-VHP TS 2 (secondary, OO toward CH_3)

C	0.60129	-1.05041	-0.42238
C	-0.62655	-0.15216	-0.65782
C	1.45868	0.22269	-0.30326
C	0.16716	1.03714	0.00325
H	1.82199	0.50020	-1.29381
H	-0.75350	0.06262	-1.71888
H	0.85741	-1.75700	-1.20595
H	0.54196	-1.58052	0.52820
C	0.02822	2.37341	-0.69976
H	-0.98195	2.77005	-0.58454
H	0.23665	2.28158	-1.76617
H	0.72422	3.10280	-0.27985
C	-0.12125	1.18233	1.49166
H	-1.12315	1.58451	1.64844
H	0.58856	1.87374	1.94799
H	-0.06119	0.23371	2.02578
C	2.61539	0.24870	0.66793
H	2.99793	1.26640	0.80820
H	2.31781	-0.08457	1.66782
C	3.78393	-0.60165	0.25104
H	4.63204	-0.61112	0.96467
O	3.84092	-1.23698	-0.76604
C	-1.94304	-0.50256	-0.08151
C	-2.28932	-1.45271	0.89400
H	-2.81303	-1.06041	1.76520
H	-1.53981	-2.19246	1.13780
O	-2.94642	0.07272	-0.66763
O	-4.14511	-0.42649	-0.16987
H	-3.48822	-1.49222	0.32443

CI-to-VHP TS 3 (secondary, OO toward ring)

C	0.51527	-1.05065	-0.46531
C	-0.80342	-0.28691	-0.39840
C	1.26889	0.27509	-0.26724
C	-0.04709	0.97271	0.18925
H	1.55378	0.67330	-1.24136
H	-1.60202	0.38975	-1.23939
H	0.73065	-1.58890	-1.38532
H	0.65633	-1.73685	0.37551
C	-0.27005	2.33424	-0.44305

H	-1.22401	2.76563	-0.14771
H	-0.24757	2.27101	-1.53133
H	0.53008	3.00958	-0.12894
C	-0.22800	1.05257	1.70070
H	-1.24930	1.35758	1.93170
H	0.44856	1.79005	2.13793
H	-0.04380	0.09287	2.18694
C	2.47402	0.30507	0.64357
H	2.79053	1.33293	0.85648
H	2.25908	-0.13463	1.62370
C	3.67595	-0.41558	0.09940
H	4.56224	-0.41104	0.76599
O	3.72366	-0.96796	-0.96558
C	-1.98612	-0.87459	0.06403
C	-2.16405	-2.23695	0.62304
H	-1.64772	-2.31963	1.58026
H	-1.71346	-2.96506	-0.05234
H	-3.21781	-2.47156	0.75004
O	-3.08822	-0.24559	-0.21103
O	-2.78518	0.90042	-0.94315

RO_2 H-shift reactions

RO_2a

C	-1.56144300	0.36140300	-0.66909400
C	-0.36368000	1.31392800	-0.58178300
C	-0.62491500	-0.82357000	-0.22280900
C	0.56723800	0.08946000	-0.64714000
H	-1.87807600	0.19331800	-1.70029200
H	0.83322000	-0.13316600	-1.68321500
H	-0.25473000	2.06262700	-1.36066800
H	-0.33267600	1.81003500	0.38642600
C	-0.76518300	-2.11846300	-1.00015500
H	-0.73021200	-1.93963300	-2.07567900
H	-1.71149200	-2.61238400	-0.77065500
H	0.04161400	-2.80685800	-0.74434100
C	-0.68120400	-1.08154900	1.27741300
H	-0.62319000	-0.16238700	1.86052900
H	0.13399100	-1.73907100	1.58172100
H	-1.61709500	-1.57547700	1.54296300
C	1.83037700	0.11105900	0.18529600
H	1.62401500	0.29269700	1.24010800
C	-2.77254100	0.63417000	0.18599400
O	2.43851300	-1.19545700	0.06977700
O	3.53843400	-1.26784200	0.76701900
C	2.80226200	1.16405600	-0.31896000
H	3.63799400	0.77800500	-0.93305300
O	2.65736600	2.33074500	-0.09913800
C	-3.96528400	-0.25611800	-0.05700200
H	-4.72393400	-0.08888900	0.70216000
H	-3.66130400	-1.30438800	-0.06176100
H	-4.38132300	-0.04249900	-1.04353900
O	-2.77813400	1.49528200	1.03093300

TSa3

C	1.49226000	-0.31217900	-0.71272400
C	0.30172400	-1.27175900	-0.59641800
C	0.61996800	0.82219400	-0.05416100
C	-0.61734900	-0.04890600	-0.43512400
H	1.70090100	-0.04178600	-1.74938600
H	-1.00318800	0.28273600	-1.39902100
H	0.10817500	-1.93662700	-1.43336600
H	0.37727900	-1.86437900	0.31485500
C	0.67533600	2.18551800	-0.71596600
H	0.53022400	2.10764000	-1.79405400
H	1.63741900	2.67003000	-0.53663900
H	-0.10694800	2.83226600	-0.31638100
C	0.84327400	0.93929200	1.44819400
H	0.84640600	-0.03032000	1.94685400
H	0.06900500	1.56092600	1.89895500
H	1.80519200	1.41174300	1.65317500
C	-1.76785300	-0.13759100	0.54920600
H	-1.45199500	-0.49084400	1.53089900
C	2.78234500	-0.66871500	-0.01990500
O	-2.48355200	1.05470700	0.73955700
O	-3.22732500	1.25179200	-0.41506100
C	-2.86521500	-1.04912300	-0.07481100
O	-2.92697100	-2.21252200	-0.18365000
H	-3.53730300	-0.00240600	-0.50939200
C	3.95032700	0.24509600	-0.29225800
H	4.77939800	0.00837400	0.36838700
H	3.65305200	1.28774400	-0.16697500
H	4.26556200	0.12834900	-1.33101800
O	2.86758700	-1.61227600	0.72751800

TSa4

C	-1.35028000	0.44359200	0.79068400
C	-0.43293000	-0.57775200	1.43114400
C	-0.09576300	1.12350900	0.12206100
C	0.80863900	0.13433200	0.93636200
H	-1.78278700	1.10681000	1.54434500
H	1.36366500	0.64585600	1.72464900
H	-0.28807300	-1.74269200	0.76033400
H	-0.55106800	-0.92544900	2.45403800
C	0.09414400	2.57140100	0.54444700
H	0.05732700	2.67781300	1.63001900
H	-0.69068600	3.19526500	0.11547500
H	1.06153400	2.94166000	0.20175600
C	-0.04734300	1.01103300	-1.39479800
H	-0.17975100	-0.01125000	-1.74475500
H	0.90755700	1.37973800	-1.77282800
H	-0.83346900	1.62584300	-1.83169300
C	1.80851800	-0.79285800	0.22805900
H	2.35642900	-1.35441100	0.99445400
C	-2.50455300	0.07148000	-0.12528100
O	1.14042400	-1.70776300	-0.61572900
O	0.36568500	-2.53957300	0.17780800
C	2.82440200	-0.05574400	-0.61774400
H	2.99466500	-0.47459400	-1.62649400
O	3.42137500	0.90322000	-0.21723100
C	-2.78503800	-1.38085100	-0.38726400

H	-3.68759400	-1.48095800	-0.98274800
H	-2.88814800	-1.92541400	0.55294800
H	-1.93947200	-1.82915700	-0.91290500
O	-3.15484800	0.95437700	-0.62892500

TSa5

C	-1.37204500	0.07556300	-0.75131900
C	-0.14711500	0.99315800	-0.88599700
C	-0.56373400	-0.82024500	0.26625400
C	0.68440000	-0.09096800	-0.24614400
H	-1.56314100	-0.49871100	-1.65882700
H	1.35146400	-0.86274700	-1.08734200
H	0.13687100	1.32304700	-1.88357900
H	-0.23446700	1.87581500	-0.24868900
C	-0.62256600	-2.32057600	0.03833500
H	-0.42366200	-2.57022200	-1.00370000
H	-1.60659300	-2.71133600	0.30393600
H	0.12197800	-2.82889600	0.65166100
C	-0.84697000	-0.47662000	1.72782500
H	-0.79712500	0.59597200	1.91557600
H	-0.12676100	-0.97727200	2.37582800
H	-1.84166300	-0.82124500	2.01458300
C	1.99445400	0.06173200	0.52668400
H	1.84507500	0.15743300	1.60495100
C	-2.66475100	0.66765400	-0.24996600
O	2.67194300	-1.15970300	0.29967400
O	2.49508600	-1.36556000	-1.07371000
C	2.80659900	1.25049900	0.04073800
H	3.72201400	0.98696200	-0.52014900
O	2.49078700	2.38493700	0.26387000
C	-3.85897700	-0.25246500	-0.26877800
H	-4.69195000	0.19674000	0.26426500
H	-3.60346200	-1.21741300	0.17259400
H	-4.14895300	-0.44453300	-1.30375100
O	-2.73224000	1.79907900	0.16227300

Pa3

C	-1.57339000	0.38024600	-0.64626700
C	-0.39056700	1.34843700	-0.53029400
C	-0.61222500	-0.80754400	-0.26481100
C	0.55777700	0.14430100	-0.66452200
H	-1.89943900	0.25374400	-1.68049400
H	0.81583800	-0.02814100	-1.71090200
H	-0.30570900	2.13386400	-1.27536500
H	-0.35811500	1.79833500	0.46068900
C	-0.73753700	-2.06959500	-1.09607500
H	-0.72344700	-1.84336900	-2.16316600
H	-1.66870900	-2.59486000	-0.87382000
H	0.09003600	-2.74691700	-0.88112800
C	-0.64320400	-1.13264400	1.22312100
H	-0.60348400	-0.23842800	1.84528800
H	0.19629600	-1.77692600	1.48506700
H	-1.56193800	-1.66392600	1.47680600
C	1.83018900	0.12837200	0.15769600
H	1.63322400	0.30508300	1.22009700
C	-2.77840600	0.59471800	0.23272600
O	2.42181900	-1.13253700	-0.02158700
O	3.53745400	-1.22138100	0.85322900

C	2.77449000	1.25214100	-0.30192900
O	2.58430700	2.40721400	-0.23245800
H	4.26204500	-0.95478100	0.27436700
C	-3.95362500	-0.31403500	-0.02723100
H	-4.70709300	-0.18949100	0.74520300
H	-3.62568000	-1.35410900	-0.07000700
H	-4.38555300	-0.07757200	-1.00165100
O	-2.79349000	1.42559400	1.10763100

Pa4

C	-1.37798000	0.51242300	0.81863200
C	-0.37971000	-0.19213100	1.66652900
C	-0.15563700	1.19481300	0.06052700
C	0.81156000	0.31247400	0.93265400
H	-2.00910400	1.25084200	1.32534200
H	1.48807400	0.93303300	1.53112400
H	-0.49272700	-0.90980800	2.46427300
C	-0.03688900	2.66561300	0.42874000
H	-0.08558200	2.80815800	1.50938700
H	-0.84115600	3.24588200	-0.02819900
H	0.91644400	3.06256000	0.07740500
C	-0.10305800	1.02655400	-1.45006600
H	-0.21008000	-0.01009700	-1.76106600
H	0.84956600	1.39782600	-1.83025900
H	-0.88746000	1.61844800	-1.92536900
C	1.71729100	-0.73276300	0.27424200
H	2.22306200	-1.29079400	1.07414300
C	-2.27428200	-0.34115700	-0.05001700
O	1.08572100	-1.65722200	-0.57913300
O	0.43684400	-2.64325800	0.20978200
C	2.82218800	-0.10219200	-0.55524200
H	3.16678100	-0.72200600	-1.40319100
O	3.31141700	0.96516200	-0.31000700
C	-3.44032800	0.35885500	-0.69029200
H	-3.86030800	-0.24942000	-1.48601100
H	-3.14080400	1.33592900	-1.06986800
H	-4.20279800	0.53230800	0.07243100
O	-2.07374300	-1.52279300	-0.23352500
H	-0.49474700	-2.35289900	0.13867400

Pa5

C	1.54791400	0.46909300	-0.70785200
C	0.30837600	-0.08985800	-1.43659800
C	0.69777500	0.61274000	0.62254600
C	-0.49383200	0.30219400	-0.23966700
H	1.83265700	1.45917700	-1.06548800
H	-4.33995500	1.34860500	-0.52444300
H	0.04506000	0.37908800	-2.38488400
H	0.38891600	-1.16954300	-1.59952000
C	0.71578800	1.99745000	1.25682700
H	0.49778000	2.77303500	0.52241300
H	1.69342400	2.20450700	1.69694100
H	-0.02570400	2.06306000	2.05493400
C	0.97160500	-0.46816600	1.67226900
H	1.00458500	-1.46193700	1.22703100
H	0.17931800	-0.46636800	2.42093300
H	1.92036800	-0.28646200	2.18104700
C	-1.92749400	0.21526600	0.08975600

H	-2.16063300	0.78143100	0.99804900
C	2.77704300	-0.39853200	-0.62406900
O	-2.64939900	0.70706600	-1.02900100
O	-4.03467300	0.47163300	-0.77956900
C	-2.26411500	-1.25404900	0.34093900
H	-2.43542900	-1.84238400	-0.58007400
O	-2.28372300	-1.74637900	1.43295100
C	3.99563600	0.25044200	-0.01621000
H	4.74819400	-0.49819100	0.21441000
H	3.72856500	0.81030700	0.88110400
H	4.40666600	0.96798200	-0.72963300
O	2.78579600	-1.54254200	-1.00693900

RO_2b

C	-0.67841700	0.43059400	-0.64941700
C	0.39476700	1.38368300	-1.18441500
C	0.44309700	-0.36571900	0.13203800
C	1.47631600	0.36250500	-0.78764700
H	0.32697200	1.65919600	-2.23413600
H	0.44026700	2.29188400	-0.58388200
H	-1.09604900	-0.20852100	-1.42602400
H	1.71137100	-0.29412000	-1.62612400
C	0.38931800	-1.87519500	-0.00916500
H	0.29010200	-2.16583300	-1.05571400
H	-0.45964400	-2.29013400	0.53512200
H	1.30687700	-2.31861300	0.37608700
C	0.54664000	0.03671700	1.59672800
H	0.53124400	1.11818600	1.73796100
H	1.46860200	-0.35538300	2.02838700
H	-0.28126700	-0.38505500	2.16998300
C	2.76344300	0.92069900	-0.21973900
H	3.24105300	1.58317100	-0.95118100
H	2.57909300	1.56078600	0.64989000
C	3.79760700	-0.08727600	0.18838500
H	4.73634600	0.34825300	0.58692900
O	3.67220900	-1.27950800	0.11017000
C	-1.78449700	1.02769400	0.16240400
C	-2.92052400	0.13815500	0.66532900
H	-3.87219900	0.58279300	0.38050400
H	-2.85226200	0.07519100	1.75089900
O	-1.81916600	2.18435400	0.49981300
O	-2.88097500	-1.21663400	0.20356400
O	-3.30169500	-1.31732900	-1.02676000

TSb1

C	0.53981800	-0.08299700	-0.56518200
C	-0.78167200	-0.18024600	-1.29970100
C	0.01232400	1.05745800	0.34542900
C	-1.41868900	0.65676700	-0.16056500
H	-0.78653000	0.33333800	-2.25815000
H	-1.16214400	-1.19088000	-1.43226100
H	1.62592100	0.33503100	-1.20754500
H	-2.00186300	1.50900000	-0.50688000
C	0.40707100	2.43377600	-0.17797800
H	0.19382700	2.53199300	-1.24275700
H	1.47221500	2.60906500	-0.02848700
H	-0.15296900	3.20570200	0.35227700
C	0.30989200	0.95108700	1.83179100

H	0.07661500	-0.03419800	2.23584700
H	-0.27524300	1.68692000	2.38602600
H	1.36445700	1.15637800	2.01767300
C	-2.24892500	-0.17858600	0.79179600
H	-1.73338500	-1.10328100	1.07402300
H	-2.44488000	0.34814300	1.73182900
C	-3.58447100	-0.57736700	0.22768700
H	-4.20335600	-1.20525500	0.89886700
O	-3.99325000	-0.26299700	-0.85676300
C	1.14549400	-1.29043800	0.06092900
C	2.63223400	-1.16855300	0.38270800
H	3.16958700	-1.93238100	-0.18566100
H	2.79645600	-1.32457800	1.44867000
O	0.54715400	-2.31643000	0.28115500
O	3.11349900	0.12476300	0.08857400
O	2.83045100	0.37336200	-1.25108600

TSb2

C	-0.80756400	1.08406200	0.63607800
C	0.05433400	0.37357400	1.70225900
C	0.48722400	1.51188800	-0.14584600
C	1.33733400	0.78790200	0.95200500
H	-0.04007900	0.80077500	2.69808700
H	-0.09806900	-0.69793400	1.78368100
H	-1.31276200	1.96465100	1.03712100
H	1.92137700	1.51421500	1.51783000
C	0.69664100	3.01935100	-0.13445400
H	0.62267500	3.42325300	0.87700000
H	-0.05421800	3.51276800	-0.75284400
H	1.68375800	3.27263300	-0.52713300
C	0.62055800	0.99057300	-1.56855400
H	0.37516000	-0.06654400	-1.66594200
H	1.63891100	1.14202200	-1.93130200
H	-0.05857400	1.52812900	-2.22886600
C	2.30008800	-0.31581500	0.55775100
H	3.14423200	0.06521900	-0.01987100
H	2.71538200	-0.76381200	1.46685800
C	1.74856900	-1.49664000	-0.21640100
O	2.38433600	-2.22534200	-0.89691300
C	-1.88385400	0.38919900	-0.16551100
C	-2.43801900	-0.98447800	0.21004100
H	-2.99332900	-1.35939500	-0.64988400
H	-3.12678500	-0.84807700	1.04856400
O	-2.40583700	0.97201000	-1.08425000
O	-1.51653100	-1.95172500	0.66260200
O	-0.66168700	-2.27793800	-0.36636000
H	0.48819400	-1.78163100	-0.13814600

TSb3

C	-0.75449400	0.32074500	0.34961800
C	-0.31764700	-0.94773500	-0.36260100
C	0.72078900	0.80641100	0.26457500
C	1.11326600	-0.71986900	0.08984100
H	-1.27557600	-1.84492300	-0.00911600
H	-0.47070600	-0.96405900	-1.44179200
H	-0.98338000	0.07098300	1.39087900
H	1.28682600	-1.13637500	1.08304400
C	1.24102300	1.48474500	1.51928700

H	1.04417100	0.87942900	2.40493700
H	0.75462600	2.45302800	1.65041000
H	2.31707900	1.63851300	1.45416500
C	1.02515000	1.63965600	-0.97288400
H	0.62076500	1.20127100	-1.88560000
H	2.10471500	1.74908100	-1.09102200
H	0.59034900	2.63203400	-0.87296500
C	2.21748700	-1.14593900	-0.84997900
H	2.17114700	-2.22669100	-1.02590000
H	2.10406500	-0.69414400	-1.84061100
C	3.61184100	-0.84349200	-0.38021800
H	4.41320000	-1.14340000	-1.08457100
O	3.88838800	-0.32524900	0.66694100
C	-1.99155500	0.94026800	-0.22101500
C	-3.22179200	0.02689200	-0.08787300
H	-3.53783000	-0.30192500	-1.07981000
H	-4.02751300	0.60353600	0.36702500
O	-2.07733200	2.01022400	-0.76164800
O	-3.01302100	-1.08722600	0.76061300
O	-2.42007900	-2.13355600	0.07014700

Pb1

C	-0.35723100	0.58348400	0.00259400
C	0.54810300	1.74929600	-0.19158200
C	0.76508500	-0.42788100	0.03889600
C	1.70560200	0.74448600	-0.42810700
H	0.28977600	2.43167700	-1.00092000
H	0.66647600	2.34529100	0.71891600
H	-4.26122600	0.75195900	-0.48879000
H	1.90464200	0.63113900	-1.49310500
C	0.66409000	-1.59176600	-0.94040100
H	0.38011100	-1.24630500	-1.93500000
H	-0.07461000	-2.32318100	-0.60979700
H	1.63218400	-2.08548100	-1.01550000
C	1.04296200	-0.93816300	1.45437900
H	1.08469000	-0.12909800	2.18394000
H	1.98911200	-1.48056100	1.47688100
H	0.25845800	-1.62629000	1.77006600
C	3.00720500	1.01984100	0.29184800
H	3.41359100	1.98883300	-0.01950400
H	2.86698000	1.11411900	1.37403400
C	4.09123800	0.00326500	0.07575300
H	5.05174400	0.23337100	0.57820200
O	3.97649200	-0.99617500	-0.58086800
C	-1.77787000	0.52899500	0.05890900
C	-2.45455000	-0.83188600	0.18292400
H	-1.99138900	-1.41203900	0.98396300
H	-2.33184900	-1.38496400	-0.75496100
O	-2.45261500	1.55889700	-0.00127900
O	-3.80519300	-0.73569600	0.53122700
O	-4.50449600	-0.18283700	-0.57904400

Pb2

C	-0.39964100	-0.43815600	0.86433300
C	0.52916000	-1.65049600	0.72454500
C	0.76716700	0.48283900	0.33776700
C	1.72801200	-0.68623600	0.71412200
H	0.49411900	-2.39941400	1.51184700

H	0.37797100	-2.13832000	-0.23772400
H	-0.60191000	-0.19276900	1.90885100
H	2.08491800	-0.52582200	1.73304500
C	0.98554400	1.78189200	1.08987600
H	1.03029000	1.61399500	2.16665600
H	0.18426100	2.49655000	0.88943500
H	1.92398600	2.24706300	0.78205400
C	0.68007100	0.73461800	-1.16283900
H	0.49030900	-0.17768500	-1.72811100
H	1.60702200	1.17692500	-1.52936400
H	-0.12763200	1.43278900	-1.38946700
C	2.91383000	-1.01730900	-0.17503200
H	3.39054700	-1.92904600	0.19186600
H	2.61921300	-1.17672900	-1.21529400
C	3.97148300	0.06502700	-0.11728600
O	4.47189500	0.65405500	-1.00248300
C	-1.68215400	-0.41008600	0.08967600
C	-2.61992200	0.74156400	0.41131000
H	-2.06467000	1.68234000	0.36384000
H	-2.98963700	0.62150800	1.43675100
O	-1.96109600	-1.22425400	-0.75886200
O	-3.67187500	0.87821900	-0.49649200
O	-4.53854900	-0.23833000	-0.33013400
H	-4.06309100	-0.91086200	-0.83946800

Pb3

C	0.36380600	0.78481400	-1.01044000
C	-0.36440600	-0.30896200	-1.71690000
C	-0.83176700	0.83217800	0.02797300
C	-1.60237200	-0.18271900	-0.89442000
H	3.50349100	0.15188100	1.42017900
H	-0.16813500	-0.82513000	-2.64706400
H	0.42714800	1.72255200	-1.57407400
H	-2.40394900	0.34235000	-1.42778700
C	-1.48848600	2.19574300	0.13411900
H	-1.74506700	2.58641400	-0.85192100
H	-0.81583800	2.90673400	0.61622000
H	-2.40624700	2.12503600	0.71811400
C	-0.47583800	0.30337000	1.40822800
H	0.02962000	-0.66311600	1.37652000
H	-1.37811000	0.19570400	2.01104300
H	0.18728000	1.00125500	1.91916700
C	-2.19512200	-1.45619400	-0.31250900
H	-2.47032600	-2.14717100	-1.11715800
H	-1.47227300	-2.00819100	0.29564000
C	-3.42506200	-1.24966500	0.52488800
H	-3.85939500	-2.17596400	0.95103300
O	-3.93727900	-0.18525300	0.74197000
C	1.74293100	0.55186900	-0.43974100
C	2.33036800	-0.83836200	-0.59803600
H	2.42809600	-1.06660400	-1.66261400
H	1.63303800	-1.56740900	-0.16744300
O	2.33904600	1.42250500	0.14765600
O	3.61205500	-0.96987700	-0.06274500
O	3.50947200	-0.81372200	1.34826400

RO_2c

C	-0.95225700	-0.22226800	-0.22536600

C	0.36289300	0.11671600	0.57014600
C	-0.12278900	-0.39810000	-1.49369400
C	1.15534100	-0.48415100	-0.63725200
C	0.55458400	1.61927700	0.73414300
H	-0.14418300	2.01726400	1.47156100
H	0.40017300	2.17029100	-0.19284300
H	1.56347200	1.81779100	1.09678800
C	0.53678800	-0.58432200	1.90712400
H	-0.19530400	-0.22703900	2.63406900
H	1.53492300	-0.37554000	2.28866600
H	0.42919600	-1.66299400	1.81927500
H	1.39827300	-1.52244200	-0.41113400
H	-0.39156300	-1.25159800	-2.11043500
H	-0.17190800	0.51110200	-2.09082700
C	2.38568000	0.20901300	-1.17985700
H	2.19304700	1.26407400	-1.40256300
H	2.66970100	-0.22835000	-2.14382900
C	3.60434800	0.16061300	-0.30503700
H	4.50353500	0.64536800	-0.73552400
C	-2.06930600	0.81425000	-0.20636700
C	-3.07446800	0.72113600	0.90841300
H	-2.57852700	0.49726500	1.85381400
H	-3.76545400	-0.09858600	0.70974600
H	-3.62699800	1.65365100	0.97479600
O	-2.08458600	1.69647400	-1.02558500
O	3.65492800	-0.34880000	0.78176600
O	-1.46004200	-1.49021900	0.25720600
O	-2.37320900	-1.97286100	-0.53777100

TSc1

C	1.09536400	0.26751100	-0.27421100
C	-0.14212300	-0.44447300	0.41211500
C	0.28240500	0.32720800	-1.57570200
C	-0.94081600	0.29160400	-0.66662900
C	-0.15387700	-1.96135600	0.20289100
H	0.57450400	-2.43612700	0.86073300
H	0.08477400	-2.25547800	-0.81658000
H	-1.14084700	-2.35018600	0.45615600
C	-0.41677400	-0.11581700	1.86950800
H	-1.38963700	-0.51378000	2.16234700
H	-0.40696900	0.95579300	2.05339200
H	-0.74934700	1.50957600	-0.21683000
H	0.43080600	1.20413700	-2.20052700
H	0.41580100	-0.57866400	-2.16423100
C	-2.36066300	0.02173300	-1.06825000
H	-2.45523100	-0.99663500	-1.45522700
H	-2.65379800	0.71757500	-1.85964500
C	-3.30992400	0.19401900	0.09022200
H	-3.31296900	1.20425000	0.54654400
C	2.43489300	-0.43681400	-0.22566200
C	3.36056100	-0.07927200	0.90027900
H	3.66442200	0.96389400	0.80926900
H	4.22961000	-0.73013300	0.88112100
H	2.83648100	-0.16627400	1.85349800
O	2.68901600	-1.28477000	-1.04426400
O	-4.01367100	-0.67501000	0.52363300
O	1.24981700	1.56015000	0.31126000
O	0.13066000	2.35806000	0.03312900

H	0.33156600	-0.58144400	2.51255200

TSc3

C	-0.78327200	-0.29398900	-0.12134000
C	-0.46238800	1.22608700	0.36339000
C	0.31579400	-0.11569800	-1.14169300
C	0.96826500	0.75885100	-0.06730500
C	-1.16078500	2.29314500	-0.46230800
H	-2.22650200	2.32083600	-0.23306300
H	-1.06647100	2.14990300	-1.53510800
H	-0.74072900	3.26730000	-0.20714400
C	-0.63900300	1.50578100	1.84385700
H	-1.69609500	1.61381600	2.09240000
H	-0.14380000	2.44203500	2.10735400
H	-0.22219900	0.70944700	2.45792400
H	1.09884100	0.14204600	0.80742100
H	0.81209300	-1.01034900	-1.50170800
H	-0.02725200	0.47642100	-1.98401200
C	2.43065200	1.07698300	-0.28227700
H	2.89252300	1.68214700	0.49998800
H	2.72699300	1.45965600	-1.25852500
C	2.98817600	-0.37523200	-0.10657800
C	-2.20375300	-0.62821900	-0.51623800
C	-3.03380900	-1.40428500	0.46521200
H	-2.63621200	-2.41548900	0.55581100
H	-4.06635500	-1.43379500	0.12971500
H	-2.96292900	-0.95631500	1.45765500
O	-2.63290700	-0.23155400	-1.57210400
O	4.06667700	-0.79059200	-0.30825500
O	-0.29694100	-1.22053300	0.90064100
O	0.84016900	-1.94391400	0.53297700
H	1.92284100	-1.21546000	0.33690100

TSc4

C	0.99656700	0.21645500	-0.01600200
C	-0.33446300	-0.44265900	0.49181600
C	0.18222500	0.92608200	-1.09343400
C	-1.10971700	0.65039200	-0.34866900
C	-0.52307100	-1.85346400	-0.04464600
H	0.15218100	-2.54523400	0.46032400
H	-0.32630000	-1.92970000	-1.11322600
H	-1.54310500	-2.18497300	0.15298800
C	-0.55571700	-0.39894400	1.99422100
H	-1.57440000	-0.71152700	2.21772400
H	-0.40826200	0.60234900	2.39138500
H	-1.36233900	1.47076200	0.32512800
H	0.29513700	0.65124600	-2.13706500
C	-2.31741200	0.28426100	-1.18307900
H	-2.11404400	-0.56596000	-1.84213700
H	-2.57236100	1.10816100	-1.85902000
C	-3.56111300	-0.04342600	-0.40756000
H	-4.44128400	-0.29848800	-1.03061800
C	2.16619000	-0.65885600	-0.43616600
C	3.28145600	-0.81015500	0.55669400
H	3.78455300	0.14940900	0.68035300
H	3.98384600	-1.56225400	0.20991500
H	2.88075800	-1.07831300	1.53567700
O	2.15678300	-1.20931400	-1.50947100

O	-3.64625600	-0.04227800	0.79012700
O	1.38259200	1.26672500	0.86385200
O	1.72171000	2.32218600	0.01133400
H	0.13630500	-1.07512000	2.50018600
H	0.84099400	2.05298400	-0.81740400

Pc1

C	0.80730600	0.29839000	-0.07370500
C	-0.21928400	-0.63149300	0.70285700
C	-0.29214700	0.63497900	-1.10416900
C	-1.11848600	-0.44220400	-0.48751300
C	0.21193500	-2.06500700	0.99982400
H	0.95384700	-2.09639900	1.79926500
H	0.61895300	-2.56090800	0.12009600
H	-0.65388300	-2.63795300	1.33634500
C	-0.77223600	0.02269000	1.97455900
H	-1.61388400	-0.57026000	2.33708300
H	-1.12754600	1.03335500	1.78986700
H	-0.70361700	1.63942300	-0.95401700
H	-0.00605100	0.51095000	-2.14909100
C	-2.49878600	-0.89039800	-0.73956900
H	-2.74016600	-1.79380100	-0.16840400
H	-2.64907300	-1.16660800	-1.79175300
C	-3.58156400	0.12526800	-0.42394700
H	-4.61104200	-0.22319700	-0.64556900
C	1.99304500	-0.47804400	-0.64466000
C	3.22657700	-0.55261400	0.21306900
H	3.74146800	0.40795100	0.17833200
H	3.88059300	-1.33366200	-0.16381200
H	2.96660200	-0.73353500	1.25550500
O	1.91291400	-1.02831600	-1.71418900
O	-3.39264300	1.22371400	0.01777800
O	1.24736000	1.34814700	0.75521600
O	1.99225600	2.25595800	-0.05586900
H	-0.01495000	0.05399600	2.75830900
H	1.34148900	2.94522000	-0.22611300

Pc3

C	0.96140400	0.25898800	-0.11621800
C	-0.38420800	-0.25094000	0.53280900
C	0.13655400	0.93045700	-1.22031100
C	-1.10631900	0.83780200	-0.31824700
C	-0.71348900	-1.67456300	0.09729500
H	-0.05269700	-2.38704800	0.59305800
H	-0.60794700	-1.82319200	-0.97654500
H	-1.73691300	-1.92204200	0.38050000
C	-0.52101600	-0.11637000	2.03975100
H	0.12812700	-0.82158000	2.56107600
H	-1.55086800	-0.33763400	2.32628900
H	-0.27891600	0.88671700	2.38311600
H	-1.20505600	1.74146800	0.28359700
H	0.46491300	1.91863500	-1.53574900
H	0.07834500	0.28214600	-2.09253400
C	-2.44183900	0.53110400	-0.97195100
H	-2.40687000	-0.37393900	-1.58356900
H	-2.72481700	1.36854300	-1.61397000
C	-3.54952300	0.39649900	0.05202800
C	1.97382500	-0.80953900	-0.51312000

C	2.92654100	-1.26256700	0.55822500
H	3.66056200	-0.47845900	0.74484700
H	3.42903900	-2.17055500	0.23783300
H	2.39501500	-1.42629400	1.49654200
O	1.96041300	-1.28676500	-1.61973900
O	-4.32434800	-0.47657600	0.18804200
O	1.53330700	1.18006300	0.79257600
O	2.63578600	1.81060500	0.14116600
H	2.27524500	2.67940100	-0.06241400

Pc4

C	-0.97372200	-0.20646700	-0.25124100
C	0.35806900	-0.62911600	0.50204400
C	-0.18845600	-0.20664300	-1.51925600
C	1.13140800	-0.38161400	-0.84581900
C	0.74480800	0.20570300	1.71221300
H	0.04057300	0.03618200	2.52818200
H	0.76367000	1.27456900	1.50481500
H	1.73294500	-0.09254200	2.05983600
C	0.37869800	-2.10789800	0.86496700
H	1.39055800	-2.37089500	1.17572000
H	0.10434900	-2.73582200	0.01867500
H	1.68944200	-1.27153800	-1.15311100
H	-0.44857100	0.14866700	-2.50627700
C	2.06425900	0.81771000	-0.94879100
H	1.59655100	1.73314300	-0.57657800
H	2.28619500	1.02921200	-2.00105700
C	3.38604000	0.63678500	-0.26181400
H	4.06212900	1.51322600	-0.31646000
C	-1.50199600	1.17044200	0.16977900
C	-2.58724100	1.20070400	1.20800300
H	-2.36764400	0.50255700	2.01531500
H	-3.52392300	0.87375000	0.75586400
H	-2.69361700	2.21237000	1.58918900
O	-1.01883900	2.17333800	-0.29659100
O	3.73701400	-0.36293800	0.30548400
O	-1.98196000	-1.19158500	-0.09882800
O	-3.03280600	-0.87741100	-1.01069900
H	-0.30644500	-2.32715700	1.68367400
H	-2.82469100	-1.45459100	-1.75323500

RO_2d

C	-0.35072600	0.09936900	0.62392600
C	0.97939600	-0.31152700	-0.10453400
C	-1.06326800	-0.13811500	-0.74772500
C	0.16251600	-0.93589300	-1.23425900
H	0.52040700	-0.74153900	-2.24032800
H	0.05217300	-2.00786800	-1.07531300
H	-1.12368200	0.81032200	-1.27981500
C	-0.42953100	1.50728300	1.19055900
H	0.22957200	1.61940200	2.05369400
H	-1.45019000	1.71217200	1.50819700
H	-0.16249100	2.25887400	0.44825300
C	-0.74245000	-0.91814100	1.68962200
H	-0.09681600	-0.83103600	2.56245900
H	-0.68036000	-1.94759200	1.33790400
H	-1.76661500	-0.72206500	2.00975500
C	-2.40074500	-0.84292100	-0.81398000

H	-2.63051600	-1.11146300	-1.85132600
H	-2.38556600	-1.79832500	-0.27810400
C	-3.57958400	-0.07263200	-0.29445300
H	-4.55288800	-0.59368600	-0.39640700
O	-3.52918500	1.01986700	0.20205100
O	1.77544500	-1.22253200	0.67973700
O	2.69779000	-1.79494100	-0.04370000
C	1.83587000	0.88173100	-0.52873800
O	1.57424100	1.47581800	-1.54265800
C	2.95406900	1.29428700	0.38764300
H	2.64194700	1.24522200	1.43051200
H	3.27615100	2.29846300	0.12852900
H	3.78925500	0.60276900	0.27018000

TSd1

C	0.35772200	-0.25141900	-1.21077800
C	-0.74536500	-0.33172100	-0.15216500
C	1.06275300	0.82877400	-0.35172800
C	-0.31074500	1.10306900	0.34507900
C	-1.05654900	2.22414700	-0.36880000
H	-2.08957700	2.29271800	-0.02466900
H	-1.07805600	2.09064700	-1.44870900
H	-0.56605600	3.17409400	-0.15076400
C	-0.34494400	1.33033800	1.84587800
H	-1.37528800	1.44249900	2.18673100
H	0.18482100	2.25153400	2.09576900
H	0.09774300	0.51228300	2.40964400
O	-0.51025400	-1.30123900	0.89259800
O	0.75901900	-1.81822100	0.88469100
C	-2.19232200	-0.49999300	-0.58760300
C	-3.17758600	-0.96370600	0.44863700
H	-2.96153100	-1.99571000	0.72535300
H	-4.18581000	-0.88545300	0.05273400
H	-3.07585100	-0.36965000	1.35834100
O	-2.51762000	-0.21509100	-1.71259300
H	-0.05638600	0.15980100	-2.12595500
H	0.89847900	-1.16310400	-1.43552600
C	2.10977000	0.26432200	0.56999800
C	3.37251900	-0.22040100	-0.01207100
O	3.56359900	-0.34626600	-1.19787700
H	4.16155400	-0.48285600	0.71649300
H	2.23748700	0.75310500	1.53345800
H	1.47912500	1.66984700	-0.91057100
H	1.51986500	-0.90368500	0.92444200

TSd2

C	-0.06640100	0.11362100	-1.55486900
C	-0.74111500	-0.28829900	-0.24317100
C	0.77212700	1.18184000	-0.81786400
C	-0.17327700	1.03725000	0.41820500
C	-1.19446900	2.16895500	0.43877800
H	-1.98073500	1.98062700	1.17194800
H	-1.67029800	2.30917000	-0.53112500
H	-0.69708500	3.10038500	0.71351000
C	0.45481200	0.87755800	1.79043400
H	-0.31575200	0.71996900	2.54626900
H	0.99951000	1.78521800	2.05643000
H	1.13803000	0.03339400	1.85543300

O	-0.22294200	-1.45131000	0.42090700
O	0.77245800	-2.09674500	-0.26709100
C	-2.26073600	-0.42708700	-0.24399100
C	-2.88160900	-1.10471200	0.94609900
H	-2.65398400	-2.17016300	0.91592600
H	-3.95685500	-0.95240600	0.93196600
H	-2.45062500	-0.72098200	1.87197000
O	-2.91845300	0.02748800	-1.14607300
H	-0.80587500	0.55034400	-2.22071100
H	0.46460800	-0.67742400	-2.07379700
C	2.25628500	0.90147700	-0.64129700
C	2.67974500	-0.43173400	-0.04618000
O	3.73195600	-0.67056400	0.43664200
H	1.77353000	-1.36499900	-0.13227500
H	2.73660500	0.91570000	-1.62512700
H	2.74084800	1.67536200	-0.04297400
H	0.70174300	2.17162900	-1.26938800

TSd4

C	0.97345600	0.34018800	-0.16844600
C	0.18774700	-0.72607100	0.71697700
C	-0.28449100	0.46794300	-1.03276800
C	-1.06568800	-0.53811300	-0.20182700
C	0.74714200	-2.13936000	0.61970900
H	1.71482600	-2.21694100	1.11872700
H	0.87000500	-2.46193800	-0.41314500
H	0.06296900	-2.83128500	1.11262100
C	0.05431700	-0.31110200	2.17238800
H	-0.62415600	-0.99179900	2.68841400
H	-0.31466500	0.70426500	2.28858700
H	-1.25845100	-1.44561900	-0.77879900
H	-0.25790400	0.45811800	-2.11700000
C	-2.37720500	-0.08257200	0.43827800
H	-2.20338900	0.82942600	1.01555700
H	-2.77264000	-0.84940500	1.10262700
C	-3.40268400	0.23023000	-0.61454300
H	-3.10838900	1.02015700	-1.33663600
C	2.25877700	-0.14465900	-0.81368700
C	3.53931100	0.13146000	-0.08145100
H	3.71503000	1.20695600	-0.04687800
H	4.36402400	-0.36873000	-0.58042600
H	3.45724100	-0.20670200	0.95299500
O	2.20671300	-0.75031700	-1.85467400
O	-4.46844000	-0.31204500	-0.71392300
O	1.24273200	1.60427200	0.41050700
O	0.02159600	2.26922700	0.48050400
H	1.02589900	-0.36975200	2.66421900
H	-0.47531500	1.66649900	-0.45796100

Pd1

C	-0.05097000	0.55488900	-1.25222500
C	0.99543300	0.27403600	-0.16723000
C	-1.11230200	-0.17328800	-0.38829000
C	-0.16848000	0.02185400	0.86047700
C	-0.07385100	-1.18088600	1.78222400
H	0.67725400	-1.02540600	2.55818400
H	0.16788000	-2.09539400	1.24153900
H	-1.03445200	-1.33141000	2.27743000

C	-0.49546100	1.27674900	1.66160900
H	0.28664500	1.47569300	2.39283100
H	-1.43445400	1.12954300	2.19656800
H	-0.59523500	2.16245700	1.03646000
O	1.81810800	1.34099400	0.24191000
O	2.71553500	1.62802100	-0.83100500
C	1.82172800	-0.98842100	-0.42401600
C	3.07595700	-1.15763900	0.38623400
H	3.83989300	-0.47856800	0.00681300
H	3.42193000	-2.18380100	0.30319600
H	2.90431000	-0.88949600	1.42814400
O	1.44280000	-1.81474200	-1.21624900
H	0.13743100	0.13389100	-2.23459900
H	-0.25454500	1.62270000	-1.32449300
C	-2.47603800	0.36201700	-0.33529300
C	-3.64146800	-0.45002900	-0.43547300
O	-4.78280700	-0.00886100	-0.36594100
H	-3.47138600	-1.53250500	-0.58135700
H	-2.63552900	1.42561900	-0.19768000
H	-1.12619900	-1.23156000	-0.64966300
H	2.32007400	2.41925100	-1.21119900

Pd2

C	0.09127500	0.62852600	-1.44638700
C	0.82865800	0.22422600	-0.16596100
C	-1.22141800	0.03929900	-0.88331700
C	-0.38856900	-0.70467800	0.21074800
C	-0.15226900	-2.15119000	-0.21011400
H	0.57711600	-2.63945100	0.43836700
H	0.20763700	-2.22821300	-1.23552800
H	-1.09270800	-2.69763400	-0.13441300
C	-0.85305000	-0.65779300	1.65756100
H	-0.09085000	-1.07976700	2.31385300
H	-1.75753400	-1.25536900	1.76890900
H	-1.05977900	0.35117700	2.00660600
O	0.87846300	1.25713000	0.80253100
C	2.18595500	-0.45813200	-0.29635200
C	2.97799200	-0.62767900	0.97074000
H	3.36436500	0.34071000	1.28885000
H	3.80069900	-1.31471700	0.79548700
H	2.33764100	-0.99179400	1.77508500
O	2.56299700	-0.87620400	-1.36191000
H	0.47368800	0.08996700	-2.30911100
H	0.09643500	1.69541100	-1.66778500
C	-2.20562000	1.09838400	-0.40838200
C	-3.49755000	0.55467900	0.15859400
O	-3.88683800	-0.55534600	0.16562200
H	-1.77262900	1.76890400	0.33507600
H	-2.50848500	1.73770500	-1.24279000
H	-1.73762900	-0.64347700	-1.55680200
O	1.85340800	2.20940500	0.37933700
H	1.30537800	2.91281300	0.01677500

Pd4

C	0.95474100	0.29884100	-0.08995300
C	-0.38832100	-0.24592900	0.55955700
C	0.12314000	0.90057100	-1.17218800
C	-1.11910100	0.18587500	-0.76250300

C	-0.44557400	-1.73476200	0.85976900
H	0.19595100	-1.99074300	1.70472100
H	-0.14438900	-2.33452900	0.00157400
H	-1.46952100	-2.00773700	1.11072500
C	-0.80165100	0.55549700	1.78583300
H	-1.81621800	0.27514300	2.07298000
H	-0.76801400	1.63024300	1.61514900
H	-1.28837900	-0.69815900	-1.38870800
H	0.40787900	1.37318100	-2.10156900
C	-2.41007400	0.98664200	-0.71034800
H	-2.63865300	1.39315500	-1.70170900
H	-2.32238300	1.86332100	-0.06139300
C	-3.62169600	0.22186600	-0.26234600
H	-4.56202900	0.80909800	-0.25417900
C	1.90844000	-0.80775200	-0.55643200
C	2.97102600	-1.24509200	0.41283300
H	2.56639100	-1.33075700	1.42070200
H	3.75315400	-0.48616400	0.44860800
H	3.39134600	-2.19106300	0.08323000
O	1.76779800	-1.31048200	-1.64278900
O	-3.62728400	-0.93193700	0.07074200
O	1.62420800	1.18651600	0.79213100
O	2.67826000	1.80895300	0.06041200
H	-0.14308300	0.33685600	2.62567400
H	2.26852300	2.63920500	-0.20510400

Ring opening reactions

CI ring opening TS 1 (OO toward CH_3, Figure 9 top)

C	0.06350	-1.34568	-0.82995
C	-1.05235	-0.34025	-0.92017
C	1.29225	-0.45954	-0.60022
C	0.69977	0.68832	0.19498
H	0.13800	-1.97402	-1.72080
H	-0.08107	-2.01285	0.02030
C	0.85887	2.09055	-0.27631
H	0.88316	2.15212	-1.36416
H	1.80069	2.51577	0.08981
H	0.04498	2.71910	0.08977
C	0.44004	0.48823	1.64987
H	-0.34968	1.15462	1.99880
H	1.33690	0.71886	2.23997
H	0.14735	-0.53510	1.88913
C	2.45938	-1.19738	0.04321
H	2.19317	-1.57815	1.03563
H	2.71935	-2.08962	-0.53800
C	3.72098	-0.39805	0.19965
H	4.55556	-0.93788	0.69061
O	3.86660	0.73707	-0.16422
C	-2.22860	-0.36003	-0.23559
C	-2.64849	-1.25281	0.86895
H	-1.90453	-2.02243	1.05107
H	-3.60518	-1.71838	0.63045
H	-2.80816	-0.67404	1.78000
O	-3.08596	0.62008	-0.59264
O	-4.19774	0.70447	0.11135
H	-0.99287	0.37180	-1.73476
H	1.62712	-0.06287	-1.56031

CI ring opening TS 2 (OO toward ring, Figure 9 bottom)

C	-0.11680	-1.28417	-0.99569
C	-1.27430	-0.33922	-0.82917
C	1.08127	-0.34993	-0.80368
C	0.56786	0.65577	0.20851
H	-0.11317	-1.79104	-1.96296
H	-0.11821	-2.05409	-0.22368
C	0.71282	2.11010	-0.07562
H	0.05080	2.70451	0.55304
H	0.49503	2.34204	-1.11838
H	1.74118	2.44071	0.12771
C	0.47677	0.24453	1.63874
H	-0.28629	0.82391	2.15989
H	1.43127	0.42360	2.14917
H	0.24180	-0.81375	1.75534
C	2.38349	-1.06445	-0.41207
H	2.27534	-1.58230	0.54072
H	2.62639	-1.79880	-1.18576
C	3.51690	-0.08485	-0.31452
H	3.79778	0.40510	-1.27022
O	4.08486	0.20622	0.70270
C	-2.33359	-0.51550	-0.00792
C	-2.61020	-1.64885	0.92263
H	-2.10791	-2.55622	0.59810
H	-3.68074	-1.84532	0.95998
H	-2.28029	-1.41417	1.93667
O	-3.29611	0.43313	0.10199
O	-3.09054	1.57215	-0.52407
H	-1.33262	0.50171	-1.50699
H	1.24867	0.18152	-1.74491

CI ring opening product 1 (OO toward CH_3, Figure 9 top)

C	-0.00298	-1.48264	0.46184
C	-1.29756	-1.28631	-0.25559
C	1.14140	-0.62005	-0.13521
C	0.87953	0.84372	0.06353
H	0.27724	-2.53650	0.39520
H	-0.10020	-1.25330	1.52474
C	0.52521	1.68431	-1.10941
H	-0.15871	1.16049	-1.78175
H	1.41698	1.93538	-1.69837
H	0.05479	2.62173	-0.80890
C	1.18002	1.48211	1.37393
H	0.55355	2.36032	1.53833
H	2.22277	1.82600	1.43699
H	1.02447	0.80127	2.21551
C	2.47702	-1.07773	0.45279
H	2.52313	-0.90736	1.53376
H	2.60657	-2.15987	0.33471
C	3.69435	-0.43833	-0.15224
H	4.65346	-0.73165	0.32108
O	3.68751	0.32361	-1.08000
C	-2.26390	-0.43579	0.08199
C	-2.34974	0.49523	1.23238
H	-1.47958	0.37879	1.87081
H	-3.25574	0.31406	1.80958

H	-2.39216	1.52645	0.88211
O	-3.33938	-0.43590	-0.80679
O	-4.29467	0.40527	-0.52321
H	-1.44804	-1.85279	-1.16772
H	1.17375	-0.81397	-1.21013

CI ring opening product 2 (OO toward ring, Figure 9 bottom)

C	-0.17479	-1.13230	0.92897
C	-1.52631	-1.02795	0.30055
C	0.95261	-0.68916	-0.03865
C	0.86247	0.77266	-0.36747
H	0.00152	-2.17023	1.21928
H	-0.10806	-0.53766	1.84148
C	0.42731	1.19670	-1.72521
H	0.00091	2.20146	-1.71560
H	-0.31899	0.51356	-2.13642
H	1.26439	1.21843	-2.43756
C	1.33367	1.78725	0.61592
H	0.79224	2.72809	0.50236
H	2.40082	2.01521	0.49454
H	1.20838	1.45137	1.64836
C	2.32291	-1.07210	0.54786
H	2.50810	-0.57883	1.50188
H	2.35366	-2.15402	0.71189
C	3.42749	-0.72065	-0.40793
H	3.30781	-1.13799	-1.43011
O	4.37858	-0.03786	-0.14267
C	-2.34702	0.00622	0.40914
C	-2.19893	1.27186	1.17796
H	-1.31354	1.24225	1.80546
H	-3.07247	1.44182	1.80768
H	-2.10539	2.12031	0.49880
O	-3.58161	0.04324	-0.26317
O	-3.84356	-0.95707	-1.05069
H	-1.84285	-1.83990	-0.34066
H	0.81965	-1.25547	-0.96597

Vinoxy radical reactant (figure 10)

C	1.12041	-0.17294	-0.74948
C	-0.02136	0.56445	0.03922
C	0.21492	-1.40105	-0.88060
C	-1.00627	-0.51723	-0.56823
H	-1.43524	-0.08653	-1.47373
H	1.26970	0.33115	-1.70629
H	0.21546	-1.91999	-1.83586
H	0.42458	-2.11754	-0.08709
C	-0.31776	1.99309	-0.36611
H	0.46475	2.66929	-0.01394
H	-1.26650	2.31899	0.06219
H	-0.39131	2.08962	-1.44963
C	0.12554	0.44233	1.54980
H	0.93414	1.08127	1.90954
H	0.34707	-0.57776	1.86340
H	-0.79288	0.76284	2.04327
C	2.44783	-0.31493	-0.05112
C	3.33630	0.90365	-0.07067

H	3.69132	1.07447	-1.08896
H	4.18578	0.76455	0.59191
H	2.77077	1.79052	0.22026
C	-2.08477	-1.02792	0.28514
H	-1.89796	-1.87363	0.93723
C	-3.36423	-0.40068	0.35259
H	-4.10039	-0.85566	1.03619
O	-3.66189	0.60011	-0.29218
O	2.77152	-1.33313	0.51070

Vinoxy radical ring opening transition state (figure 10)

C	-0.17652	0.75124	0.12867
C	1.18318	-0.71440	-0.60188
C	-1.06652	-0.18357	-0.68816
C	-0.15198	-1.40430	-0.74424
H	-0.24444	-1.99241	-1.65744
H	-0.34975	-2.06127	0.10176
H	-1.19764	0.24926	-1.68259
C	2.15453	-1.05555	0.29476
H	1.97146	-1.81346	1.04734
C	3.42984	-0.36574	0.32733
H	4.16485	-0.75992	1.05407
O	3.72119	0.58957	-0.36749
C	0.17885	2.09729	-0.40567
H	1.11181	2.45075	0.03433
H	-0.59998	2.82993	-0.15714
H	0.29252	2.08950	-1.48911
C	-0.20359	0.61211	1.61586
H	-0.37815	-0.41526	1.93243
H	-1.00384	1.22855	2.04230
H	0.73686	0.95549	2.04778
C	-2.44225	-0.39108	-0.07729
C	-3.39667	0.77026	-0.19964
H	-4.29028	0.58805	0.39023
H	-3.67169	0.90350	-1.24770
H	-2.91556	1.69528	0.12267
O	-2.74239	-1.41097	0.49068
H	1.49027	-0.07447	-1.42284

Vinoxy radical product (figure 10)

C	-2.14454	-0.84665	0.13954
C	-2.67491	-1.56512	1.32931
H	-2.47549	-1.02212	2.25563
H	-2.20914	-2.55459	1.44252
H	-3.75048	-1.72970	1.25318
C	-2.76545	-1.05614	-1.19650
H	-2.40730	-1.98183	-1.66806
H	-2.53728	-0.24102	-1.88476
H	-3.84995	-1.14555	-1.11693
C	-0.82875	-0.12706	0.23567
H	-0.46162	-0.20845	1.26146
C	0.23623	-0.69203	-0.72365
H	-0.10159	-0.52505	-1.74767
H	0.31824	-1.76748	-0.56319
C	-1.12637	1.34957	-0.04089
C	-1.65589	2.14647	1.12219
H	-2.41186	1.58072	1.66702
H	-2.06511	3.09204	0.77792

H	-0.83381	2.34084	1.81499
O	-0.97404	1.83185	-1.13694
C	1.56291	-0.03903	-0.53797
H	1.61797	1.01411	-0.80234
C	2.65527	-0.63543	-0.06591
H	2.66758	-1.68321	0.21235
C	3.90722	0.11027	0.09810
H	3.85757	1.17508	-0.20879
O	4.93004	-0.35846	0.53036

Ring-opening product of alkoxy radical ROc (Figure 11 top)

C	-1.52909	-1.04195	0.36370
C	0.51832	0.82466	0.01795
C	-0.27811	-1.53661	-0.31018
C	0.88941	-0.63056	0.14955
C	0.56188	1.47788	-1.31839
H	-0.09537	2.34750	-1.35400
H	0.25707	0.80265	-2.11971
H	1.57332	1.83675	-1.55704
C	0.44251	1.66191	1.24527
H	-0.10844	2.58678	1.06674
H	1.44672	1.93564	1.59207
H	-0.03561	1.12570	2.06895
H	1.06071	-0.83701	1.20768
H	-0.09745	-2.57048	-0.01805
H	-0.39989	-1.47717	-1.39152
C	2.15541	-1.01606	-0.61660
H	2.05137	-0.81077	-1.68738
H	2.33317	-2.09555	-0.55334
C	3.41648	-0.34448	-0.15465
H	4.32018	-0.60819	-0.74024
C	-2.36346	0.01005	-0.39903
C	-3.16259	0.95565	0.44352
H	-2.48997	1.52272	1.08910
H	-3.82338	0.39141	1.10124
H	-3.73245	1.62678	-0.19202
O	-2.37719	-0.00489	-1.60474
O	3.49700	0.41686	0.77036
O	-1.89039	-1.40444	1.45446

Ring-opening product of alkoxy radical ROd (Figure 11 bottom)

C	0.52909	-0.47209	0.80658
C	-1.65164	0.96559	-0.01727
C	0.77598	0.42528	-0.37719
C	-0.31832	1.51392	-0.45842
H	-0.40097	1.88302	-1.48262
H	-0.09427	2.35926	0.19205
H	0.71580	-0.18303	-1.27834
C	0.50427	-1.94960	0.63743
H	-0.11739	-2.42487	1.40018
H	1.51089	-2.37553	0.73010
H	0.13508	-2.23770	-0.34743
C	0.65394	0.08763	2.18181
H	0.03068	-0.46080	2.88992
H	0.37043	1.14010	2.23338
H	1.68629	0.01099	2.55193
C	2.14758	1.10686	-0.35761
H	2.22233	1.84691	-1.16318

H	2.29226	1.68055	0.56449
C	3.33135	0.19542	-0.50874
H	4.31416	0.70497	-0.44330
O	3.27685	-0.98875	-0.69786
O	-2.34486	1.48441	0.82124
C	-2.15572	-0.30562	-0.72966
O	-1.80666	-0.51901	-1.86370
C	-3.09955	-1.17252	0.04367
H	-2.59376	-1.53919	0.93876
H	-3.42689	-2.00570	-0.57092
H	-3.94911	-0.58137	0.38398