

Pressure-Dependent Rate Rules for Cycloaddition, Intramolecular H-shift, and Concerted Elimination Reactions of Alkenyl Peroxy Radicals in Low Temperature

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1. Detailed Description of the Master Equation Method

The time evolution of the molecular population for reactant molecules is given by the time-dependent master equation:¹

$$\frac{d\rho_i^\alpha}{dt} = \omega \sum_j P_{ij}^\alpha \rho_j^\alpha - \omega \sum_j P_{ji}^\alpha \rho_i^\alpha - k_i^\alpha \rho_i^\alpha + \sum_\beta k_l^\beta \rho_l^\beta + R_i \quad (1)$$

where ω is the collision frequency, which is proportional to the concentration of the third body M, P_{ij}^α is the collision energy transfer probability from energy level j to energy level i of isomer α , ρ_j^α is the molecular population of the isomer α at energy level E_j , ρ_i^α is the molecular population of the isomer α at energy level E_i , k_i^α is the sum of rates for all the decomposition and isomerization channels from energy level E_i , k_l^β is the rate of isomerization from isomer β at energy level E_l to isomer α at energy level E_i and R_i is the chemical activation flux, which is assumed to be constant. Index l for isomer β corresponds to the same energy as i for α , i.e. $E_l = E_i$. The master equation can also be written in the matrix form:

$$\frac{d\rho}{dt} = B\rho + R \quad (2)$$

All the eigenvalues of the matrix B are negative, and the overall pressure-dependent thermal rate constant $k_{\text{uni}}(T,P)$ can be derived as the negative of the largest eigenvalue of the matrix B for the single-reaction channel case. This eigenvalue is the chemically significant eigenvalue, which corresponds to the slow mode describing the “chemical reaction”, and for the multi-reaction channels case, there is one chemically significant eigenvalue for each reaction channel. All calculations are carried out with a series of energy grain sizes and variations in the maximum system energy to ensure that the results have converged.

[1] R. G. Gilbert, S. C. Smith, Theory of Unimolecular and Recombination Reactions; Blackwell: Oxford, U.K., 1990.

2. Reaction List

Table S1. List of Cycloaddition Reactions

Reaction class	No.	Reaction equation
1,5-endo-cycloaddition	R1	$C=CCOO\bullet \rightarrow YCC\bullet COO$
	R2	$C=CC(C)OO\bullet \rightarrow YCC\bullet C(C)OO$
	R3	$C=CC(CC)OO\bullet \rightarrow YCC\bullet C(CC)OO$
	R4	$C=C(C)COO\bullet \rightarrow YCC\bullet (C)COO$
	R5	$C=C(CC)COO\bullet \rightarrow YCC\bullet (CC)COO$
	R6	$cis-CC=CCOO\bullet \rightarrow CYCC\bullet COO$
	R7	$trans-CC=CCOO\bullet \rightarrow CYCC\bullet COO$
	R8	$cis-CCC=CCOO\bullet \rightarrow CCYCC\bullet COO$
	R9	$trans-CCC=CCOO\bullet \rightarrow CCYCC\bullet OO$
	R10	$C=C(C)C(C)OO\bullet \rightarrow YCC\bullet (C)C(C)OO$
	R11	$C=C(CC)C(C)OO\bullet \rightarrow YCC\bullet (CC)C(C)OO$
1,6-endo-cycloaddition	R12	$C=CCCCOO\bullet \rightarrow YCC\bullet CCOO$
	R13	$C=CCC(C)OO\bullet \rightarrow YCC\bullet CC(C)OO$
	R14	$C=CCC(CC)OO\bullet \rightarrow YCC\bullet CC(CC)OO$
	R15	$C=CC(C)COO\bullet \rightarrow YCC\bullet C(C)COO$
	R16	$C=CC(CC)COO\bullet \rightarrow YCC\bullet C(CC)COO$
	R17	$C=C(C)CCOO\bullet \rightarrow YCC\bullet (C)CCOO$
	R18	$C=C(CC)CCOO\bullet \rightarrow YCC\bullet (CC)CCOO$
	R19	$cis-CC=CCCCOO\bullet \rightarrow CYCC\bullet CCOO$
	R20	$trans-CC=CCCCOO\bullet \rightarrow CYCC\bullet CCOO$
	R21	$cis-CCC=CCCCOO\bullet \rightarrow CCYCC\bullet CCOO$
	R22	$trans-CCC=CCCCOO\bullet \rightarrow CCYCC\bullet CCOO$
	R23	$C=CC(C)C(C)OO\bullet \rightarrow YCC\bullet C(C)C(C)OO$
1,7-endo-cycloaddition	R24	$C=CCCCOO\bullet \rightarrow YCC\bullet CCCC$
	R25	$C=CC(C)CCOO\bullet \rightarrow YCC\bullet C(C)CCOO$

	R26	$C=CC(CC)CCOO \bullet \rightarrow YCC \bullet C(CC)CCOO$
	R27	$C=CCC(C)COO \bullet \rightarrow YCC \bullet CC(C)COO$
	R28	$C=CCC(CC)COO \bullet \rightarrow YCC \bullet CC(CC)COO$
	R29	$C=CCCC(C)OO \bullet \rightarrow YCC \bullet CCC(C)OO$
	R30	$C=CCCC(CC)OO \bullet \rightarrow YCC \bullet CCC(CC)OO$
	R31	$C=C(C)CCCCOO \bullet \rightarrow YCC \bullet (C)CCCCOO$
	R32	$C=C(CC)CCCCOO \bullet \rightarrow YCC \bullet (CC)CCCCOO$
	R33	$cis-CC=CCCCOO \bullet \rightarrow CYCC \bullet CCCC$
	R34	$trans-CC=CCCCOO \bullet \rightarrow CYCC \bullet CCCC$
	R35	$cis-CCC=CCCCOO \bullet \rightarrow CCYCC \bullet CCCC$
	R36	$trans-CCC=CCCCOO \bullet \rightarrow CCYCC \bullet CCCC$
1,5-exo-cycloaddition	R37	$C=CCOO \bullet \rightarrow \bullet CYCCOO$
	R38	$C=CC(C)OO \bullet \rightarrow \bullet CYCC(C)OO$
	R39	$C=CC(CC)OO \bullet \rightarrow \bullet CYCC(CC)OO$
	R40	$C=C(C)COO \bullet \rightarrow \bullet CYC(C)COO$
	R41	$C=C(CC)COO \bullet \rightarrow \bullet CYC(CC)COO$
	R42	$cis-CC=CCOO \bullet \rightarrow CC \bullet YCCOO$
	R43	$trans-CC=CCOO \bullet \rightarrow CC \bullet YCCOO$
	R44	$cis-CCC=CCOO \bullet \rightarrow CC \bullet CYCCOO$
	R45	$trans-CCC=CCOO \bullet \rightarrow CC \bullet CYCCOO$
	R46	$C=C(C)C(C)OO \bullet \rightarrow \bullet CYC(C)C(C)OO$
	R47	$C=C(CC)C(C)OO \bullet \rightarrow \bullet CYC(CC)C(C)OO$
1,6-exo-cycloaddition	R48	$C=CCCCOO \bullet \rightarrow \bullet CYCCCCOO$
	R49	$C=CCC(C)OO \bullet \rightarrow \bullet CYCCC(C)OO$
	R50	$C=CCC(CC)OO \bullet \rightarrow \bullet CYCCC(CC)OO$
	R51	$C=CC(C)COO \bullet \rightarrow \bullet CYCC(C)COO$
	R52	$C=CC(CC)COO \bullet \rightarrow \bullet CYCC(CC)COO$
	R53	$C=C(C)CCOO \bullet \rightarrow \bullet CYC(C)CCOO$
	R54	$C=C(CC)CCOO \bullet \rightarrow \bullet CYC(CC)CCOO$

1,7-exo-cycloaddition	R55	cis-CC=CCCCOO•→CC•YCCCCOO
	R56	trans-CC=CCCCOO•→CC•YCCCCOO
	R57	cis-CCC=CCCCOO•→CC•CYCCCCOO
	R58	trans-CCC=CCCCOO•→CC•CYCCCCOO
	R59	C=CC(C)C(C)OO•→•CYCC(C)C(C)OO
	R60	C=CCCCOO•→•CYCCCCOO
	R61	C=CC(C)CCOO•→•CYCC(C)CCOO
	R62	C=CC(CC)CCOO•→•CYCC(CC)CCOO
	R63	C=CCC(C)COO•→•CYCCC(C)COO
	R64	C=CCC(CC)COO•→•CYCCC(CC)COO
	R65	C=CCCC(C)OO•→•CYCCCC(C)OO
	R66	C=CCCC(CC)OO•→•CYCCCC(CC)OO
	R67	C=C(C)CCCCOO•→•CYC(C)CCCCOO
	R68	C=C(CC)CCCCOO•→•CYC(CC)CCCCOO
	R69	cis-CC=CCCCOO•→CC•YCCCCOO
	R70	trans-CC=CCCCOO•→CC•YCCCCOO
	R71	cis-CCC=CCCCOO•→CCC•YCCCCOO
	R72	trans-CCC=CCCCOO•→CCC•YCCCCOO

Table S2. List of Intramolecular H-shift Reactions

Reaction class	No.	Reaction equation
1,4-H(as)	R1	C=CCCCOO•→C=CC•COO
	R2	C=CCC(C)OO•→C=CC•C(C)OO
	R3	C=C(C)CCOO•→C=C(C)C•COO
	R4	cis-CC=CCCCOO•→CC=CC•COO
	R5	trans-CC=CCCCOO•→CC=CC•COO
	R6	C=CC(C)COO•→C=CC•(C)COO
	R7	C=CC(CC)COO•→C=CC•(CC)COO
	R8	C=CC(C)C(C)OO•→C=CC•(C)C(C)OO

1,4-H(s)	R9	$C=CCCCOO\bullet \rightarrow C=CCC\bullet COO$
	R10	$C=CC(C)CCOO\bullet \rightarrow C=CC(C)C\bullet COO$
	R11	$C=CCCC(C)OO\bullet \rightarrow C=CCC\bullet C(C)OO$
	R12	$C=C(C)CCCCOO\bullet \rightarrow C=C(C)CC\bullet COO$
	R13	$cis-CC=CCCCOO\bullet \rightarrow CC=CCC\bullet COO$
	R14	$trans-CC=CCCCOO\bullet \rightarrow CC=CCC\bullet COO$
1,4-H(vt)	R15	$C=CCC(C)COO\bullet \rightarrow C=CCC\bullet (C)COO$
	R16	$C=CCC(CC)COO\bullet \rightarrow C=CCC\bullet (CC)COO$
	R17	$trans-CC=COO\bullet \rightarrow C\bullet C=COO$
	R18	$trans-CCC=COO\bullet \rightarrow CC\bullet C=COO$
	R19	$C=CCOO\bullet \rightarrow C=C\bullet COO$
	R20	$C=CC(C)OO\bullet \rightarrow C=C\bullet C(C)OO$
1,4-H(vi)	R21	$cis-CC=CCOO\bullet \rightarrow CC=C\bullet COO$
	R22	$trans-CC=CCOO\bullet \rightarrow CC=C\bullet COO$
1,5-H(as)	R23	$C=CCCCOO\bullet \rightarrow C=CC\bullet CCOO$
	R24	$cis-CC=CCCCOO\bullet \rightarrow CC=CC\bullet CCOO$
	R25	$trans-CC=CCCCOO\bullet \rightarrow CC=CC\bullet CCOO$
	R26	$C=CCC(C)COO\bullet \rightarrow C=CC\bullet C(C)COO$
	R27	$C=CCCC(C)OO\bullet \rightarrow C=CC\bullet CC(C)OO$
	R28	$C=C(C)CCCCOO\bullet \rightarrow C=C(C)C\bullet CCOO$
1,5-H(s)	R29	$C=CC(C)CCOO\bullet \rightarrow C=CC\bullet (C)CCOO$
	R30	$C=CC(CC)CCOO\bullet \rightarrow C=CC\bullet (CC)CCOO$
	R31	$C=CCCCCOO\bullet \rightarrow C=CCC\bullet CCOO$
	R32	$C=CCC(C)CCOO\bullet \rightarrow C=CCC\bullet (C)CCOO$
1,5-H(vt)	R33	$C=CCOO\bullet \rightarrow \bullet C=CCOO$
	R34	$trans-CC=CCOO\bullet \rightarrow CC\bullet =CCOO$
	R35	$trans-CCC=CCOO\bullet \rightarrow CC\bullet C=CCOO$
1,5-H(vi)	R36	$C=CC(C)COO\bullet \rightarrow C=C\bullet C(C)COO$
	R37	$C=CCCCOO\bullet \rightarrow C=C\bullet CCOO$

	R38	$C=CCC(C)OO\bullet \rightarrow C=C\bullet CC(C)OO$
	R39	$C=CC(C)C(C)OO\bullet \rightarrow C=C\bullet C(C)C(C)OO$
	R40	$cis-CC=CCCCOO\bullet \rightarrow CC=C\bullet CCOO$
	R41	$trans-CC=CCCCOO\bullet \rightarrow CC=C\bullet CCOO$
1,6-H(as)	R42	$C=CCCCCOO\bullet \rightarrow C=CC\bullet CCCCCO$
	R43	$C=CC(C)CCCCOO\bullet \rightarrow C=CC\bullet (C)CCCCO$
1,6-H(s)	R44	$C=CCCCCOO\bullet \rightarrow C=CCC\bullet CCCCCO$
1,6-H(vt)	R45	$C=CCCOO\bullet \rightarrow \bullet CCCCCO$
	R46	$C=CCC(C)OO\bullet \rightarrow \bullet C=CCC(C)OO$
	R47	$C=CC(C)COO\bullet \rightarrow \bullet C=CC(C)COO$
	R48	$C=CC(C)C(C)OO\bullet \rightarrow \bullet C=CC(C)C(C)OO$
	R49	$trans-CC=CCCCOO\bullet \rightarrow CC\bullet =CCCCO$
1,6-H(vi)	R50	$C=CCCCOO\bullet \rightarrow C=C\bullet CCCCCO$
	R51	$C=CC(C)CCOO\bullet \rightarrow C=C\bullet C(C)CCOO$
	R52	$C=CCC(C)COO\bullet \rightarrow C=C\bullet CC(C)COO$
	R53	$C=CCCC(C)OO\bullet \rightarrow C=C\bullet CCC(C)OO$

Table S3. List of Concerted Elimination Reactions

Reaction class	No.	Reaction equation
Allylic Secondary C-H	R1	$C=CCCCOO\bullet \rightarrow C=CC=C+HO_2\bullet$
	R2	$C=CC(C)COO\bullet \rightarrow C=CC(C)=C+HO_2\bullet$
	R3	$C=CC(C)C(C)OO\bullet \rightarrow C=CC(C)=CC+HO_2\bullet$
	R4	$C=CC(C)C(C_2)OO\bullet \rightarrow C=CC(C)=CC_2+HO_2\bullet$
	R5	$C_2C=CCCCOO\bullet \rightarrow C_2C=CC=C+HO_2\bullet$
	R6	$C_2C=CCC(C)OO\bullet \rightarrow C_2C=CC=CC+HO_2\bullet$
	R7	$C_2C=CC(C)COO\bullet \rightarrow C_2C=CC(C)=C+HO_2\bullet$
	R8	$cis-CC=CCC(C)OO\bullet \rightarrow CC=CC=CC+HO_2\bullet$
	R9	$trans-CC=CCC(C)OO\bullet \rightarrow CC=CC=CC+HO_2\bullet$

Secondary C-H	R10	$\text{C=CCCCOO}\cdot \rightarrow \text{C=CCC=C}+\text{HO}_2\cdot$
	R11	$\text{C=CC(C)CCOO}\cdot \rightarrow \text{C=CC(C)C=C}+\text{HO}_2\cdot$
	R12	$\text{C=CC(C}_2\text{)CCOO}\cdot \rightarrow \text{C=CC(C}_2\text{)C=C}+\text{HO}_2\cdot$
	R13	$\text{C=CCC(C)COO}\cdot \rightarrow \text{C=CCC(C)=C}+\text{HO}_2\cdot$
	R14	$\text{C=CC(C)C(C)COO}\cdot \rightarrow \text{C=CC(C)C(C)=C}+\text{HO}_2\cdot$
	R15	$\text{C}_2\text{C=CCCCOO}\cdot \rightarrow \text{C}_2\text{C=CCC=C}+\text{HO}_2\cdot$
	R16	$\text{cis-CC=CCCCOO}\cdot \rightarrow \text{CC=CCC=C}+\text{HO}_2\cdot$
Vinylic C-H	R17	$\text{trans-CC=CCCCOO}\cdot \rightarrow \text{CC=CCC=C}+\text{HO}_2\cdot$
	R18	$\text{C=CCOO}\cdot \rightarrow \text{C=C=C}+\text{HO}_2\cdot$
	R19	$\text{C=CC(C)OO}\cdot \rightarrow \text{C=C=CC}+\text{HO}_2\cdot$
	R20	$\text{cis-CC=CCOO}\cdot \rightarrow \text{CC=C=C}+\text{HO}_2\cdot$
	R21	$\text{trans-CC=CCOO}\cdot \rightarrow \text{CC=C=C}+\text{HO}_2\cdot$

3. Energy Barriers

Table S4. Forward and Reverse Energy Barriers and Reaction Enthalpies for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction class	Reaction	E_1^a	E_{-1}^b	ΔH^c
		(kcal/mol)	(kcal/mol)	(kcal/mol)
1,5-endo-cycloaddition	R1	33.32(1.84) ^d	30.11(0.68)	2.76(1.08)
	R2	32.08(0.60)	29.36(0.07)	2.41(0.73)
	R3	31.43(0.05)	29.22(0.21)	1.90(0.22)
	R4	31.40(0.08)	28.05(1.38)	2.97(1.29)
	R5	31.29(0.19)	28.06(1.37)	2.84(1.16)
	R6	31.39(0.09)	31.47(2.04)	-0.54(2.22)
	R7	31.51(0.03)	29.72(0.29)	1.28(0.40)
	R8	31.21(0.27)	31.32(1.89)	-0.55(2.23)
	R9	31.12(0.36)	29.77(0.34)	0.94(0.74)
	R10	30.50(0.98)	28.09(1.34)	2.28(0.60)
	R11	31.03(0.45)	28.54(0.89)	2.22(0.54)
1,6-endo-cycloaddition	R12	17.39(1.19) ^d	16.60(0.25)	-0.11(1.31)

	R13	17.25(1.05)	16.69(0.16)	-0.17(1.25)
	R14	17.40(1.20)	17.30(0.45)	-0.58(0.84)
	R15	17.03(0.83)	16.69(0.16)	-0.49(0.93)
	R16	16.04(0.16)	16.89(0.04)	-1.71(0.29)
	R17	15.68(0.52)	16.23(0.62)	-1.21(0.21)
	R18	15.26(0.94)	15.59(1.26)	-0.98(0.44)
	R19	16.32(0.12)	18.88(2.03)	-3.42(2.00)
	R20	14.94(1.26)	16.20(0.65)	-2.08(0.66)
	R21	15.65(0.55)	18.13(1.28)	-3.23(1.81)
	R22	15.09(1.11)	16.13(0.72)	-1.80(0.38)
	R23	16.31(0.11)	16.88(0.03)	-1.26(0.16)
1,7-endo-cycloaddition	R24	18.48(0.66) ^d	18.73(0.22)	-1.26(0.39)
	R25	17.73(0.09)	16.83(1.68)	-0.08(1.57)
	R26	17.95(0.13)	16.78(1.73)	0.20(1.85)
	R27	18.84(1.02)	17.17(1.34)	0.73(2.38)
	R28	17.96(0.14)	17.30(1.21)	-0.28(1.37)
	R29	18.62(0.80)	18.93(0.42)	-1.16(0.49)
	R30	18.64(0.82)	19.73(1.22)	-1.98(0.33)
	R31	16.88(0.94)	17.33(1.18)	-1.31(0.34)
	R32	16.77(1.04)	17.34(1.17)	-1.51(0.14)
	R33	18.34(0.52)	21.48(2.97)	-4.18(2.53)
	R34	16.72(1.10)	18.47(0.04)	-2.80(1.15)
	R35	18.15(0.33)	21.67(3.16)	-4.49(2.84)
	R36	16.56(1.26)	18.92(0.41)	-3.32(1.67)
1,5-exo-cycloaddition	R37	31.94(2.02) ^d	12.33(0.03)	19.34(1.96)
	R38	30.64(0.72)	13.38(1.02)	17.13(0.25)
	R39	29.80(0.12)	13.33(0.97)	16.39(0.99)
	R40	29.55(0.37)	12.11(0.25)	17.20(0.18)
	R41	29.08(0.84)	12.03(0.33)	16.88(0.50)

1,6-exo-cycloaddition	R42	29.11(0.81)	11.53(0.83)	17.39(0.01)
	R43	30.84(0.92)	11.40(0.96)	19.22(1.84)
	R44	32.51(2.59)	14.53(2.17)	17.72(0.34)
	R45	30.34(0.42)	10.90(1.46)	19.20(1.82)
	R46	27.85(2.07)	12.23(0.13)	15.53(1.85)
	R47	27.43(2.49)	12.16(0.20)	15.22(2.16)
	R48	18.09(0.85) ^d	15.73(0.10)	1.82(0.70)
	R49	17.91(0.67)	15.42(0.21)	2.06(0.94)
	R50	17.80(0.56)	15.74(0.11)	1.66(0.54)
	R51	18.90(1.66)	15.68(0.05)	2.74(1.62)
	R52	17.50(0.26)	15.95(0.32)	1.06(0.06)
	R53	17.08(0.16)	16.55(0.92)	0.09(1.03)
	R54	16.12(1.12)	16.13(0.50)	-0.48(1.60)
	R55	16.35(0.89)	16.05(0.42)	-0.25(1.37)
	R56	16.67(0.57)	15.07(0.56)	1.09(0.03)
	R57	16.24(1.00)	16.08(0.45)	-0.37(1.49)
	R58	16.83(0.41)	15.22(0.41)	1.06(0.06)
	R59	17.34(0.10)	13.97(1.66)	2.93(1.81)
1,7-exo-cycloaddition	R60	16.10(0.99) ^d	17.72(0.27)	-2.40(0.69)
	R61	14.90(0.21)	17.51(0.06)	-3.39(0.30)
	R62	15.54(0.43)	17.75(0.30)	-2.97(0.12)
	R63	15.96(0.85)	16.78(0.67)	-1.51(1.58)
	R64	14.93(0.18)	16.85(0.60)	-2.64(0.45)
	R65	15.68(0.57)	17.89(0.44)	-2.83(0.26)
	R66	15.61(0.50)	18.55(1.10)	-3.58(0.49)
	R67	15.10(0.01)	16.75(0.70)	-2.44(0.65)
	R68	14.85(0.26)	16.46(0.99)	-2.40(0.69)
	R69	14.31(0.80)	18.12(0.67)	-4.53(1.44)
	R70	14.85(0.26)	17.26(0.19)	-3.16(0.07)

R71	14.32(0.79)	18.22(0.77)	-4.73(1.64)
R72	14.25(0.86)	16.98(0.47)	-3.56(0.47)

^aE₁ is the forward energy barriers. ^bE₋₁ is the reverse energy barriers. ^cΔH is the reaction enthalpies. ^dValues in parentheses are the absolute values of deviation between calculation values and average values.

Table S5. Average Energy Barriers at 0K and Maximun Absolute Deviation for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction class		E ₁ ^a (kcal/mol)	E ₋₁ ^b (kcal/mol)	ΔH ^c (kcal/mol)
1,5-endo-cycloaddition	Avg ^d	31.48	29.43	1.68
	Mad ^e	1.84	2.04	2.23
1,6-endo-cycloaddition	Avg ^d	16.20	16.85	-1.42
	Mad ^e	1.26	2.03	2.00
1,7-endo-cycloaddition	Avg ^d	17.82	18.51	-1.65
	Mad ^e	1.26	2.97	2.84
1,5-exo-cycloaddition	Avg ^d	29.92	12.36	17.38
	Mad ^e	2.59	2.17	2.16
1,6-exo-cycloaddition	Avg ^d	17.24	15.63	1.12
	Mad ^e	1.66	1.66	1.62
1,7-exo-cycloaddition	Avg ^d	15.11	17.45	-3.09
	Mad ^e	0.99	1.10	1.64

^aE₁ is the forward energy barrier. ^bE₋₁ is the reverse energy barrier. ^cΔH is the reaction enthalpy. ^dAvg is the average energy barrier for a calss. ^eMad is the maximum absolute deviation of energy barriers between the calculated values and the average values within a class.

Table S6. Forward and Reverse Energy Barriers and Reaction Enthalpies for Intramolecular H-shift Reactions of Alkenyl Peroxy Radicals

Reaction class	Reaction	E ₁ ^a (kcal/mol)	E ₋₁ ^b (kcal/mol)	ΔH ^c (kcal/mol)
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1,4-H(as)	R1	30.07(0.74) ^d	29.96(0.32)	0.34(0.36)
	R2	30.64(1.31)	28.90(0.74)	1.94(1.96)
	R3	29.42(0.09)	28.15(1.49)	1.59(1.61)
	R4	31.19(1.86)	31.69(2.05)	-0.16(0.14)
	R5	29.37(0.04)	29.24(0.40)	0.47(0.49)
	R6	28.16(1.17)	29.63(0.01)	-1.06(1.04)
	R7	27.29(2.04)	30.13(0.49)	-2.67(2.65)
	R8	28.47(0.86)	29.45(0.19)	-0.63(0.61)
1,4-H(s)	R9	32.69(0.74) ^d	19.32(0.05)	13.75(0.66)
	R10	32.94(0.99)	20.14(0.87)	13.23(0.14)
	R11	32.76(0.81)	19.11(0.16)	14.04(0.95)
	R12	32.56(0.61)	19.51(0.24)	13.39(0.30)
	R13	32.90(0.95)	19.30(0.03)	13.97(0.88)
	R14	32.87(0.92)	19.27(0.00)	13.94(0.85)
	R15	29.86(2.10)	18.36(0.91)	12.10(0.99)
	R16	29.06(2.90)	19.12(0.15)	10.31(2.78)
1,4-H(vt)	R17	36.58(0.17) ^d	11.55(0.23)	25.58(0.05)
	R18	36.23(0.18)	11.09(0.23)	25.68(0.05)
1,4-H(vi)	R19	39.39(0.63) ^d	15.25(0.64)	24.54(0.01)
	R20	37.71(1.05)	13.64(0.97)	24.53(0.02)
	R21	38.29(0.47)	14.47(0.14)	24.18(0.37)
	R22	39.65(0.89)	15.09(0.48)	24.95(0.40)
1,5-H(as)	R23	19.44(0.59) ^d	20.13(0.15)	-0.46(0.41)
	R24	18.74(0.10)	20.24(0.26)	-1.08(0.21)
	R25	19.12(0.28)	19.70(0.28)	-0.31(0.56)
	R26	20.90(2.06)	21.09(1.11)	0.08(0.95)
	R27	18.89(0.05)	19.20(0.78)	-0.10(0.77)
	R28	19.43(0.59)	18.39(1.59)	1.30(2.17)
	R29	18.01(0.83)	20.71(0.73)	-2.35(1.48)

	R30	16.22(2.62)	20.40(0.42)	-4.01(3.14)
1,5-H(s)	R31	22.15(1.39) ^d	9.16(0.58)	6.32(2.83)
	R32	19.37(1.39)	8.00(0.58)	11.97(2.82)
1,5-H(vt)	R33	30.96(1.70) ^d	5.29(0.41)	25.97(2.06)
	R34	28.55(0.71)	6.09(0.34)	22.84(1.07)
	R35	28.27(0.99)	5.73(0.03)	22.91(1.00)
1,5-H(vi)	R36	27.90(0.11) ^d	5.86(0.33)	22.44(0.22)
	R37	28.25(0.46)	6.38(0.85)	22.26(0.40)
	R38	27.96(0.17)	5.56(0.03)	22.80(0.15)
	R39	26.90(0.89)	4.58(0.95)	22.72(0.07)
	R40	27.48(0.31)	5.22(0.31)	22.62(0.04)
	R41	28.23(0.44)	5.60(0.07)	23.09(0.44)
1,6-H(as)	R42	20.35(1.52) ^d	20.78(0.48)	-0.19(1.05)
	R43	17.31(1.52)	19.81(0.49)	-2.09(1.05)
1,6-H(s)	R44	21.67(0.00) ^d	8.67(0.00)	13.52(0.00)
1,6-H(vt)	R45	63.36(0.83) ^d	38.34(0.48)	25.32(0.32)
	R46	63.52(0.99)	37.82(0.04)	26.02(1.02)
	R47	62.28(0.25)	37.20(0.66)	25.36(0.36)
	R48	61.70(0.83)	36.21(1.65)	25.76(0.76)
	R49	61.78(0.75)	39.73(1.87)	22.52(2.48)
1,6-H(vi)	R50	26.70(0.28) ^d	4.87(0.45)	22.22(0.19)
	R51	25.67(0.76)	3.64(0.79)	22.44(0.03)
	R52	26.58(0.16)	4.75(0.33)	22.25(0.16)
	R53	26.75(0.33)	4.44(0.02)	22.72(0.31)

^aE₁ is the forward energy barriers. ^bE₋₁ is the reverse energy barriers. ^cΔH is the reaction enthalpies.

^dValues in parentheses are the absolute values of deviation between calculation values and average values.

Table S7. Average Energy Barriers and Maximun Absolute Deviation for Intramolecular H-shift

Reactions of Alkenyl Peroxy Radicals

Reaction class		E_1^a	E_{-1}^b	ΔH^c
		(kcal/mol)	(kcal/mol)	(kcal/mol)
1,4-H(as)	Avg ^d	29.33	29.64	-0.02
	Mad ^e	2.04	2.05	2.65
1,4-H(s)	Avg ^d	31.96	19.27	13.09
	Mad ^e	2.90	0.91	2.78
1,4-H(vt)	Avg ^d	36.41	11.32	25.63
	Mad ^e	0.18	0.23	0.05
1,4-H(vi)	Avg ^d	38.76	14.61	24.55
	Mad ^e	1.05	0.97	0.40
1,5-H(as)	Avg ^d	18.84	20.40	-0.87
	Mad ^e	2.62	1.59	3.14
1,5-H(s)	Avg ^d	20.76	8.58	9.15
	Mad ^e	1.39	0.58	2.83
1,5-H(vt)	Avg ^d	29.26	5.70	23.91
	Mad ^e	1.70	0.41	2.06
1,5-H(vi)	Avg ^d	27.79	5.53	22.66
	Mad ^e	0.89	0.95	0.44
1,6-H(as)	Avg ^d	18.83	20.30	-1.14
	Mad ^e	1.52	0.49	1.05
1,6-H(s)	Avg ^d	21.67	8.67	13.52
	Mad ^e	--	--	--
1,6-H(vt)	Avg ^d	62.53	37.86	25.00
	Mad ^e	0.99	1.87	2.48
1,6-H(vi)	Avg ^d	26.43	4.43	22.41
	Mad ^e	0.76	0.79	0.31

^aE₁ is the forward energy barrier. ^bE₋₁ is the reverse energy barrier. ^cΔH is the reaction enthalpy. ^dAvg is the average energy barrier. ^eMad is the maximum absolute deviation of energy barriers between calculation values and average values within a class.

Table S8. Forward and Reverse Energy Barriers and Reaction Enthalpies for Concerted Elimination Reactions of Alkenyl Peroxy Radicals

Reaction class	Reaction	E_1^a (kcal/mol)	E_{-1}^b (kcal/mol)	ΔH^c (kcal/mol)
Allylic	R1	27.39(0.68) ^d	12.95(1.76)	15.24(2.25)
Secondary C-H	R2	27.28(0.79)	14.25(3.06)	13.83(3.66)
	R3	27.44(0.63)	10.84(0.35)	17.63(0.14)
	R4	27.82(0.25)	8.00(3.19)	21.17(3.68)
	R5	27.77(0.30)	12.66(1.47)	15.89(1.60)
	R6	28.76(0.69)	9.58(1.61)	20.14(2.65)
	R7	30.21(2.14)	11.99(0.80)	18.86(1.37)
	R8	28.43(0.36)	10.05(1.14)	19.58(2.09)
	R9	27.50(0.57)	10.40(0.79)	15.10(2.39)
	R10	31.01(0.05) ^d	12.33(0.07)	19.50(0.13)
Secondary C-H	R11	31.45(0.49)	12.59(0.19)	19.68(0.31)
	R12	29.71(1.25)	10.73(1.67)	19.70(0.33)
	R13	31.57(0.61)	14.35(1.95)	18.06(1.31)
	R14	31.37(0.41)	14.47(2.07)	17.82(1.55)
	R15	30.65(0.31)	11.12(1.28)	20.32(0.95)
	R16	30.87(0.09)	11.70(0.70)	19.96(0.59)
	R17	31.02(0.06)	11.90(0.50)	19.92(0.55)
Vinylic C-H	R18	41.08(0.65) ^d	14.33(1.91)	27.84(1.55)
	R19	39.60(0.84)	9.92(2.50)	30.81(1.42)
	R20	39.63(0.81)	12.75(0.33)	29.23(0.16)
	R21	41.43(0.99)	12.68(0.26)	29.68(0.29)

^a E_1 is the forward energy barriers. ^b E_{-1} is the reverse energy barriers. ^c ΔH is the reaction enthalpies.
^dValues in parentheses are the absolute values of deviation between calculation values and average values.

Table S9. Average Energy Barriers and Maximun Absolute Deviation for Concerted Elimination

Reactions of Alkenyl Peroxy Radicals

Reaction class		E_1^a	E_{-1}^b	ΔH^c
		(kcal/mol)	(kcal/mol)	(kcal/mol)
Allylic Secondary C-H	Avg ^d	28.07	11.19	17.49
	Mad ^e	2.14	3.19	3.68
Secondary C-H	Avg ^d	30.96	12.40	19.37
	Mad ^e	1.25	2.07	1.55
Vinyllic C-H	Avg ^d	40.44	12.42	29.39
	Mad ^e	0.99	2.50	1.55

^a E_1 is the forward energy barrier. ^b E_{-1} is the reverse energy barrier. ^c ΔH is the reaction enthalpy. ^dAvg is the average energy barrier. ^eMad is the maximum absolute deviation of energy barriers between calculation values and average values within a class.

4. High Pressure Limit Rate Constants and Rate Rules

Table S10. High Pressure Limit Rate Constants and Ratio of the Rate Constants from TST to the Values from the Rate Rules for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction	modified Arrhenius parameters			500K		1000K	
	A(s ⁻¹)	n	E(kcal/mol)	k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
1,5-endo-cycloaddition	7.23 × 10⁻¹⁶	7.93	15.98	9.53 × 10⁻²	1.00	2.09 × 10⁵	1.00
R1	2.01 × 10 ⁻¹⁴	7.44	18.94	7.94 × 10 ⁻³	0.08	4.22 × 10 ⁴	0.20
R2	4.03 × 10 ⁻¹³	7.19	18.36	6.20 × 10 ⁻²	0.65	2.01 × 10 ⁵	0.96
R3	8.51 × 10 ⁻¹²	6.82	18.42	1.27 × 10 ⁻¹	1.33	3.14 × 10 ⁵	1.50
R4	6.99 × 10 ⁻⁴	4.40	22.82	4.32 × 10 ⁻²	0.45	1.39 × 10 ⁵	0.67
R5	2.42 × 10 ⁻⁴	4.58	22.40	6.79 × 10 ⁻²	0.71	2.04 × 10 ⁵	0.98
R6	2.38 × 10 ⁻²⁰	9.06	13.83	3.33 × 10 ⁻²	0.35	4.94 × 10 ⁴	0.24
R7	2.18 × 10 ⁻²¹	9.47	13.05	8.63 × 10 ⁻²	0.91	1.20 × 10 ⁵	0.57
R8	1.48 × 10 ⁻¹⁷	8.20	15.46	1.99 × 10 ⁻²	0.21	3.35 × 10 ⁴	0.16
R9	5.91 × 10 ⁻²²	9.70	12.27	2.08 × 10 ⁻¹	2.18	2.32 × 10 ⁵	1.11

R10	7.72×10^{-4}	4.51	21.91	2.31×10^{-1}	2.42	5.11×10^5	2.44
R11	1.82×10^{-4}	4.71	22.05	1.63×10^{-1}	1.71	4.56×10^5	2.18
1,6-endo-cycloaddition	3.55	3.05	9.17	5.13×10^4	1.00	5.56×10^7	1.00
R12	2.70	3.03	10.37	1.04×10^4	0.20	2.08×10^7	0.37
R13	9.16	3.00	10.51	2.50×10^4	0.49	5.24×10^7	0.94
R14	7.08	3.07	10.60	2.50×10^4	0.49	5.74×10^7	1.03
R15	3.88	3.02	10.13	1.78×10^4	0.35	3.14×10^7	0.56
R16	5.24	2.93	9.28	3.18×10^4	0.62	3.38×10^7	0.61
R17	1.38×10^2	2.65	9.59	1.11×10^5	2.16	1.11×10^8	2.00
R18	1.09×10^2	2.63	9.16	1.18×10^5	2.30	9.30×10^7	1.67
R19	7.82×10^2	2.22	11.15	9.26×10^3	0.18	1.43×10^7	0.26
R20	8.20×10	2.64	8.94	1.15×10^5	2.24	8.14×10^7	1.46
R21	1.40×10^3	2.10	10.74	1.17×10^4	0.23	1.33×10^7	0.24
R22	3.26×10	2.67	8.94	5.55×10^4	1.08	4.02×10^7	0.72
R23	2.50×10	2.93	9.83	8.46×10^4	1.65	1.18×10^8	2.12
1,7-endo-cycloaddition	2.60×10^{-1}	3.27	10.22	5.12×10^3	1.00	1.13×10^7	1.00
R24	8.88×10^{-2}	3.39	10.76	2.03×10^3	0.40	6.60×10^6	0.58
R25	3.14×10^{-1}	3.24	10.28	4.56×10^3	0.89	1.02×10^7	0.90
R26	1.46×10^{-1}	3.33	10.27	3.79×10^3	0.74	9.13×10^6	0.81
R27	5.80×10^{-1}	3.20	11.57	1.88×10^3	0.37	7.89×10^6	0.70
R28	3.67×10^{-1}	3.25	10.63	4.04×10^3	0.79	1.10×10^7	0.97
R29	1.18×10^{-1}	3.45	10.97	3.28×10^3	0.64	1.25×10^7	1.11
R30	4.83×10^{-2}	3.50	10.82	2.00×10^3	0.39	7.32×10^6	0.65
R31	1.09×10	2.81	10.41	1.02×10^4	1.99	1.75×10^7	1.55
R32	2.60	3.00	9.91	1.33×10^4	2.60	2.06×10^7	1.82
R33	3.39×10	2.69	12.46	1.91×10^3	0.37	8.35×10^6	0.74
R34	2.08×10	2.69	10.57	7.86×10^3	1.54	1.32×10^7	1.17
R35	8.54×10^{-3}	3.89	10.15	8.07×10^3	1.58	2.89×10^7	2.56
R36	2.12×10	2.70	10.43	9.74×10^3	1.90	1.54×10^7	1.36

1,5-exo-cycloaddition	1.47×10^{-4}	4.68	18.88	2.89	1.00	1.36×10^6	1.00
R37	2.41×10^{-5}	4.86	20.87	1.92×10^{-1}	0.07	2.90×10^5	0.21
R38	1.48×10^{-6}	5.29	18.96	1.15	0.40	9.45×10^5	0.69
R39	2.51×10^{-6}	5.27	18.23	3.60	1.25	2.03×10^6	1.49
R40	3.08×10^{-3}	4.26	20.62	7.46×10^{-1}	0.26	6.49×10^5	0.48
R41	5.39×10^{-3}	4.25	20.22	1.83	0.63	1.29×10^6	0.95
R42	2.10×10^{-2}	4.00	20.32	1.41	1.91×10^3	0.37	8.35×10^6
R43	6.15×10^{-3}	4.19	21.36	4.76×10^{-1}	7.86×10^3	1.54	1.32×10^7
R44	7.78×10^{-7}	5.09	21.46	1.32×10^{-2}	8.07×10^3	1.58	2.89×10^7
R45	6.07×10^{-2}	3.95	21.43	9.72×10^{-1}	9.74×10^3	1.90	1.54×10^7
R46	1.27×10^{-2}	4.20	19.30	7.96	2.75	3.41×10^6	2.51
R47	1.98×10^{-2}	4.15	18.95	1.35×10	4.67	4.71×10^6	3.46
1,6-exo-cycloaddition	1.35×10^{-3}	4.20	8.01	7.24×10^4	1.00	1.09×10^8	1.00
R48	2.26×10^{-4}	4.40	8.53	2.50×10^4	0.35	5.77×10^7	0.53
R49	9.85×10^{-4}	4.32	8.66	5.74×10^4	0.79	1.32×10^8	1.21
R50	6.48×10^{-4}	4.39	8.43	7.51×10^4	1.04	1.64×10^8	1.50
R51	9.89×10^{-5}	4.46	9.09	9.08×10^3	0.13	2.92×10^7	0.27
R52	9.74×10^{-5}	4.37	7.80	1.86×10^4	0.26	2.90×10^7	0.27
R53	3.97×10^{-2}	3.73	9.17	3.75×10^4	0.52	7.08×10^7	0.66
R54	8.76×10^{-2}	3.55	8.56	4.88×10^4	0.67	5.83×10^7	0.53
R55	5.98×10^{-3}	4.02	7.65	1.58×10^5	2.18	1.74×10^8	1.60
R56	2.97×10^{-2}	3.86	8.27	1.53×10^5	2.11	2.03×10^8	1.86
R57	8.31×10^{-3}	3.90	7.69	9.75×10^4	1.35	9.94×10^7	0.91
R58	1.60×10^{-2}	3.90	8.30	1.01×10^5	1.40	1.40×10^8	1.28
R59	7.44×10^{-3}	4.03	8.48	8.81×10^4	1.22	1.47×10^8	1.35
1,7-exo-cycloaddition	5.75×10^{-3}	3.79	6.43	1.25×10^5	1.00	6.17×10^7	1.00
R60	2.00×10^{-4}	4.19	6.80	3.39×10^4	0.27	2.79×10^7	0.45
R61	8.05×10^{-4}	3.99	5.98	9.43×10^4	0.75	4.37×10^7	0.71
R62	5.14×10^{-4}	4.06	6.52	5.25×10^4	0.42	3.36×10^7	0.54

R63	1.13×10^{-3}	4.02	7.08	5.29×10^4	0.42	4.38×10^7	0.71
R64	2.69×10^{-3}	3.92	6.28	1.45×10^5	1.16	7.37×10^7	1.19
R65	5.24×10^{-4}	4.16	6.62	8.87×10^4	0.71	6.48×10^7	1.05
R66	3.15×10^{-4}	4.15	6.46	6.05×10^4	0.48	4.07×10^7	0.66
R67	7.22×10^{-2}	3.35	7.69	2.93×10^4	0.23	1.93×10^7	0.31
R68	9.25×10^{-2}	3.28	7.57	2.69×10^4	0.22	1.57×10^7	0.25
R69	5.80×10^{-2}	3.53	6.45	2.42×10^5	1.94	9.89×10^7	1.60
R70	3.84×10^{-2}	3.58	6.84	1.45×10^5	1.16	7.45×10^7	1.21
R71	1.02×10^{-1}	3.52	6.50	3.84×10^5	3.07	1.59×10^8	2.58
R72	1.36×10^{-1}	3.42	6.53	2.74×10^5	2.19	1.07×10^8	1.73

Table S11. The Impact of the Substitute Groups on the High Pressure Limit Rate Constants for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction	Substitute group	500K		1000K	
		k_{TST}	k_{TST}/k_{rule}	k_{TST}	k_{TST}/k_{rule}
1,5-endo	C=CC(R)OO•	9.53×10^{-2}	1.00	2.09×10^5	1.00
R1	-H	7.94×10^{-3}	0.08	4.22×10^4	0.20
R2	-CH ₃	6.20×10^{-2}	0.65	2.01×10^5	0.96
R3	-C ₂ H ₅	1.27×10^{-1}	1.33	3.14×10^5	1.50
1,6-endo	C=CCC(R)OO•	5.13×10^4	1.00	5.56×10^7	1.00
R12	-H	1.04×10^4	0.20	2.08×10^7	0.37
R13	-CH ₃	2.50×10^4	0.49	5.24×10^7	0.94
R14	-C ₂ H ₅	2.50×10^4	0.49	5.74×10^7	1.03
1,7-endo	C=CC(R)CCOO•	5.12×10^3	1.00	1.13×10^7	1.00
R24	-H	2.03×10^3	0.40	6.60×10^6	0.58
R25	-CH ₃	4.56×10^3	0.89	1.02×10^7	0.90
R26	-C ₂ H ₅	3.79×10^3	0.74	9.13×10^6	0.81
1,5-exo	C=CC(R)OO•	2.89	1.00	1.36×10^6	1.00
R37	-H	1.92×10^{-1}	0.07	2.90×10^5	0.21

R38	-CH ₃	1.15	0.40	9.45×10^5	0.69
R39	-C ₂ H ₅	3.60	1.25	2.03×10^6	1.49
1,6-exo	C=CCC(R)OO•	7.24×10^4	1.00	1.09×10^8	1.00
R48	-H	2.50×10^4	0.35	5.77×10^7	0.53
R49	-CH ₃	5.74×10^4	0.79	1.32×10^8	1.21
R50	-C ₂ H ₅	7.51×10^4	1.04	1.64×10^8	1.50
1,7-exo	C=CC(R)CCOO•	1.25×10^5	1.00	6.17×10^7	1.00
R60	-H	3.39×10^4	0.27	2.79×10^7	0.45
R61	-CH ₃	9.43×10^4	0.75	4.37×10^7	0.71
R62	-C ₂ H ₅	5.25×10^4	0.42	3.36×10^7	0.54

R is the substituent group in a reactant molecule.

Table S12. The Impact of the Configurations of Reactant Molecules on the High Pressure Limit

Rate Constants for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction	Configuration	500K		1000K	
		k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
1,5-endo	CC=CCOO•	9.53×10^{-2}	1.00	2.09×10^5	1.00
R6	cis-	3.33×10^{-2}	0.35	4.94×10^4	0.24
R7	trans-	8.63×10^{-2}	0.91	1.20×10^5	0.57
	CCC=CCOO•				
R8	cis-	1.99×10^{-2}	0.21	3.35×10^4	0.16
R9	trans-	2.08×10^{-1}	2.18	2.32×10^5	1.11
1,6-endo	CC=CCCCOO•	5.13×10^4	1.00	5.56×10^7	1.00
R19	cis-	9.26×10^3	0.18	1.43×10^7	0.26
R20	trans-	1.15×10^5	2.24	8.14×10^7	1.46
	CCC=CCCCOO•				
R21	cis-	1.17×10^4	0.23	1.33×10^7	0.24
R22	trans-	5.55×10^4	1.08	4.02×10^7	0.72
1,7-endo	CC=CCCCOO•	5.12×10^3	1.00	1.13×10^7	1.00

R33	cis-	1.91×10^3	0.37	8.35×10^6	0.74
R34	trans-	7.86×10^3	1.54	1.32×10^7	1.17
CCC=CCCCOO•					
R35	cis-	8.07×10^3	1.58	2.89×10^7	2.56
R36	trans-	9.74×10^3	1.90	1.54×10^7	1.36
1,5-exo	CC=CCOO•	2.89	1.00	1.36×10^6	1.00
R42	cis-	1.41	1.91×10^3	0.37	8.35×10^6
R43	trans-	4.76×10^{-1}	7.86×10^3	1.54	1.32×10^7
CCC=CCOO•					
R44	cis-	1.32×10^{-2}	8.07×10^3	1.58	2.89×10^7
R45	trans-	9.72×10^{-1}	9.74×10^3	1.90	1.54×10^7
1,6-exo	CC=CCCCOO•	7.24×10^4	1.00	1.09×10^8	1.00
R55	cis-	1.58×10^5	2.18	1.74×10^8	1.60
R56	trans-	1.53×10^5	2.11	2.03×10^8	1.86
CCC=CCCCOO•					
R57	cis-	9.75×10^4	1.35	9.94×10^7	0.91
R58	trans-	1.01×10^5	1.40	1.40×10^8	1.28
1,7-exo	CC=CCCCOO•	1.25×10^5	1.00	6.17×10^7	1.00
R69	cis-	2.42×10^5	1.94	9.89×10^7	1.60
R70	trans-	1.45×10^5	1.16	7.45×10^7	1.21
CCC=CCCCOO•					
R71	cis-	3.84×10^5	3.07	1.59×10^8	2.58
R72	trans-	2.74×10^5	2.19	1.07×10^8	1.73

Table S13. High Pressure Limit Rate Constants and Ratio of the Rate Constants from TST to the Values from the Rate Rules for Intramolecular H-shift Reactions for Alkenyl Peroxy Radicals

Reaction	modified Arrhenius parameters			500K		1000K	
	A(s ⁻¹)	n	E(kcal/mol)	k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
1,4-H(as) rate rule	5.94×10^{-11}	6.36	13.76	2.90	1.00	9.20×10^5	1.00
R1	9.32×10^{-12}	6.54	14.12	8.48×10^{-1}	0.29	4.14×10^5	0.45

R2	9.25×10^{-12}	6.63	14.63	8.99×10^{-1}	0.31	5.99×10^5	0.65
R3	5.96×10^{-11}	6.43	14.21	2.76	0.95	1.17×10^6	1.28
R4	1.19×10^{-11}	6.42	15.62	1.13×10^{-1}	0.04	1.11×10^5	0.12
R5	9.00×10^{-11}	6.30	14.40	1.56	0.54	6.65×10^5	0.72
R6	4.71×10^{-10}	6.10	13.88	4.18	1.44	1.12×10^6	1.22
R7	5.14×10^{-10}	6.04	13.07	7.09	2.45	1.20×10^6	1.30
R8	1.24×10^{-9}	6.10	14.52	5.73	1.98	2.08×10^6	2.26
1,4-H(s) rate rule	3.26×10^{-15}	7.82	15.37	5.50×10^{-1}	1.00	5.42×10^5	1.00
R9	1.15×10^{-14}	7.69	17.77	7.19×10^{-2}	0.13	2.25×10^5	0.42
R10	3.48×10^{-16}	8.08	17.29	4.07×10^{-2}	0.07	1.38×10^5	0.25
R11	3.43×10^{-14}	7.62	18.13	1.08×10^{-1}	0.18	9.62×10^4	0.66
R12	1.28×10^{-14}	7.71	17.66	1.05×10^{-1}	0.19	3.17×10^5	0.58
R13	1.17×10^{-14}	7.64	18.05	4.27×10^{-2}	0.08	1.49×10^5	0.28
R14	3.10×10^{-14}	7.56	18.06	6.80×10^{-2}	0.12	2.25×10^5	0.41
R15	1.12×10^{-11}	6.84	16.74	1.09	1.97	1.04×10^6	1.93
R16	2.57×10^{-12}	7.06	15.61	2.89	5.25	1.88×10^6	3.46
1,4-H(vt) rate rule	9.61×10^{-1}	3.85	29.18	3.42×10^{-3}	1.00	1.55×10^5	1.00
R17	5.04×10^{-1}	3.93	29.19	2.89×10^{-3}	0.85	1.41×10^5	0.91
R18	1.72	3.77	29.18	3.95×10^{-3}	1.15	1.70×10^5	1.10
1,4-H(vi) rate rule	8.97×10^{-7}	5.49	27.82	3.22×10^{-4}	1.00	2.68×10^4	1.00
R19	2.00×10^{-8}	5.94	28.10	8.24×10^{-5}	0.26	1.14×10^4	0.43
R20	1.16×10^{-5}	5.26	27.91	9.27×10^{-4}	2.88	6.76×10^4	2.53
R21	4.56×10^{-7}	5.52	27.74	2.12×10^{-4}	0.66	1.77×10^4	0.66
R22	9.91×10^{-8}	5.74	28.68	6.56×10^{-5}	0.20	1.04×10^4	0.39
1,5-H(as) rate rule	3.91×10^{-7}	5.26	7.70	2.13×10^4	1.00	5.85×10^7	1.00
R23	2.56×10^{-6}	5.04	9.71	4.54×10^3	0.21	3.04×10^7	0.52
R24	1.43×10^{-5}	4.80	9.49	7.21×10^3	0.34	3.57×10^7	0.61
R25	2.26×10^{-5}	4.77	9.92	6.04×10^3	0.28	3.62×10^7	0.62
R26	9.27×10^{-7}	5.16	10.96	9.87×10^2	0.05	1.38×10^7	0.24

R27	2.60×10^{-5}	4.83	9.71	1.29×10^4	0.61	7.35×10^7	1.26
R28	4.37×10^{-5}	4.69	10.43	4.22×10^3	0.20	3.05×10^7	0.52
R29	8.32×10^{-5}	4.61	9.19	1.78×10^4	0.84	6.55×10^7	1.12
R30	1.09×10^{-3}	4.30	7.99	1.17×10^5	5.48	1.82×10^8	3.12
1,5-H(s) rate rule	1.24	3.47	10.26	8.66×10^4	1.00	2.04×10^8	1.00
R31	7.48×10	2.97	10.58	1.64×10^5	1.89	3.20×10^8	1.57
R32	9.86×10^2	2.69	14.33	8.72×10^3	0.10	8.89×10^7	0.44
1,5-H(vt) rate rule	4.60×10^4	2.19	24.79	2.07×10^{-1}	1.00	6.65×10^5	1.00
R33	1.68×10^6	1.74	28.13	3.98×10^{-2}	0.03	2.00×10^5	0.21
R34	1.98×10^5	2.02	25.00	6.06×10^{-1}	0.44	7.87×10^5	0.81
R35	3.28×10^5	1.97	24.84	8.76×10^{-1}	0.63	1.01×10^6	1.03
1,5-H(vi) rate rule	4.21×10^5	1.96	24.30	1.87	1.00	1.62×10^6	1.00
R36	1.83×10^5	2.02	24.44	9.99×10^{-1}	0.53	9.79×10^5	0.60
R37	5.96×10^4	2.13	24.51	6.20×10^{-1}	0.33	6.88×10^5	0.42
R38	5.27×10^5	1.98	24.76	1.70	0.91	1.90×10^6	1.17
R39	3.98×10^6	1.77	24.21	6.01	3.21	4.30×10^6	2.65
R40	4.86×10^5	1.85	24.35	1.06	0.57	8.73×10^5	0.54
R41	4.55×10^5	1.93	24.98	8.32×10^{-1}	0.44	9.94×10^5	0.61
1,6-H(as) rate rule	3.83×10^{-5}	4.59	8.40	8.29×10^3	1.00	2.26×10^7	1.00
R42	3.16×10^{-8}	9.67	5.46	7.51×10^2	0.09	6.88×10^6	0.30
R43	3.83×10^{-5}	4.59	8.40	1.58×10^4	1.91	3.83×10^7	1.69
1,6-H(s) rate rule	4.96×10	2.91	15.93	3.41×10^2	--	9.26×10^6	--
R44	4.96×10	2.91	15.93	3.41×10^2	--	9.26×10^6	--
1,6-H(vt) rate rule	5.49×10^{-15}	7.20	42.96	2.92×10^{-15}	1.00	1.25×10^{-2}	1.00
R45	3.82×10^{-15}	7.19	43.65	9.44×10^{-16}	0.25	5.84×10^{-3}	0.46
R46	1.18×10^{-14}	7.18	44.15	1.65×10^{-15}	0.43	1.24×10^{-2}	0.97
R47	2.63×10^{-14}	6.99	43.27	3.02×10^{-15}	0.79	1.21×10^{-2}	0.95
R48	1.08×10^{-13}	6.87	43.56	4.70×10^{-15}	1.22	1.87×10^{-2}	1.46
R49	2.48×10^{-15}	7.26	42.12	4.27×10^{-15}	1.11	1.35×10^{-2}	1.05

1,6-H(vi) rate rule	2.62×10^5	1.87	23.22	2.02	1.00	9.48×10^5	1.00
R50	2.16×10^5	1.86	23.38	1.35	0.67	6.82×10^5	0.72
R51	1.30×10^6	1.61	22.91	2.65	1.31	8.64×10^5	0.92
R52	4.75×10^5	1.83	23.49	2.08	1.03	1.08×10^6	1.14
R53	9.96×10^5	1.75	23.83	1.99	0.99	1.16×10^6	1.23

Table S14. The Impact of the Substitute Groups On the High Pressure Limit Rate Constants for Intramolecular H-Shift Reactions of Alkenyl Peroxy Radicals

Reaction	Substitute group	500K		1000K	
		k_{TST}	$k_{\text{TST}}/k_{\text{rule}}$	k_{TST}	$k_{\text{TST}}/k_{\text{rule}}$
1,4-H(as)	C=CCC(R)OO•	2.90	1.00	9.20×10^5	1.00
R1	-H	8.48×10^{-1}	0.29	4.14×10^5	0.45
R2	-CH ₃	8.99×10^{-1}	0.31	5.99×10^5	0.65
	C=C(R)CCOO•				
R3	-CH ₃	2.76	0.95	1.17×10^6	1.28
	C=CC(R)COO•				
R6	-CH ₃	4.18	1.44	1.12×10^6	1.22
R7	-C ₂ H ₅	7.09	2.45	1.20×10^6	1.30
1,4-H(s)	C=CC(R)CCOO•	5.50×10^{-1}	1.00	5.42×10^5	1.00
R9	-H	7.19×10^{-2}	0.13	2.25×10^5	0.42
R10	-CH ₃	4.07×10^{-2}	0.07	1.38×10^5	0.25
	C=CCCC(R)OO•				
R11	-CH ₃	1.08×10^{-1}	0.18	9.62×10^4	0.66
	C=C(R)CCCOO•				
R12	-CH ₃	1.05×10^{-1}	0.19	3.17×10^5	0.58
	C=CCC(R)COO•				
R15	-CH ₃	1.09	1.97	1.04×10^6	1.93
R16	-C ₂ H ₅	2.89	5.25	1.88×10^6	3.46
1,5-H(as)	C=CCC(R)COO•	2.13×10^4	1.00	5.85×10^7	1.00

R26	-CH ₃	9.87×10^2	0.05	1.38×10^7	0.24
	C=CCCC(R)OO•				
R27	-CH ₃	1.29×10^4	0.61	7.35×10^7	1.26
	C=C(R)CCCCOO•				
R28	-CH ₃	4.22×10^3	0.20	3.05×10^7	0.52
	C=CC(R)CCOO•				
R29	-CH ₃	1.78×10^4	0.84	6.55×10^7	1.12
R30	-C ₂ H ₅	1.17×10^5	5.48	1.82×10^8	3.12
1,5-H(s)	C=CCC(R)CCOO•	8.66×10^4	1.00	2.04×10^8	1.00
R31	-H	1.64×10^5	1.89	3.20×10^8	1.57
R32	-CH ₃	8.72×10^3	0.10	8.89×10^7	0.44
1,6-H(as)	C=CC(R)CCCCOO•	8.29×10^3	1.00	2.26×10^7	1.00
R42	-H	7.51×10^2	0.09	6.88×10^6	0.30
R43	-CH ₃	1.58×10^4	1.91	3.83×10^7	1.69

R is the substitute group in a reactant molecule.

Table S15. The Impact of the Configurations of Reactant Molecules on the High Pressure Limit

Rate Constants for Intramolecular H-Shift Reactions of Alkenyl Peroxy Radicals

Reaction	Configuration	500K		1000K	
		k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
1,4-H(as)	CC=CCCCOO•	2.90	1.00	9.20×10^5	1.00
R4	cis-	1.13×10^{-1}	0.04	1.11×10^5	0.12
R5	trans-	1.56	0.54	6.65×10^5	0.72
1,4-H(s)	CC=CCCCOO•	5.50×10^{-1}	1.00	5.42×10^5	1.00
R13	cis-	4.27×10^{-2}	0.08	1.49×10^5	0.28
R14	trans-	6.80×10^{-2}	0.12	2.25×10^5	0.41
1,5-H(as)	CC=CCCCOO•	2.13×10^4	1.00	5.85×10^7	1.00
R24	cis-	7.21×10^3	0.34	3.57×10^7	0.61
R25	trans-	6.04×10^3	0.28	3.62×10^7	0.62

Table S16. High Pressure Limit Rate Constants and Ratio of the Rate Constants from TST to the Values from the Rate Rules for Concerted Elimination Reactions of Alkenyl Peroxy Radicals

Reaction	modified Arrhenius parameters			500K		1000K	
	A(s ⁻¹)	n	E(kcal/mol)	k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
rate rule-1	1.63 × 10⁷	1.85	25.78	8.35	1.00	1.45 × 10⁷	1.00
R1	7.08 × 10 ⁵	2.05	24.64	3.71	0.44	4.18 × 10 ⁶	0.29
R2	8.58 × 10 ⁵	1.99	24.74	2.98	0.36	3.39 × 10 ⁶	0.23
R3	1.82 × 10 ⁷	1.77	25.46	7.58	0.91	1.04 × 10 ⁷	0.72
R4	7.58 × 10 ⁸	1.58	26.35	4.11 × 10	4.92	7.65 × 10 ⁷	5.28
R5	1.00 × 10 ⁶	2.01	25.14	2.56	0.31	3.61 × 10 ⁶	0.25
R6	4.93 × 10 ⁷	1.74	26.75	4.79	0.57	1.23 × 10 ⁷	0.85
R7	6.79 × 10 ⁵	2.02	27.67	1.48 × 10 ⁻¹	0.02	7.48 × 10 ⁵	0.05
R8	2.01 × 10 ⁷	1.77	26.33	3.47	0.42	7.35 × 10 ⁶	0.51
R9	1.50 × 10 ⁷	1.80	25.34	8.75	1.05	1.16 × 10 ⁷	0.80
rate rule-2	2.19 × 10⁵	2.28	27.79	2.12 × 10⁻¹	1.00	1.40 × 10⁶	1.00
R10	9.50 × 10 ⁵	2.09	28.33	1.66 × 10 ⁻¹	0.78	1.24 × 10 ⁶	0.89
R11	4.97 × 10 ⁵	2.05	28.68	4.74 × 10 ⁻²	0.22	4.10 × 10 ⁵	0.29
R12	1.12 × 10 ⁶	2.03	27.14	4.25 × 10 ⁻¹	2.00	1.65 × 10 ⁶	1.18
R13	1.90 × 10 ⁶	2.07	29.07	1.31 × 10 ⁻¹	0.62	1.39 × 10 ⁶	0.99
R14	1.70 × 10 ⁶	1.99	28.86	9.24 × 10 ⁻²	0.44	8.32 × 10 ⁵	0.59
R15	3.24 × 10 ⁶	2.03	28.11	4.59 × 10 ⁻¹	2.17	2.91 × 10 ⁶	2.08
R16	1.36 × 10 ⁶	2.06	28.24	2.12 × 10 ⁻¹	1.00	1.48 × 10 ⁶	1.06
R17	1.20 × 10 ⁶	2.07	28.39	1.66 × 10 ⁻¹	0.78	1.25 × 10 ⁶	0.89
rate rule-3	1.44 × 10⁶	2.15	37.39	3.74 × 10⁻⁵	1.00	2.76 × 10⁴	1.00
R18	2.33 × 10 ⁵	2.31	38.23	7.35 × 10 ⁻⁶	0.20	9.50 × 10 ³	0.34
R19	1.43 × 10 ⁷	1.96	37.45	1.14 × 10 ⁻⁴	3.05	7.57 × 10 ⁴	2.74
R20	1.12 × 10 ⁶	2.10	37.38	2.24 × 10 ⁻⁵	0.60	1.60 × 10 ⁴	0.58
R21	6.24 × 10 ⁵	2.21	38.84	5.74 × 10 ⁻⁶	0.15	9.32 × 10 ³	0.34

Table S17. The Impact of the Configurations of Reactant Molecules on the High Pressure Limit

Rate Constants for Concerted Elimination Reactions of Alkenyl Peroxy Radicals

Reaction	Configuration	500K		1000K	
		k _{TST}	k _{TST} /k _{rule}	k _{TST}	k _{TST} /k _{rule}
rate-1	CC=CCC(C)OO•	8.35	1.00	1.45×10⁷	1.00
R8	cis-	3.47	0.42	7.35×10 ⁶	0.51
R9	trans-	8.75	1.05	1.16×10 ⁷	0.80
Rate-2	CC=CCCCOO•	2.12×10⁻¹	1.00	1.40×10⁶	1.00
R16	cis-	2.12×10 ⁻¹	1.00	1.48×10 ⁶	1.06
R17	trans-	1.66×10 ⁻¹	0.78	1.25×10 ⁶	0.89
rate -3	CC=CCOO•	3.74×10⁻⁵	1.00	2.76×10⁴	1.00
R20	cis-	2.24×10 ⁻⁵	0.60	1.60×10 ⁴	0.58
R21	trans-	5.74×10 ⁻⁶	0.15	9.32×10 ³	0.34

5. Pressure-Dependent Rate Constants and Rate Rules

Table S18. Pressure-Dependent Rate Constants, Rate Rules and Ratios of the Individually Calculated Rate Constants for Cycloaddition Reactions of Alkenyl Peroxy Radicals

Reaction	Pressure(atm)	modified Arrhenius parameters			500K		1000K	
		A(s ⁻¹)	n	E(kcal/mol)	k	k/k _{rule}	k	k/k _{rule}
1,5-endo-cycloaddition	0.01	7.38×10⁵	1.08	22.30	4.70×10⁻²	1.00	2.88×10⁴	1.00
rate rule								
	0.1	7.60×10⁻³	3.70	20.23	4.74×10⁻²	1.00	6.48×10⁴	1.00
	1	9.35×10⁻⁹	5.61	18.56	4.75×10⁻²	1.00	9.45×10⁴	1.00
	10	8.11×10⁻¹¹	6.27	17.96	4.75×10⁻²	1.00	1.04×10⁵	1.00
	100	3.81×10⁻¹¹	6.37	17.87	4.75×10⁻²	1.00	1.05×10⁵	1.00
R1	0.01	3.31×10 ⁴	1.44	24.09	3.59×10 ⁻³	0.08	5.91×10 ³	0.21
	0.1	5.94×10 ⁻⁴	3.99	22.10	3.70×10 ⁻³	0.08	1.30×10 ⁴	0.20
	1	8.66×10 ⁻¹¹	6.19	20.16	3.72×10 ⁻³	0.08	1.91×10 ⁴	0.20
	10	1.44×10 ⁻¹⁴	7.39	19.03	3.72×10 ⁻³	0.08	2.15×10 ⁴	0.21
	100	2.02×10 ⁻¹⁵	7.66	18.77	3.72×10 ⁻³	0.08	2.18×10 ⁴	0.21

R2	0.01	8.08×10^{10}	-0.39	24.88	4.48×10^{-2}	0.95	3.14×10^4	1.09
	0.1	2.38×10^2	2.42	22.70	4.55×10^{-2}	0.96	7.87×10^4	1.21
	1	2.34×10^{-6}	5.00	20.43	4.56×10^{-2}	0.96	1.26×10^5	1.33
	10	1.87×10^{-10}	6.31	19.21	4.56×10^{-2}	0.96	1.44×10^5	1.39
	100	3.49×10^{-11}	6.54	18.99	4.56×10^{-2}	0.96	1.47×10^5	1.40
R3	0.01	1.64×10^{11}	-0.46	24.77	8.05×10^{-2}	1.71	4.79×10^4	1.66
	0.1	2.35×10^2	2.43	22.43	8.10×10^{-2}	1.71	1.15×10^5	1.78
	1	1.98×10^{-4}	4.9	20.71	8.11×10^{-2}	1.71	1.74×10^5	1.84
	10	1.06×10^{-5}	4.80	20.35	8.11×10^{-2}	1.71	1.91×10^5	1.84
	100	7.65×10^{-6}	4.85	20.32	8.11×10^{-2}	1.71	1.93×10^5	1.84
R4	0.01	2.53×10^{15}	-1.72	28.06	1.82×10^{-2}	0.36	1.86×10^4	0.46
	0.1	9.15×10^7	1.03	25.78	1.83×10^{-2}	0.36	3.71×10^4	0.37
	1	5.32	3.02	23.95	1.83×10^{-2}	0.36	4.85×10^4	0.32
	10	8.36×10^{-2}	3.59	23.42	1.83×10^{-2}	0.36	5.11×10^4	0.30
	100	4.97×10^{-2}	3.67	23.35	1.83×10^{-2}	0.36	5.14×10^4	0.30
R5	0.01	3.83×10^{17}	-2.32	28.50	3.99×10^{-2}	0.39	3.60×10^4	0.44
	0.1	7.03×10^8	0.53	26.15	4.01×10^{-2}	0.39	7.79×10^4	0.34
	1	5.31×10^3	2.18	24.70	4.01×10^{-2}	0.39	1.06×10^5	0.29
	10	6.60×10^2	2.47	24.45	4.01×10^{-2}	0.39	1.13×10^5	0.27
	100	5.28×10^2	2.50	24.42	4.01×10^{-2}	0.39	1.13×10^5	0.27
R6	0.01	1.67×10^{-4}	3.90	18.61	1.71×10^{-2}	0.39	1.33×10^4	0.65
	0.1	6.12×10^{-13}	6.63	16.27	1.72×10^{-2}	0.39	2.41×10^4	0.57
	1	1.72×10^{-18}	8.41	14.63	1.72×10^{-2}	0.39	2.98×10^4	0.51
	10	7.88×10^{-20}	8.84	14.23	1.72×10^{-2}	0.39	3.09×10^4	0.49
	100	5.50×10^{-20}	8.89	14.18	1.72×10^{-2}	0.39	3.10×10^4	0.49
R7	0.01	1.78×10^{-6}	4.47	17.52	1.83×10^{-2}	0.85	1.26×10^4	1.25
	0.1	8.03×10^{-15}	7.17	15.20	1.83×10^{-2}	0.85	2.22×10^4	1.20
	1	4.54×10^{-20}	8.85	13.65	1.83×10^{-2}	0.84	2.69×10^4	1.13
	10	2.94×10^{-21}	9.23	13.29	1.83×10^{-2}	0.84	2.78×10^4	1.09

R8	100	2.15×10^{-21}	9.27	13.25	1.83×10^{-2}	0.84	2.79×10^4	1.08
	0.01	2.89×10^{-5}	4.14	19.02	9.27×10^{-3}	0.20	9.13×10^3	0.32
	0.1	7.95×10^{-11}	5.93	17.45	9.27×10^{-3}	0.20	1.27×10^4	0.20
	1	6.72×10^{-12}	6.27	17.14	9.27×10^{-3}	0.20	1.35×10^4	0.14
	10	5.13×10^{-12}	6.31	17.11	9.27×10^{-3}	0.20	1.36×10^4	0.13
R9	100	5.00×10^{-12}	6.32	17.11	9.27×10^{-3}	0.20	1.37×10^4	0.13
	0.01	4.76×10^{-5}	4.08	17.36	4.78×10^{-2}	1.02	2.45×10^4	0.85
	0.1	2.03×10^{-13}	6.79	15.05	4.79×10^{-2}	1.01	4.56×10^4	0.70
	1	5.92×10^{-17}	7.93	14.04	4.79×10^{-2}	1.01	5.58×10^4	0.59
	10	1.88×10^{-17}	8.09	13.90	4.79×10^{-2}	1.01	5.75×10^4	0.55
R10	100	1.67×10^{-17}	8.10	13.89	4.79×10^{-2}	1.01	5.77×10^4	0.55
	0.01	5.65×10^{21}	-3.58	28.81	1.78×10^{-1}	3.79	7.03×10^4	2.44
	0.1	1.71×10^{13}	-0.77	26.67	1.81×10^{-1}	3.81	1.90×10^5	2.93
	1	5.69×10^5	1.65	24.59	1.81×10^{-1}	3.81	3.22×10^5	3.41
	10	3.23×10^3	2.38	23.96	1.81×10^{-1}	3.81	3.72×10^5	3.58
R11	100	1.73×10^3	2.46	23.89	1.81×10^{-1}	3.81	3.78×10^5	3.60
	0.01	4.29×10^{17}	-2.32	28.19	5.95×10^{-2}	1.27	4.73×10^4	1.64
	0.1	1.07×10^{11}	-0.16	26.47	5.97×10^{-2}	1.26	9.57×10^4	1.48
	1	4.91×10^9	0.29	26.15	5.97×10^{-2}	1.26	1.17×10^5	1.24
	10	3.59×10^9	0.33	26.13	5.97×10^{-2}	1.26	1.20×10^5	1.16
1,6-endo-cycloaddition	100	3.48×10^9	0.34	26.12	5.97×10^{-2}	1.26	1.21×10^5	1.15
	0.01	2.19×10^{12}	-1.20	11.24	1.56×10^4	1.00	1.75×10^6	1.00
	0.1	1.17×10^{11}	-0.57	11.72	2.23×10^4	1.00	6.25×10^6	1.00
	1	5.57×10^7	0.61	11.25	2.43×10^4	1.00	1.55×10^7	1.00
	10	2.96×10^6	1.07	11.08	2.46×10^4	1.00	2.36×10^7	1.00
R12	100	2.19×10^6	1.12	11.08	2.46×10^4	1.00	2.56×10^7	1.00
	0.01	8.92×10^{13}	-1.73	12.80	5.02×10^3	0.32	9.10×10^5	0.52
	0.1	1.80×10^{12}	-0.95	13.17	7.25×10^3	0.33	3.45×10^6	0.55
	1	5.21×10^7	0.62	12.34	8.01×10^3	0.33	9.04×10^6	0.58

R13	10	1.93×10^3	2.09	11.22	8.13×10^3	0.33	1.46×10^7	0.62
	100	1.35×10^2	2.46	10.92	8.14×10^3	0.33	1.65×10^7	0.65
	0.01	8.28×10^{14}	-1.94	13.11	9.38×10^3	0.60	1.59×10^6	0.91
	0.1	1.12×10^{13}	-1.12	13.42	1.27×10^4	0.57	5.92×10^6	0.95
	1	2.97×10^8	0.46	12.56	1.35×10^4	0.56	1.52×10^7	0.98
R14	10	6.51×10^5	1.36	11.96	1.36×10^4	0.55	2.35×10^7	1.00
	100	3.24×10^5	1.46	11.91	1.36×10^4	0.55	2.56×10^7	1.00
	0.01	1.96×10^{15}	-2.02	13.15	1.28×10^4	0.82	2.01×10^6	1.15
	0.1	5.00×10^{13}	-1.29	13.57	1.74×10^4	0.78	7.68×10^6	1.23
	1	5.57×10^9	0.11	12.94	1.86×10^4	0.77	2.06×10^7	1.33
R15	10	7.36×10^8	0.45	12.92	1.88×10^4	0.76	3.26×10^7	1.38
	100	7.80×10^8	0.45	12.97	1.88×10^4	0.76	3.55×10^7	1.39
	0.01	6.33×10^{13}	-1.62	12.79	6.84×10^3	0.44	1.33×10^6	0.76
	0.1	1.64×10^{11}	-0.59	12.82	8.61×10^3	0.39	4.60×10^6	0.74
	1	2.56×10^6	1.04	11.81	8.99×10^3	0.37	1.07×10^7	0.69
R16	10	2.70×10^4	1.71	11.37	9.04×10^3	0.37	1.50×10^7	0.64
	100	1.69×10^4	1.78	11.34	9.04×10^3	0.37	1.59×10^7	0.62
	0.01	1.01×10^{12}	-1.09	12.05	5.96×10^3	0.38	1.25×10^6	0.72
	0.1	4.66×10^8	0.15	11.73	6.84×10^3	0.31	3.85×10^6	0.62
	1	4.86×10^6	0.86	11.49	6.98×10^3	0.29	7.50×10^6	0.48
R17	10	5.41×10^6	0.87	11.60	6.99×10^3	0.28	8.90×10^6	0.38
	100	5.63×10^6	0.86	11.61	7.00×10^3	0.28	9.08×10^6	0.36
	0.01	1.43×10^{13}	-1.44	11.22	2.45×10^4	1.57	2.18×10^6	1.24
	0.1	1.71×10^{12}	-0.92	11.82	3.62×10^4	1.62	7.96×10^6	1.27
	1	3.12×10^8	0.40	11.23	3.97×10^4	1.63	1.99×10^7	1.28
R18	10	2.49×10^6	1.12	10.80	4.02×10^4	1.63	3.03×10^7	1.28
	100	1.55×10^6	1.20	10.78	4.02×10^4	1.63	3.29×10^7	1.29
	0.01	6.09×10^{12}	-1.31	10.69	4.10×10^4	2.62	2.96×10^6	1.69
	0.1	1.74×10^{12}	-0.90	11.42	6.18×10^4	2.77	1.09×10^7	1.75

R19	1	3.60×10^9	0.10	11.19	6.82×10^4	2.81	2.83×10^7	1.83
	10	3.40×10^9	0.16	11.43	6.91×10^4	2.81	4.33×10^7	1.84
	100	4.47×10^9	0.13	11.50	6.92×10^4	2.81	4.65×10^7	1.82
	0.01	3.34×10^{14}	-1.84	13.81	3.17×10^3	0.20	9.11×10^5	0.52
	0.1	6.95×10^{10}	-0.51	13.36	3.63×10^3	0.16	2.74×10^6	0.44
R20	1	6.00×10^6	0.86	12.44	3.70×10^3	0.15	5.17×10^6	0.33
	10	1.03×10^6	1.12	12.30	3.71×10^3	0.15	6.20×10^6	0.26
	100	8.74×10^5	1.15	12.29	3.71×10^3	0.15	6.35×10^6	0.25
	0.01	3.82×10^{11}	-0.99	11.34	8.72×10^3	0.56	1.30×10^6	0.74
	0.1	6.06×10^8	0.09	11.24	1.08×10^4	0.48	4.26×10^6	0.68
R21	1	1.44×10^4	1.66	10.25	1.12×10^4	0.46	9.18×10^6	0.59
	10	4.59×10^2	2.16	9.93	1.12×10^4	0.46	1.22×10^7	0.52
	100	3.30×10^2	2.21	9.91	1.12×10^4	0.46	1.28×10^7	0.50
	0.01	9.11×10^{13}	-1.68	13.23	4.26×10^3	0.27	1.03×10^6	0.59
	0.1	6.04×10^{10}	-0.52	12.88	4.71×10^3	0.21	2.81×10^6	0.45
R22	1	2.19×10^{10}	-0.32	13.01	4.77×10^3	0.20	4.56×10^6	0.29
	10	2.80×10^{10}	-0.34	13.09	4.78×10^3	0.19	4.98×10^6	0.21
	100	2.89×10^{10}	-0.34	13.10	4.78×10^3	0.19	5.03×10^6	0.20
	0.01	2.42×10^{12}	-1.20	10.63	3.38×10^4	2.16	2.64×10^6	1.51
	0.1	2.55×10^{11}	-0.66	11.20	4.84×10^4	2.17	9.39×10^6	1.50
R23	1	5.05×10^8	0.33	10.92	5.24×10^4	2.16	2.32×10^7	1.49
	10	5.32×10^8	0.37	11.13	5.29×10^4	2.15	3.35×10^7	1.42
	100	6.51×10^8	0.35	11.19	5.30×10^4	2.15	3.55×10^7	1.39
	0.01	1.55×10^{14}	-1.71	11.71	3.21×10^4	2.06	2.87×10^6	1.64
	0.1	4.88×10^{13}	-1.30	12.52	4.97×10^4	2.23	1.14×10^7	1.82
1,7-endo-cycloaddition	1	2.46×10^{10}	-0.09	12.17	5.57×10^4	2.29	3.29×10^7	2.12
	10	2.69×10^9	0.29	12.19	5.66×10^4	2.30	5.80×10^7	2.46
	100	3.49×10^9	0.27	12.28	5.67×10^4	2.30	6.53×10^7	2.55
	0.01	1.06×10^{12}	-1.09	13.39	1.50×10^3	1.00	7.14×10^5	1.00

rate rule	0.1	1.35×10^9	-0.03	13.07	1.60×10^3	1.00	1.87×10^6	1.00
	1	2.29×10^8	0.27	13.06	1.62×10^3	1.00	2.84×10^6	1.00
	10	2.45×10^8	0.27	13.11	1.62×10^3	1.00	3.07×10^6	1.00
	100	2.47×10^8	0.27	13.12	1.62×10^3	1.00	3.09×10^6	1.00
	R24	0.01	2.33×10^{12}	-1.23	14.03	6.87×10^2	0.46	4.28×10^5
	0.1	4.57×10^7	0.40	13.17	7.44×10^2	0.46	1.17×10^6	0.63
	1	4.66×10^4	1.42	12.52	7.53×10^2	0.47	1.97×10^6	0.69
	10	2.01×10^4	1.55	12.47	7.54×10^2	0.47	2.23×10^6	0.73
	100	1.86×10^4	1.56	12.46	7.54×10^2	0.47	2.27×10^6	0.73
	R25	0.01	5.87×10^{12}	-1.30	13.41	2.19×10^3	1.46	8.62×10^5
	0.1	7.11×10^8	0.09	12.82	2.37×10^3	1.48	2.40×10^6	1.29
	1	5.79×10^7	0.50	12.76	2.40×10^3	1.48	4.02×10^6	1.41
	10	6.28×10^7	0.50	12.83	2.40×10^3	1.48	4.45×10^6	1.45
	100	6.40×10^7	0.50	12.83	2.40×10^3	1.48	4.50×10^6	1.45
	R26	0.01	3.29×10^{11}	-0.92	13.46	1.14×10^3	0.76	6.81×10^5
	0.1	2.84×10^{10}	-0.46	13.66	1.19×10^3	0.74	1.64×10^6	0.88
	1	1.17×10^{11}	-0.62	13.99	1.19×10^3	0.74	2.13×10^6	0.75
	10	1.47×10^{11}	-0.65	14.04	1.19×10^3	0.74	2.20×10^6	0.72
	100	1.51×10^{11}	-0.65	14.05	1.19×10^3	0.74	2.21×10^6	0.71
	R27	0.01	4.34×10^{14}	-1.83	15.14	1.07×10^3	0.71	7.18×10^5
	0.1	2.16×10^{10}	-0.32	14.42	1.14×10^3	0.71	2.00×10^6	1.07
	1	1.41×10^9	0.12	14.33	1.15×10^3	0.71	3.33×10^6	1.17
	10	1.45×10^9	0.13	14.38	1.15×10^3	0.71	3.67×10^6	1.20
	100	1.46×10^9	0.13	14.39	1.15×10^3	0.71	3.71×10^6	1.20
	R28	0.01	1.39×10^{12}	-1.11	13.91	9.95×10^2	0.66	6.51×10^5
	0.1	2.36×10^{11}	-0.74	14.18	1.03×10^3	0.64	1.53×10^6	0.82
	1	9.52×10^{11}	-0.90	14.50	1.03×10^3	0.64	1.95×10^6	0.69
	10	1.18×10^{12}	-0.92	14.55	1.03×10^3	0.64	2.01×10^6	0.66
	100	1.20×10^{12}	-0.93	14.55	1.03×10^3	0.64	2.01×10^6	0.65

R29	0.01	4.79×10^{13}	-1.55	14.47	1.28×10^3	0.85	7.55×10^5	1.06
	0.1	3.08×10^9	-0.07	13.79	1.37×10^3	0.85	2.12×10^6	1.13
	1	2.32×10^8	0.35	13.72	1.38×10^3	0.86	3.53×10^6	1.24
	10	2.45×10^8	0.35	13.78	1.38×10^3	0.86	3.90×10^6	1.27
	100	2.49×10^8	0.35	13.78	1.38×10^3	0.86	3.94×10^6	1.27
R30	0.01	7.44×10^{12}	-1.30	14.31	1.08×10^3	0.72	7.42×10^5	1.04
	0.1	1.21×10^{11}	-0.59	14.33	1.12×10^3	0.70	1.94×10^6	1.04
	1	5.53×10^{11}	-0.76	14.72	1.13×10^3	0.70	2.71×10^6	0.96
	10	7.43×10^{11}	-0.79	14.78	1.13×10^3	0.70	2.83×10^6	0.92
	100	7.67×10^{11}	-0.80	14.79	1.13×10^3	0.70	2.85×10^6	0.92
R31	0.01	1.21×10^{13}	-1.41	13.07	3.32×10^3	2.21	9.52×10^5	1.33
	0.1	4.73×10^9	-0.18	12.64	3.63×10^3	2.26	2.58×10^6	1.38
	1	5.93×10^8	0.16	12.60	3.67×10^3	2.27	4.16×10^6	1.46
	10	1.31×10^9	0.06	12.77	3.68×10^3	2.27	4.54×10^6	1.48
	100	1.34×10^9	0.06	12.78	3.68×10^3	2.27	4.59×10^6	1.48
R32	0.01	1.09×10^{12}	-1.09	12.72	2.97×10^3	1.98	9.52×10^5	1.33
	0.1	1.14×10^{11}	-0.64	13.00	3.17×10^3	1.97	2.42×10^6	1.29
	1	8.17×10^{11}	-0.87	13.44	3.19×10^3	1.97	3.32×10^6	1.17
	10	1.15×10^{12}	-0.91	13.51	3.19×10^3	1.97	3.46×10^6	1.13
	100	1.19×10^{12}	-0.92	13.51	3.19×10^3	1.97	3.47×10^6	1.12
R33	0.01	6.44×10^{15}	-2.16	16.05	8.06×10^2	0.54	6.66×10^5	0.93
	0.1	1.36×10^{11}	-0.53	15.22	8.56×10^2	0.53	1.91×10^6	1.02
	1	2.94×10^9	0.06	14.99	8.63×10^2	0.53	3.27×10^6	1.15
	10	2.68×10^9	0.09	15.03	8.63×10^2	0.53	3.65×10^6	1.19
	100	2.68×10^9	0.09	15.04	8.63×10^2	0.53	3.69×10^6	1.19
R34	0.01	9.23×10^{12}	-1.37	13.35	2.40×10^3	1.60	8.44×10^5	1.18
	0.1	1.84×10^9	-0.06	12.81	2.59×10^3	1.62	2.27×10^6	1.21
	1	3.79×10^8	0.22	12.85	2.62×10^3	1.62	3.62×10^6	1.27
	10	4.30×10^8	0.21	12.91	2.62×10^3	1.62	3.93×10^6	1.28

R35	100	4.39×10^8	0.21	12.92	2.62×10^3	1.62	3.97×10^6	1.28
	0.01	1.08×10^{11}	-0.77	14.90	2.02×10^2	0.13	3.33×10^5	0.47
	0.1	9.46×10^{10}	-0.67	15.24	2.04×10^2	0.13	6.35×10^5	0.34
	1	1.79×10^{11}	-0.74	15.39	2.04×10^2	0.13	7.20×10^5	0.25
	10	1.94×10^{11}	-0.75	15.41	2.04×10^2	0.13	7.30×10^5	0.24
R36	100	1.96×10^{11}	-0.75	15.41	2.04×10^2	0.13	7.31×10^5	0.24
	0.01	5.48×10^{11}	-1.00	13.34	1.38×10^3	0.92	7.00×10^5	0.98
	0.1	4.15×10^{10}	-0.52	13.52	1.44×10^3	0.90	1.68×10^6	0.90
	1	1.70×10^{11}	-0.68	13.86	1.44×10^3	0.89	2.20×10^6	0.77
	10	2.14×10^{11}	-0.70	13.91	1.44×10^3	0.89	2.27×10^6	0.74
1,5-exo-cycloaddition	100	2.19×10^{11}	-0.71	13.91	1.44×10^3	0.89	2.28×10^6	0.74
	0.01	2.01×10^{21}	-3.60	25.55	1.80	1.00	9.89×10^4	1.00
	0.1	1.07×10^{14}	-1.15	23.92	1.86	1.00	3.07×10^5	1.00
	1	3.60×10^6	1.29	21.94	1.86	1.00	6.19×10^5	1.00
	10	6.51×10^2	2.50	20.89	1.86	1.00	7.97×10^5	1.00
R37	100	9.43×10	2.77	20.65	1.86	1.00	8.31×10^5	1.00
	0.01	2.47×10^{17}	-2.41	26.92	8.41×10^{-2}	0.05	2.40×10^4	0.24
	0.1	4.32×10^9	0.17	25.06	8.79×10^{-2}	0.05	6.53×10^4	0.21
	1	5.98×10	2.72	22.89	8.84×10^{-2}	0.05	1.15×10^5	0.19
	10	1.84×10^{-4}	4.48	21.26	8.85×10^{-2}	0.05	1.40×10^5	0.18
R38	100	2.13×10^{-6}	5.09	20.67	8.85×10^{-2}	0.05	1.45×10^5	0.18
	0.01	6.95×10^{19}	-3.13	25.88	7.59×10^{-1}	0.42	7.86×10^4	0.79
	0.1	1.28×10^{12}	-0.54	24.09	7.86×10^{-1}	0.42	2.40×10^5	0.78
	1	5.33×10^3	2.19	21.82	7.90×10^{-1}	0.42	4.74×10^5	0.77
	10	4.52×10^{-3}	4.13	20.04	7.91×10^{-1}	0.42	6.16×10^5	0.77
R39	100	9.51×10^{-5}	4.67	19.54	7.91×10^{-1}	0.42	6.47×10^5	0.78
	0.01	5.17×10^{22}	-3.97	25.73	3.57	1.98	1.74×10^5	1.76
	0.1	2.17×10^{15}	-1.48	24.12	3.70	2.00	5.91×10^5	1.93
	1	6.25×10^6	1.31	21.87	3.72	2.00	1.34×10^6	2.17

R40	10	2.28×10	3.07	20.34	3.72	2.00	1.91×10^6	2.40
	100	2.17	3.40	20.06	3.72	2.00	2.05×10^6	2.46
	0.01	4.50×10^{20}	-3.36	26.98	4.09×10^{-1}	0.31	6.16×10^4	0.68
	0.1	4.90×10^{12}	-0.71	25.05	4.20×10^{-1}	0.31	1.69×10^5	0.61
	1	4.86×10^4	1.88	22.82	4.22×10^{-1}	0.30	2.95×10^5	0.49
R41	10	1.27	3.35	21.47	4.22×10^{-1}	0.30	3.52×10^5	0.43
	100	0.16	3.63	21.20	4.22×10^{-1}	0.30	3.62×10^5	0.42
	0.01	6.28×10^{22}	-3.97	27.05	1.14	0.09	1.14×10^5	0.41
	0.1	6.21×10^{14}	-1.31	25.13	1.17	0.09	3.31×10^5	0.32
	1	1.34×10^7	1.18	23.03	1.17	0.09	6.03×10^5	0.25
R42	10	3.00×10^4	2.04	22.29	1.17	0.09	7.22×10^5	0.22
	100	1.39×10^4	2.14	22.20	1.17	0.09	7.40×10^5	0.21
	0.01	1.63×10^{19}	-2.91	26.14	5.54×10^{-1}	0.23	6.67×10^4	0.62
	0.1	1.49×10^{11}	-0.26	24.13	5.65×10^{-1}	0.23	1.88×10^5	0.55
	1	3.75×10^3	2.20	21.99	5.67×10^{-1}	0.23	3.01×10^5	0.48
R43	10	0.81	3.37	20.90	5.67×10^{-1}	0.23	3.43×10^5	0.44
	100	0.20	3.56	20.72	5.67×10^{-1}	0.23	3.49×10^5	0.44
	0.01	1.63×10^{19}	-2.91	27.37	1.56×10^{-1}	0.64	4.06×10^4	1.16
	0.1	7.78×10^{10}	-0.17	25.25	1.59×10^{-1}	0.63	9.92×10^4	1.08
	1	1.84×10^3	2.28	23.07	1.59×10^{-1}	0.63	1.54×10^5	0.97
R44	10	0.50	3.42	22.02	1.59×10^{-1}	0.63	1.73×10^5	0.91
	100	0.13	3.61	21.84	1.59×10^{-1}	0.63	1.76×10^5	0.89
	0.01	7.32×10^5	1.11	25.18	4.03×10^{-3}	2.24×10^{-3}	6.77×10^3	0.07
	0.1	1.14	2.97	23.52	4.04×10^{-3}	2.18×10^{-3}	1.02×10^4	0.03
	1	7.75×10^{-2}	3.35	23.19	4.04×10^{-3}	2.17×10^{-3}	1.09×10^4	0.02
R45	10	5.77×10^{-2}	3.39	23.16	4.04×10^{-3}	2.17×10^{-3}	1.10×10^4	0.01
	100	5.60×10^{-2}	3.40	23.15	4.04×10^{-3}	2.17×10^{-3}	1.10×10^4	0.01
	0.01	4.77×10^{22}	-3.91	28.15	4.28×10^{-1}	0.24	8.16×10^4	0.83
	0.1	1.82×10^{14}	-1.12	26.05	4.34×10^{-1}	0.23	2.22×10^5	0.72

R46	1	4.34×10^6	1.34	23.93	4.35×10^{-1}	0.23	3.81×10^5	0.62	
	10	1.47×10^4	2.14	23.24	4.35×10^{-1}	0.23	4.43×10^5	0.56	
	100	7.23×10^3	2.24	23.15	4.35×10^{-1}	0.23	4.52×10^5	0.54	
	0.01	1.83×10^{32}	-6.81	30.40	3.23	1.80	1.59×10^5	1.61	
	0.1	3.80×10^{15}	-1.57	24.28	3.33	1.79	4.98×10^5	1.62	
R47	1	5.00×10^7	1.00	22.17	3.34	1.79	9.96×10^5	1.61	
	10	3.00×10^4	2.04	21.28	3.34	1.79	1.26×10^6	1.58	
	100	1.11×10^4	2.18	21.16	3.34	1.79	1.31×10^6	1.58	
	0.01	5.99×10^{25}	-4.88	26.26	9.46	5.25	2.81×10^5	2.84	
	0.1	4.84×10^{18}	-2.47	24.75	9.75	5.26	9.60×10^5	3.13	
1,6-exo-cycloaddition	1	1.37×10^{12}	-0.31	23.12	9.79	5.26	2.14×10^6	3.46	
	10	5.58×10^{10}	0.16	22.81	9.80	5.26	2.80×10^6	3.51	
	100	4.11×10^{10}	0.21	22.79	9.80	5.26	2.90×10^6	3.49	
	0.01	1.05×10^{11}	-0.80	10.40	2.09×10^4	1.00	2.10×10^6	1.00	
	0.1	8.52×10^9	-0.21	11.00	3.09×10^4	1.00	8.14×10^6	1.00	
rate rule	1	2.14×10^6	1.09	10.53	3.43×10^4	1.00	2.29×10^7	1.00	
	10	4.60×10^3	2.00	10.01	3.49×10^4	1.00	4.05×10^7	1.00	
	100	1.62×10^3	2.16	9.95	3.49×10^4	1.00	4.68×10^7	1.00	
	R48	0.01	1.70×10^{11}	-0.88	11.38	7.13×10^3	0.34	1.22×10^6	0.58
	0.1	1.64×10^9	-0.01	11.68	9.89×10^3	0.32	4.77×10^6	0.59	
R49	1	2.38×10^4	1.67	10.78	1.07×10^4	0.31	1.31×10^7	0.57	
	10	1.24×10^{-1}	3.41	9.41	1.09×10^4	0.31	2.22×10^7	0.55	
	100	1.72×10^{-3}	4.01	8.90	1.09×10^4	0.31	2.56×10^7	0.55	
	0.01	2.53×10^{12}	-1.20	12.40	1.99×10^4	0.95	2.18×10^6	1.04	
	0.1	3.48×10^{11}	-0.66	11.91	3.06×10^4	0.99	9.12×10^6	1.12	
R50	1	4.78×10^7	0.73	11.43	3.46×10^4	1.01	2.82×10^7	1.23	
	10	1.22×10^3	2.27	10.37	3.52×10^4	1.01	5.57×10^7	1.38	
	100	1.07×10^2	2.63	10.15	3.53×10^4	1.01	6.89×10^7	1.47	
	0.01	1.79×10^{12}	-1.13	11.00	2.59×10^4	1.24	2.67×10^6	1.27	

R51	0.1	3.12×10^8	0.27	10.67	3.89×10^4	1.26	1.10×10^7	1.36
	1	4.20×10^7	0.77	11.27	4.34×10^4	1.26	3.42×10^7	1.50
	10	2.19×10^5	1.58	10.94	4.40×10^4	1.26	6.73×10^7	1.66
	100	2.14×10^5	1.60	11.03	4.41×10^4	1.26	8.01×10^7	1.71
	0.01	5.30×10^{11}	-0.99	12.60	3.03×10^3	0.15	9.86×10^5	0.47
R52	0.1	1.36×10^8	0.34	12.28	3.53×10^3	0.11	3.42×10^6	0.41
	1	5.83×10^2	2.14	11.06	3.63×10^3	0.11	7.49×10^6	0.33
	10	5.10	2.83	10.58	3.64×10^3	0.10	1.02×10^7	0.25
	100	3.07	2.90	10.53	3.64×10^3	0.10	1.08×10^7	0.23
	0.01	4.60×10^9	-0.40	10.81	6.58×10^3	0.32	1.31×10^6	0.62
R53	0.1	2.18×10^6	0.84	10.52	7.54×10^3	0.24	4.10×10^6	0.50
	1	1.32×10^4	1.63	10.22	7.69×10^3	0.22	8.24×10^6	0.36
	10	1.42×10^4	1.64	10.33	7.71×10^3	0.22	9.96×10^6	0.25
	100	1.49×10^4	1.64	10.35	7.71×10^3	0.22	1.02×10^7	0.22
	0.01	5.85×10^{12}	-1.31	11.80	1.19×10^4	0.57	1.70×10^6	0.81
R54	0.1	1.05×10^{11}	-0.53	12.17	1.63×10^4	0.53	6.44×10^6	0.79
	1	2.98×10^6	1.05	11.34	1.75×10^4	0.51	1.70×10^7	0.74
	10	2.34×10^3	2.10	10.63	1.77×10^4	0.51	2.76×10^7	0.68
	100	9.36×10^2	2.23	10.56	1.77×10^4	0.51	3.06×10^7	0.65
	0.01	5.28×10^{11}	-1.00	10.93	1.79×10^4	0.86	2.05×10^6	0.98
R55	0.1	7.12×10^9	-0.19	11.20	2.33×10^4	0.75	7.17×10^6	0.88
	1	8.67×10^6	0.86	10.82	2.45×10^4	0.71	1.71×10^7	0.75
	10	8.74×10^6	0.90	10.99	2.46×10^4	0.71	2.37×10^7	0.59
	100	1.00×10^7	0.88	11.03	2.47×10^4	0.71	2.48×10^7	0.53
	0.01	1.04×10^{10}	-0.52	9.51	2.94×10^4	1.41	2.32×10^6	1.11
	0.1	1.35×10^9	0.01	10.18	4.47×10^4	1.44	9.07×10^6	1.11
	1	1.96×10^5	1.38	9.63	4.99×10^4	1.45	2.54×10^7	1.11
	10	5.11×10	2.59	8.82	5.07×10^4	1.46	4.45×10^7	1.10
	100	1.39×10	2.79	8.72	5.08×10^4	1.46	5.13×10^7	1.10

R56	0.01	1.85×10^{11}	-0.88	10.18	2.89×10^4	1.39	2.38×10^6	1.13
	0.1	3.81×10^{10}	-0.41	10.93	4.52×10^4	1.46	9.56×10^6	1.17
	1	7.89×10^6	0.92	10.46	5.12×10^4	1.49	2.78×10^7	1.21
	10	1.22×10^3	2.21	9.61	5.22×10^4	1.50	5.07×10^7	1.25
	100	2.67×10^2	2.44	9.49	5.23×10^4	1.50	5.97×10^7	1.28
R57	0.01	2.03×10^{10}	-0.58	9.78	2.94×10^4	1.41	2.52×10^6	1.20
	0.1	1.15×10^9	0.05	10.29	4.13×10^4	1.34	9.35×10^6	1.15
	1	4.00×10^5	1.29	9.82	4.46×10^4	1.30	2.47×10^7	1.08
	10	1.33×10^5	1.50	9.92	4.51×10^4	1.29	3.88×10^7	0.96
	100	1.58×10^5	1.48	9.98	4.51×10^4	1.29	4.20×10^7	0.90
R58	0.01	1.16×10^{12}	-1.10	10.64	2.95×10^4	1.41	2.67×10^6	1.27
	0.1	5.87×10^{10}	-0.44	11.20	4.36×10^4	1.41	1.05×10^7	1.30
	1	1.19×10^7	0.89	10.72	4.81×10^4	1.40	3.05×10^7	1.33
	10	5.16×10^5	1.40	10.61	4.88×10^4	1.40	5.41×10^7	1.34
	100	5.85×10^5	1.40	10.69	4.88×10^4	1.40	6.13×10^7	1.31
R59	0.01	2.63×10^{12}	-1.19	10.61	4.12×10^4	1.97	3.19×10^6	1.52
	0.1	1.33×10^{12}	-0.83	11.52	6.63×10^4	2.14	1.32×10^7	1.62
	1	7.85×10^8	0.37	11.25	7.61×10^4	2.22	4.09×10^7	1.79
	10	7.86×10^6	1.10	11.01	7.77×10^4	2.23	8.09×10^7	2.00
	100	9.04×10^6	1.10	11.12	7.79×10^4	2.23	9.67×10^7	2.06
1,7-exo-cycloaddition	0.01	5.35×10^7	0.11	7.88	3.74×10^4	1.00	2.26×10^6	1.00
rate rule	0.1	2.64×10^6	0.74	8.29	5.55×10^4	1.00	7.28×10^6	1.00
	1	5.18×10^5	1.09	8.59	6.27×10^4	1.00	1.62×10^7	1.00
	10	2.92×10^6	0.91	9.01	6.39×10^4	1.00	2.29×10^7	1.00
	100	5.11×10^6	0.84	9.12	6.40×10^4	1.00	2.43×10^7	1.00
R60	0.01	1.35×10^8	-0.03	9.16	9.91×10^3	0.27	1.09×10^6	0.48
	0.1	4.08×10^5	0.96	9.14	1.24×10^4	0.22	3.46×10^6	0.48
	1	8.98×10	2.22	8.44	1.30×10^4	0.21	7.32×10^6	0.45
	10	1.79×10	2.47	8.37	1.30×10^4	0.20	9.58×10^6	0.42

R61	100	1.60×10	2.49	8.37	1.30×10^4	0.20	9.97×10^6	0.41
	0.01	1.69×10^7	0.29	7.74	4.07×10^4	1.09	2.48×10^6	1.10
	0.1	5.41×10^5	0.96	8.07	5.37×10^4	0.97	7.91×10^6	1.09
	1	9.30×10^3	1.63	7.98	5.67×10^4	0.90	1.69×10^7	1.04
	10	1.66×10^4	1.59	8.19	5.70×10^4	0.89	2.14×10^7	0.94
R62	100	1.91×10^4	1.57	8.22	5.71×10^4	0.89	2.21×10^7	0.91
	0.01	7.97×10^{13}	-1.67	11.73	9.98×10^3	0.27	1.36×10^6	0.60
	0.1	6.17×10^5	0.89	9.15	1.10×10^4	0.20	3.58×10^6	0.49
	1	7.35×10^6	0.60	9.71	1.11×10^4	0.18	5.23×10^6	0.32
	10	1.19×10^7	0.54	9.80	1.11×10^4	0.17	5.51×10^6	0.24
R63	100	1.26×10^7	0.54	9.81	1.11×10^4	0.17	5.54×10^6	0.23
	0.01	7.57×10^8	-0.19	9.44	1.67×10^4	0.45	1.77×10^6	0.79
	0.1	3.35×10^6	0.75	9.46	2.02×10^4	0.36	5.47×10^6	0.75
	1	1.88×10^3	1.84	8.76	2.09×10^4	0.33	1.08×10^7	0.67
	10	1.68×10^5	1.28	9.55	2.10×10^4	0.33	1.30×10^7	0.57
R64	100	1.83×10^5	1.27	9.58	2.10×10^4	0.33	1.33×10^7	0.55
	0.01	2.18×10^7	0.26	8.31	2.40×10^4	0.64	2.01×10^6	0.89
	0.1	1.39×10^6	0.82	8.64	2.84×10^4	0.51	5.80×10^6	0.80
	1	2.91×10^7	0.47	9.37	2.92×10^4	0.47	9.79×10^6	0.60
	10	6.87×10^7	0.37	9.54	2.93×10^4	0.46	1.07×10^7	0.47
R65	100	7.58×10^7	0.36	9.55	2.93×10^4	0.46	1.08×10^7	0.44
	0.01	2.00×10^8	-0.02	8.71	2.73×10^4	0.73	2.20×10^6	0.98
	0.1	3.41×10^6	0.75	8.96	3.51×10^4	0.63	7.15×10^6	0.98
	1	4.23×10^4	1.46	8.83	3.68×10^4	0.59	1.54×10^7	0.95
	10	1.36×10^5	1.33	9.10	3.70×10^4	0.58	1.96×10^7	0.86
R66	100	8.03×10^4	1.41	9.07	3.70×10^4	0.58	2.02×10^7	0.83
	0.01	4.90×10^7	0.17	8.65	2.17×10^4	0.58	2.04×10^6	0.91
	0.1	1.50×10^6	0.83	8.92	2.60×10^4	0.47	6.16×10^6	0.85
	1	2.35×10^7	0.54	9.65	2.67×10^4	0.43	1.11×10^7	0.69

R67	10	6.40×10^7	0.42	9.85	2.68×10^4	0.42	2.83×10^6	0.54
	100	7.19×10^7	0.41	9.87	2.68×10^4	0.42	1.25×10^7	0.51
	0.01	1.34×10^9	-0.28	9.84	1.08×10^4	0.29	1.35×10^6	0.60
	0.1	2.65×10^6	0.73	9.64	1.23×10^4	0.22	3.68×10^6	0.51
	1	1.09×10^6	0.92	9.81	1.26×10^4	0.20	6.10×10^6	0.38
R68	10	1.53×10^6	0.89	9.91	1.26×10^4	0.20	6.73×10^6	0.29
	100	1.60×10^6	0.88	9.92	1.26×10^4	0.20	6.80×10^6	0.28
	0.01	5.62×10^7	0.10	9.78	4.62×10^3	0.12	8.41×10^5	0.37
	0.1	4.71×10^8	-0.09	10.51	4.84×10^3	0.09	1.71×10^6	0.24
	1	2.04×10^9	-0.27	10.80	4.87×10^3	0.08	2.00×10^6	0.12
R69	10	2.45×10^9	-0.29	10.83	4.87×10^3	0.08	2.03×10^6	0.09
	100	2.50×10^9	-0.29	10.84	4.87×10^3	0.08	2.04×10^6	0.08
	0.01	4.50×10^7	0.16	7.74	5.07×10^4	1.36	2.72×10^6	1.21
	0.1	3.13×10^6	0.74	8.18	6.95×10^4	1.25	8.74×10^6	1.20
	1	4.89×10^4	1.42	8.09	7.41×10^4	1.18	1.89×10^7	1.17
R70	10	8.80×10^4	1.38	8.31	7.47×10^4	1.17	2.44×10^7	1.07
	100	1.02×10^5	1.36	8.35	7.48×10^4	1.17	2.52×10^7	1.04
	0.01	2.13×10^8	-0.04	8.37	3.73×10^4	1.00	2.41×10^6	1.07
	0.1	7.04×10^6	0.63	8.69	4.93×10^4	0.89	7.62×10^6	1.05
	1	1.31×10^5	1.29	8.61	5.20×10^4	0.83	1.60×10^7	0.99
R71	10	2.24×10^5	1.25	8.80	5.23×10^4	0.82	2.01×10^7	0.88
	100	5.40×10^5	1.13	8.94	5.24×10^4	0.82	2.07×10^7	0.85
	0.01	2.10×10^{22}	-4.37	11.74	1.71×10^5	4.58	5.83×10^6	2.58
	0.1	5.30×10^8	0.15	8.26	3.15×10^5	5.67	2.28×10^7	3.14
	1	2.28×10^7	0.77	8.57	3.87×10^5	6.18	6.82×10^7	4.21
R72	10	3.29×10^8	0.49	9.30	4.00×10^5	6.27	1.24×10^8	5.42
	100	9.52×10^8	0.36	9.51	4.02×10^5	6.28	1.39×10^8	5.69
	0.01	3.93×10^7	0.19	7.67	6.11×10^4	1.63	2.09×10^6	1.42
	0.1	1.03×10^7	0.60	8.36	8.41×10^4	1.51	1.05×10^7	1.44

1	3.58×10^7	0.55	9.02	8.97×10^4	1.43	2.29×10^7	1.41
10	2.21×10^8	0.33	9.39	9.04×10^4	1.42	2.80×10^7	1.22
100	2.84×10^8	0.30	9.43	9.05×10^4	1.41	2.87×10^7	1.18

Table S19. Pressure-Dependent Rate Rules for Cycloaddition Reactions of Alkenyl Peroxy

Radicals

Reaction	Pressure(atm)	Modified Arrhenius parameters			500K	1000K
class		A(s ⁻¹)	n	E(kcal/mol)	f^a	f^a
1,5-endo	0.01	7.38×10^5	1.08	22.30	49.58	11.90
	0.1	7.60×10^{-3}	3.70	20.23	48.92	14.96
	1	9.35×10^{-9}	5.61	18.56	48.66	23.85
	10	8.11×10^{-11}	6.27	17.96	48.66	27.35
	100	3.81×10^{-11}	6.37	17.87	48.66	27.59
1,6-endo	0.01	2.19×10^{12}	-1.20	11.24	12.93	3.25
	0.1	1.17×10^{11}	-0.57	11.72	17.02	4.16
	1	5.57×10^7	0.61	11.25	18.43	7.21
	10	2.96×10^6	1.07	11.08	18.63	11.65
	100	2.19×10^6	1.12	11.08	18.65	12.98
1,7-endo	0.01	1.06×10^{12}	-1.09	13.39	16.44	2.86
	0.1	1.35×10^9	-0.03	13.07	17.79	4.06
	1	2.29×10^8	0.27	13.06	17.99	5.78
	10	2.45×10^8	0.27	13.11	18.04	6.22
	100	2.47×10^8	0.27	13.12	18.04	6.28
1,5-exo	0.01	2.01×10^{21}	-3.60	25.55	2347.39	41.51
	0.1	1.07×10^{14}	-1.15	23.92	2413.37	94.12
	1	3.60×10^6	1.29	21.94	2423.27	196.33
	10	6.51×10^2	2.50	20.89	2425.74	254.55
	100	9.43×10	2.77	20.65	2425.74	263.64
1,6-exo	0.01	1.05×10^{11}	-0.80	10.40	13.60	3.24

	0.1	8.52×10^9	-0.21	11.00	18.78	3.95
	1	2.14×10^6	1.09	10.53	20.96	5.46
	10	4.60×10^3	2.00	10.01	21.35	8.12
	100	1.62×10^3	2.16	9.95	21.40	9.48
1,7-exo	0.01	5.35×10^7	0.11	7.88	37.01	6.93
	0.1	2.64×10^6	0.74	8.29	65.08	13.33
	1	5.18×10^5	1.09	8.59	79.47	34.10
	10	2.92×10^6	0.91	9.01	82.14	61.08
	100	5.11×10^6	0.84	9.12	82.55	68.14

^a $f=k_{\max}/k_{\min}$ for each class.

Table S20. Pressure-Dependent Rate constants, Rate rules and Ratios of the Individually Calculated Rate Constants for Intramolecular H-shift Reactions of Alkenyl Peroxy Radicals

Reaction	Pressure(atm)	modified Arrhenius parameters			500K		1000K	
		A(s ⁻¹)	n	E(kcal/mol)	k	k/k _{rule}	k	k/k _{rule}
1,4-H(as) rate rule	0.01	1.93×10^{-1}	2.90	15.04	1.43	1.00	8.15×10^4	1.00
	0.1	1.52×10^{-11}	6.21	12.38	1.44	1.00	2.06×10^5	1.00
	1	8.34×10^{-15}	7.28	11.57	1.44	1.00	3.24×10^5	1.00
	10	3.57×10^{-16}	7.73	11.19	1.44	1.00	3.58×10^5	1.00
	100	2.35×10^{-16}	7.78	11.14	1.44	1.00	3.62×10^5	1.00
R1	0.01	7.33×10^{-6}	4.22	14.35	3.57×10^{-1}	0.25	4.27×10^4	0.52
	0.1	1.62×10^{-11}	6.31	14.09	3.60×10^{-1}	0.25	1.02×10^5	0.50
	1	2.45×10^{-9}	5.61	14.70	3.60×10^{-1}	0.25	1.57×10^5	0.49
	10	6.20×10^{-11}	6.15	14.37	3.60×10^{-1}	0.25	1.76×10^5	0.49
	100	3.31×10^{-11}	6.24	14.31	3.60×10^{-1}	0.25	1.79×10^5	0.49
R2	0.01	8.95×10^{-6}	4.26	15.25	2.14×10^{-1}	0.15	4.64×10^4	0.57
	0.1	1.09×10^{-14}	7.17	12.88	2.15×10^{-1}	0.15	1.06×10^5	0.51
	1	4.81×10^{-9}	5.56	15.54	2.15×10^{-1}	0.15	1.53×10^5	0.47
	10	9.45×10^{-10}	5.80	15.39	2.15×10^{-1}	0.15	1.65×10^5	0.46

R3	100	7.92×10^{-10}	5.82	15.38	2.15×10^{-1}	0.15	1.67×10^5	0.46
	0.01	1.02×10^2	2.14	17.28	7.28×10^{-1}	0.51	7.69×10^4	0.95
	0.1	3.30×10^{-7}	4.94	15.10	7.34×10^{-1}	0.51	1.92×10^5	0.93
	1	7.88×10^{-14}	7.08	13.25	7.34×10^{-1}	0.51	3.00×10^5	0.93
	10	1.93×10^{-15}	7.60	12.79	7.34×10^{-1}	0.51	3.33×10^5	0.93
R4	100	1.27×10^{-15}	7.65	12.74	7.34×10^{-1}	0.51	3.37×10^5	0.93
	0.01	3.00×10^{-10}	5.60	14.86	4.47×10^{-2}	0.03	2.15×10^4	0.27
	0.1	4.14×10^{-14}	6.93	14.21	4.48×10^{-2}	0.03	3.89×10^4	0.19
	1	2.39×10^{-9}	5.54	16.28	4.48×10^{-2}	0.03	4.70×10^4	0.15
	10	1.42×10^{-9}	5.62	16.24	4.48×10^{-2}	0.03	4.82×10^4	0.14
R5	100	1.37×10^{-9}	5.63	16.24	4.48×10^{-2}	0.03	4.84×10^4	0.13
	0.01	3.95×10^{-3}	3.44	15.36	5.71×10^{-1}	0.40	6.42×10^4	0.79
	0.1	9.39×10^{-12}	6.27	13.11	5.74×10^{-1}	0.40	1.52×10^5	0.74
	1	7.10×10^{-18}	8.24	11.39	5.74×10^{-1}	0.40	2.26×10^5	0.70
	10	3.45×10^{-19}	8.67	11.02	5.74×10^{-1}	0.40	2.47×10^5	0.69
R6	100	2.47×10^{-19}	8.71	10.98	5.74×10^{-1}	0.40	2.49×10^5	0.69
	0.01	9.47	2.40	15.32	2.40	1.68	1.05×10^5	1.29
	0.1	7.64×10^{-8}	5.07	13.28	2.42	1.68	2.67×10^5	1.30
	1	4.82×10^{-14}	7.07	11.56	2.42	1.68	4.21×10^5	1.30
	10	1.89×10^{-15}	7.53	11.18	2.42	1.68	4.67×10^5	1.31
R7	100	1.31×10^{-15}	7.58	11.13	2.42	1.68	4.73×10^5	1.31
	0.01	3.22×10^{-1}	2.84	14.34	3.32	2.32	1.26×10^5	1.55
	0.1	1.66×10^{-8}	5.24	12.51	3.33	2.32	3.05×10^5	1.48
	1	1.10×10^{-10}	5.97	12.00	3.34	2.32	4.33×10^5	1.34
	10	6.65×10^{-11}	6.05	11.96	3.34	2.32	4.57×10^5	1.28
R8	100	6.33×10^{-11}	6.05	11.96	3.34	2.32	4.60×10^5	1.27
	0.01	3.81×10^4	1.37	16.79	3.80	2.66	1.68×10^5	2.07
	0.1	3.94×10^{-4}	4.03	14.86	3.83	2.66	4.84×10^5	2.35
	1	7.26×10^{-9}	5.59	13.66	3.84	2.66	8.52×10^5	2.63

1,4-H(s) rate rule	10	1.59×10^{-9}	5.81	13.51	3.84	2.66	9.68×10^5	2.71
	100	1.37×10^{-9}	5.83	13.50	3.84	2.66	9.83×10^5	2.71
	0.01	6.55×10^8	0.19	22.01	2.48×10^{-1}	1.00	5.74×10^4	1.00
	0.1	6.30×10	2.50	20.25	2.49×10^{-1}	1.00	1.33×10^5	1.00
	1	2.48×10^{-1}	3.30	19.65	2.49×10^{-1}	1.00	1.79×10^5	1.00
	10	1.05×10^{-1}	3.42	19.55	2.49×10^{-1}	1.00	1.88×10^5	1.00
	100	9.61×10^{-2}	3.43	19.54	2.49×10^{-1}	1.00	1.89×10^5	1.00
R9	0.01	1.73×10^9	0.13	24.36	4.01×10^{-2}	0.16	3.31×10^4	0.58
	0.1	1.69	3.06	21.94	4.03×10^{-2}	0.16	7.24×10^4	0.55
	1	2.56×10^{-6}	4.94	20.28	4.03×10^{-2}	0.16	1.01×10^5	0.56
	10	1.78×10^{-7}	5.31	19.95	4.03×10^{-2}	0.16	1.08×10^5	0.58
	100	1.33×10^{-7}	5.35	19.92	4.03×10^{-2}	0.16	1.09×10^5	0.58
R10	0.01	1.55×10^6	1.07	23.58	2.52×10^{-2}	0.10	3.04×10^4	0.53
	0.1	2.79×10^{-1}	3.27	21.79	2.53×10^{-2}	0.10	5.74×10^4	0.43
	1	1.19×10^{-2}	3.72	21.44	2.53×10^{-2}	0.10	6.81×10^4	0.38
	10	8.51×10^{-3}	3.77	21.41	2.53×10^{-2}	0.10	6.95×10^4	0.37
	100	8.23×10^{-3}	3.77	21.40	2.53×10^{-2}	0.10	6.97×10^4	0.37
R11	0.01	9.65×10^9	-0.05	24.82	4.39×10^{-2}	0.18	4.20×10^4	0.73
	0.1	1.81×10^2	2.47	22.77	4.40×10^{-2}	0.18	8.89×10^4	0.67
	1	1.65	3.14	22.25	4.40×10^{-2}	0.18	1.13×10^5	0.63
	10	9.92×10^{-1}	3.21	22.20	4.40×10^{-2}	0.18	1.17×10^5	0.63
	100	9.42×10^{-1}	3.22	22.19	4.40×10^{-2}	0.18	1.18×10^5	0.62
R12	0.01	8.33×10^{10}	-0.34	24.69	7.27×10^{-2}	0.29	5.37×10^4	0.94
	0.1	2.62×10^2	2.44	22.46	7.28×10^{-2}	0.29	1.26×10^5	0.95
	1	2.16×10^{-1}	3.45	21.66	7.28×10^{-2}	0.29	1.76×10^5	0.98
	10	9.27×10^{-2}	3.58	21.57	7.28×10^{-2}	0.29	1.85×10^5	0.99
	100	8.52×10^{-2}	3.59	21.56	7.28×10^{-2}	0.29	1.87×10^5	0.99
R13	0.01	5.89×10^8	0.31	24.58	3.19×10^{-2}	0.13	3.50×10^4	0.61
	0.1	1.81×10	2.75	22.57	3.20×10^{-2}	0.13	7.00×10^4	0.53

R14	1	2.44×10^{-1}	3.37	22.09	3.20×10^{-2}	0.13	8.63×10^4	0.48
	10	1.53×10^{-1}	3.44	22.04	3.20×10^{-2}	0.13	8.88×10^4	0.47
	100	1.46×10^{-1}	3.44	22.04	3.20×10^{-2}	0.13	8.90×10^4	0.47
	0.01	9.44×10^6	0.84	24.25	2.00×10^{-2}	0.08	2.79×10^4	0.49
	0.1	1.17	3.09	22.40	2.00×10^{-2}	0.08	5.22×10^4	0.39
	1	3.99×10^{-2}	3.58	22.03	2.00×10^{-2}	0.08	6.18×10^4	0.35
R15	10	2.79×10^{-2}	3.63	21.99	2.00×10^{-2}	0.08	6.31×10^4	0.34
	100	2.69×10^{-2}	3.63	21.98	2.00×10^{-2}	0.08	6.33×10^4	0.34
	0.01	2.53×10^{13}	-1.20	23.51	5.40×10^{-1}	2.18	9.33×10^4	1.63
	0.1	4.17×10^5	1.41	21.49	5.42×10^{-1}	2.18	2.28×10^5	1.72
	1	6.95×10^2	2.32	20.80	5.42×10^{-1}	2.18	3.29×10^5	1.84
	10	3.42×10^2	2.43	20.73	5.42×10^{-1}	2.18	3.49×10^5	1.86
R16	100	3.19×10^2	2.44	20.73	5.42×10^{-1}	2.18	3.52×10^5	1.86
	0.01	3.83×10^{13}	-1.21	22.71	1.21	4.88	1.44×10^5	2.50
	0.1	1.83×10^8	0.58	21.54	1.21	4.88	3.66×10^5	2.76
	1	5.11×10^7	0.79	21.51	1.21	4.88	4.99×10^5	2.78
	10	4.80×10^7	0.81	21.52	1.21	4.88	5.20×10^5	2.77
	100	4.78×10^7	0.81	21.52	1.21	4.88	5.22×10^5	2.77
1,4-H(vt) rate rule	0.01	9.15×10^{27}	-5.30	36.93	2.03×10^{-3}	1.00	1.33×10^4	1.00
	0.1	3.82×10^{19}	-2.51	34.89	2.13×10^{-3}	1.00	3.79×10^4	1.00
	1	6.98×10^{10}	0.32	32.48	2.15×10^{-3}	1.00	7.15×10^4	1.00
	10	1.65×10^4	2.44	30.53	2.15×10^{-3}	1.00	9.27×10^4	1.00
	100	4.77×10	3.24	29.77	2.15×10^{-3}	1.00	9.82×10^4	1.00
	0.01	5.42×10^{26}	-4.98	36.42	1.57×10^{-3}	0.77	9.05×10^3	0.68
R17	0.1	1.19×10^{19}	-2.41	34.66	1.69×10^{-3}	0.80	2.67×10^4	0.71
	1	5.61×10^{10}	0.31	32.41	1.72×10^{-3}	0.80	5.26×10^4	0.74
	10	1.03×10^4	2.46	30.45	1.72×10^{-3}	0.80	7.04×10^4	0.76
	100	4.73	3.52	29.43	1.72×10^{-3}	0.80	7.56×10^4	0.77
	R18	0.01	5.02×10^{28}	-5.49	37.22	2.50×10^{-3}	1.23	1.76×10^4

1,4-H(vi) rate rule	0.1	8.27×10^{19}	-2.58	35.04	2.57×10^{-3}	1.20	4.91×10^4	1.30
	1	8.52×10^{10}	0.33	32.53	2.58×10^{-3}	1.20	9.04×10^4	1.26
	10	2.35×10^4	2.42	30.59	2.58×10^{-3}	1.20	1.15×10^5	1.24
	100	2.54×10^2	3.05	30.00	2.58×10^{-3}	1.20	1.21×10^5	1.23
	0.01	3.22×10^{18}	-2.47	34.84	2.18×10^{-4}	1.00	4.49×10^3	1.00
	0.1	7.22×10^9	0.36	32.57	2.21×10^{-4}	1.00	1.00×10^4	1.00
	1	1.45×10^3	2.52	30.71	2.21×10^{-4}	1.00	1.58×10^4	1.00
	10	1.23×10^{-3}	4.45	28.87	2.21×10^{-4}	1.00	1.84×10^4	1.00
	100	7.17×10^{-5}	4.85	28.49	2.21×10^{-4}	1.00	1.89×10^4	1.00
R19	0.01	6.49×10^{13}	-1.12	34.21	3.81×10^{-5}	0.18	1.44×10^3	0.32
	0.1	4.94×10^5	1.55	32.12	3.92×10^{-5}	0.18	3.19×10^3	0.32
	1	1.75×10^{-2}	3.95	30.00	3.94×10^{-5}	0.18	4.94×10^3	0.31
	10	1.85×10^{-7}	5.54	28.52	3.94×10^{-5}	0.18	5.79×10^3	0.31
	100	4.09×10^{-9}	6.06	28.02	3.94×10^{-5}	0.18	5.98×10^3	0.32
R20	0.01	4.30×10^{22}	-3.66	35.80	6.89×10^{-4}	3.16	1.05×10^4	2.33
	0.1	2.79×10^{13}	-0.64	33.41	6.98×10^{-4}	3.17	2.62×10^4	2.61
	1	4.99×10^7	1.24	31.91	6.99×10^{-4}	3.17	4.37×10^4	2.77
	10	5.56×10^{-2}	4.07	29.15	7.00×10^{-4}	3.17	5.24×10^4	2.86
	100	1.86×10^{-3}	4.54	28.71	7.00×10^{-4}	3.17	5.43×10^4	2.87
R21	0.01	3.00×10^{14}	-1.23	33.88	1.14×10^{-4}	0.53	3.85×10^3	0.86
	0.1	1.28×10^{10}	0.23	32.90	1.15×10^{-4}	0.52	6.88×10^3	0.69
	1	1.02×10^{-2}	4.07	29.18	1.15×10^{-4}	0.52	9.62×10^3	0.61
	10	1.75×10^{-5}	4.95	28.34	1.15×10^{-4}	0.52	1.03×10^4	0.56
	100	6.95×10^{-6}	5.08	28.22	1.15×10^{-4}	0.52	1.03×10^4	0.55
R22	0.01	1.74×10^{12}	-0.53	34.40	2.99×10^{-5}	0.14	2.21×10^3	0.49
	0.1	6.31×10^3	2.20	32.04	3.00×10^{-5}	0.14	3.86×10^3	0.39
	1	3.57×10^{-4}	4.50	29.87	3.00×10^{-5}	0.14	4.79×10^3	0.30
	10	2.95×10^{-6}	5.17	29.24	3.00×10^{-5}	0.14	5.01×10^3	0.27
	100	1.57×10^{-6}	5.25	29.16	3.00×10^{-5}	0.14	5.04×10^3	0.27

1,5-H(as) rate rule	0.01	9.53×10^9	-0.47	11.12	6.43×10^3	1.00	1.35×10^6	1.00
	0.1	4.94×10^7	0.47	11.28	8.49×10^3	1.00	4.95×10^6	1.00
	1	1.46×10^4	1.73	10.76	9.02×10^3	1.00	1.27×10^7	1.00
	10	4.92×10^3	1.93	10.83	9.09×10^3	1.00	1.91×10^7	1.00
	100	5.37×10^3	1.92	10.88	9.09×10^3	1.00	2.05×10^7	1.00
R23	0.01	9.21×10^{11}	-1.04	14.04	8.68×10^2	0.14	6.55×10^5	0.49
	0.1	1.74×10^7	0.63	13.30	9.55×10^2	0.11	2.11×10^6	0.43
	1	3.32×10	2.53	11.91	9.68×10^2	0.11	4.40×10^6	0.35
	10	5.87×10^{-1}	3.12	11.49	9.70×10^2	0.11	5.65×10^6	0.30
	100	3.82×10^{-1}	3.18	11.45	9.70×10^2	0.11	5.87×10^6	0.29
R24	0.01	2.07×10^{13}	-1.42	13.53	3.28×10^3	0.51	1.22×10^6	0.91
	0.1	8.09×10^9	-0.14	13.31	3.84×10^3	0.45	4.41×10^6	0.89
	1	2.01×10^5	1.44	12.40	3.95×10^3	0.44	1.09×10^7	0.86
	10	3.73×10^4	1.71	12.35	3.96×10^3	0.44	1.56×10^7	0.82
	100	3.57×10^4	1.73	12.38	3.96×10^3	0.44	1.65×10^7	0.81
R25	0.01	2.58×10^{14}	-1.74	14.04	3.54×10^3	0.55	1.31×10^6	0.97
	0.1	1.95×10^{11}	-0.53	13.95	4.26×10^3	0.50	4.93×10^6	1.00
	1	2.54×10^6	1.15	12.99	4.40×10^3	0.49	1.30×10^7	1.02
	10	2.29×10^5	1.53	12.89	4.42×10^3	0.49	1.99×10^7	1.04
	100	2.15×10^5	1.54	12.91	4.42×10^3	0.49	2.14×10^7	1.05
R26	0.01	5.18×10^{13}	-1.50	15.85	4.28×10^2	0.07	6.25×10^5	0.46
	0.1	2.84×10^8	0.33	14.90	4.53×10^2	0.05	1.98×10^6	0.40
	1	1.57×10^5	1.45	14.25	4.56×10^2	0.05	3.90×10^6	0.31
	10	9.12×10^4	1.54	14.26	4.57×10^2	0.05	4.65×10^6	0.24
	100	8.85×10^4	1.55	14.26	4.57×10^2	0.05	4.75×10^6	0.23
R27	0.01	5.98×10^{14}	-1.85	13.66	6.52×10^3	1.01	1.69×10^6	1.25
	0.1	3.35×10^{12}	-0.90	13.90	8.42×10^3	0.99	6.72×10^6	1.36
	1	5.73×10^7	0.76	13.05	8.89×10^3	0.99	1.94×10^7	1.52
	10	1.47×10^6	1.33	12.85	8.95×10^3	0.99	3.37×10^7	1.76

R28	100	1.41×10^6	1.35	12.90	8.96×10^3	0.99	3.77×10^7	1.84
	0.01	3.84×10^{14}	-1.78	14.71	1.94×10^3	0.30	1.05×10^6	0.78
	0.1	4.70×10^{10}	-0.35	14.31	2.21×10^3	0.26	3.71×10^6	0.75
	1	1.13×10^6	1.23	13.36	2.26×10^3	0.25	8.94×10^6	0.70
	10	2.58×10^5	1.47	13.33	2.26×10^3	0.25	1.27×10^7	0.65
R29	100	2.45×10^5	1.48	13.35	2.26×10^3	0.25	1.30×10^7	0.64
	0.01	6.16×10^{12}	-1.29	12.72	5.31×10^3	0.83	1.38×10^6	1.02
	0.1	5.58×10^8	-0.12	12.59	6.31×10^3	0.74	4.77×10^6	0.97
	1	1.57×10^6	1.12	11.97	6.50×10^3	0.72	1.10×10^7	0.87
	10	9.11×10^5	1.23	12.05	6.52×10^3	0.72	1.48×10^7	0.77
R30	100	9.44×10^5	1.23	12.07	6.52×10^3	0.72	1.54×10^7	0.75
	0.01	3.44×10^{11}	-0.92	10.55	2.96×10^4	4.60	2.87×10^6	2.13
	0.1	2.31×10^{10}	-0.30	11.12	4.14×10^4	4.88	1.09×10^7	2.21
	1	2.92×10^8	0.45	11.17	4.47×10^4	4.96	3.04×10^7	2.38
	10	2.19×10^9	0.23	11.68	4.52×10^4	4.97	4.63×10^7	2.42
1,5-H(s) rate rule	100	3.52×10^9	0.18	11.78	4.52×10^4	4.97	4.92×10^7	2.40
	0.01	1.14×10^{15}	-1.98	12.54	2.03×10^4	1.00	2.19×10^6	1.00
	0.1	1.43×10^{15}	-1.74	13.55	3.48×10^4	1.00	8.93×10^6	1.00
	1	1.47×10^{13}	-0.93	13.65	4.12×10^4	1.00	2.68×10^7	1.00
	10	1.93×10^{11}	-0.24	13.47	4.23×10^4	1.00	5.29×10^7	1.00
R31	100	2.42×10^{11}	-0.24	13.60	4.25×10^4	1.00	6.43×10^7	1.00
	0.01	3.06×10^{16}	-2.38	12.72	3.93×10^4	1.93	3.31×10^6	1.51
	0.1	4.43×10^{16}	-2.15	13.79	6.81×10^4	1.96	1.42×10^7	1.59
	1	5.50×10^{13}	-1.04	13.65	8.09×10^4	1.96	4.63×10^7	1.72
	10	3.78×10^{11}	-0.25	13.41	8.32×10^4	1.96	9.70×10^7	1.84
R32	100	4.75×10^{11}	-0.26	13.55	8.34×10^4	1.96	1.20×10^8	1.86
	0.01	9.85×10^{22}	-4.23	19.34	1.35×10^3	0.07	1.07×10^6	0.49
	0.1	2.06×10^{19}	-2.88	18.97	1.49×10^3	0.04	3.62×10^6	0.41
	1	1.02×10^{19}	-2.69	19.28	1.51×10^3	0.04	7.44×10^6	0.28

1,5-H(vt) rate rule	10	2.24×10^{19}	-2.77	19.47	1.51×10^3	0.04	8.68×10^6	0.16
	100	2.48×10^{19}	-2.79	19.49	1.51×10^3	0.04	8.83×10^6	0.14
	0.01	2.01×10^{28}	-5.60	31.26	2.45×10^{-1}	1.00	5.35×10^4	1.00
	0.1	1.78×10^{20}	-2.93	29.30	2.52×10^{-1}	1.00	1.49×10^5	1.00
	1	3.29×10^{12}	-0.42	27.16	2.52×10^{-1}	1.00	2.63×10^5	1.00
	10	9.99×10^8	0.71	26.15	2.52×10^{-1}	1.00	3.14×10^5	1.00
R33	100	1.39×10^8	0.98	25.89	2.52×10^{-1}	1.00	3.22×10^5	1.00
	0.01	1.75×10^{28}	-5.57	34.05	1.66×10^{-2}	0.07	1.42×10^4	0.27
	0.1	1.89×10^{21}	-3.22	32.48	1.85×10^{-2}	0.07	4.03×10^4	0.27
	1	5.06×10^{13}	-0.75	30.44	1.88×10^{-2}	0.07	7.55×10^4	0.29
	10	8.26×10^7	1.10	28.76	1.89×10^{-2}	0.07	9.75×10^4	0.31
	100	4.90×10^5	1.81	28.09	1.89×10^{-2}	0.07	1.03×10^5	0.32
R34	0.01	1.15×10^{27}	-5.22	31.03	1.90×10^{-1}	0.77	4.87×10^4	0.91
	0.1	9.29×10^{18}	-2.54	29.01	1.95×10^{-1}	0.77	1.25×10^5	0.84
	1	1.79×10^{11}	-0.05	26.84	1.95×10^{-1}	0.77	2.03×10^5	0.77
	10	3.69×10^7	1.12	25.75	1.95×10^{-1}	0.77	2.33×10^5	0.74
	100	9.14×10^6	1.32	25.57	1.95×10^{-1}	0.77	2.38×10^5	0.74
R35	0.01	1.44×10^{30}	-6.11	31.61	5.30×10^{-1}	2.16	9.75×10^4	1.82
	0.1	1.07×10^{22}	-3.40	29.64	5.42×10^{-1}	2.15	2.81×10^5	1.89
	1	2.21×10^{14}	-0.91	27.53	5.43×10^{-1}	2.15	5.11×10^5	1.94
	10	6.08×10^{11}	-0.08	26.82	5.43×10^{-1}	2.15	6.11×10^5	1.95
	100	2.93×10^{11}	0.02	26.74	5.43×10^{-1}	2.15	6.26×10^5	1.94
1,5-H(vi) rate rule	0.01	9.39×10^{30}	-6.39	31.03	1.13	1.00	1.12×10^5	1.00
	0.1	3.08×10^{23}	-3.88	29.31	1.16	1.00	3.38×10^5	1.00
	1	4.14×10^{16}	-1.63	27.51	1.17	1.00	6.65×10^5	1.00
	10	3.16×10^{14}	-0.94	26.95	1.17	1.00	8.24×10^5	1.00
	100	1.66×10^{14}	-0.85	26.88	1.17	1.00	8.49×10^5	1.00
R36	0.01	3.72×10^{28}	-5.64	30.93	4.71×10^{-1}	0.42	8.75×10^4	0.78
	0.1	1.94×10^{20}	-2.91	28.87	4.78×10^{-1}	0.41	2.35×10^5	0.69

R37	1	2.84×10^{13}	-0.69	26.99	4.79×10^{-1}	0.41	3.93×10^5	0.59
	10	5.26×10^{11}	-0.13	26.51	4.79×10^{-1}	0.41	4.47×10^5	0.54
	100	3.34×10^{11}	-0.07	26.46	4.79×10^{-1}	0.41	4.55×10^5	0.54
	0.01	1.74×10^{27}	-5.31	30.65	2.41×10^{-1}	0.21	4.64×10^4	0.42
	0.1	4.43×10^{19}	-2.78	28.84	2.52×10^{-1}	0.22	1.27×10^5	0.38
R38	1	7.90×10^{11}	-0.27	26.71	2.54×10^{-1}	0.22	2.26×10^5	0.34
	10	7.68×10^7	1.02	25.56	2.54×10^{-1}	0.22	2.75×10^5	0.33
	100	1.56×10^7	1.25	25.36	2.54×10^{-1}	0.22	2.84×10^5	0.34
	0.01	1.26×10^{32}	-6.69	31.89	9.55×10^{-1}	0.85	1.25×10^5	1.12
	0.1	1.92×10^{24}	-4.07	30.07	9.84×10^{-1}	0.85	3.86×10^5	1.14
R39	1	2.02×10^{16}	-1.48	27.92	9.87×10^{-1}	0.85	7.61×10^5	1.14
	10	1.57×10^{13}	-0.47	27.06	9.88×10^{-1}	0.85	9.54×10^5	1.16
	100	6.17×10^{12}	-0.34	26.95	9.88×10^{-1}	0.85	9.87×10^5	1.16
	0.01	3.86×10^{34}	-7.44	31.56	4.24	3.75	2.44×10^5	2.18
	0.1	2.25×10^{27}	-4.98	30.00	4.38	3.77	8.37×10^5	2.47
R40	10	6.00×10^{20}	-2.81	28.36	4.40	3.77	1.87×10^6	2.81
	10	2.49×10^{19}	-2.35	28.05	4.41	3.77	2.43×10^6	2.94
	100	1.83×10^{19}	-2.30	28.03	4.41	3.77	2.51×10^6	2.96
	0.01	8.21×10^{27}	-5.46	30.55	4.83×10^{-1}	0.43	8.31×10^4	0.74
	0.1	4.42×10^{19}	-2.73	28.47	4.90×10^{-1}	0.42	2.16×10^5	0.64
R41	1	1.46×10^{13}	-0.63	26.68	4.91×10^{-1}	0.42	3.49×10^5	0.52
	10	4.43×10^{11}	-0.14	26.27	4.91×10^{-1}	0.42	3.90×10^5	0.47
	100	3.00×10^{11}	-0.08	26.22	4.91×10^{-1}	0.42	3.96×10^5	0.47
	0.01	2.32×10^{29}	-5.87	31.59	3.86×10^{-1}	0.34	8.45×10^4	0.76
	0.1	1.36×10^{21}	-3.14	29.55	3.93×10^{-1}	0.34	2.30×10^5	0.68
1,6-H(as) rate rule	1	1.06×10^{14}	-0.84	27.58	3.94×10^{-1}	0.34	3.92×10^5	0.59
	10	1.21×10^{12}	-0.21	27.05	3.94×10^{-1}	0.34	4.50×10^5	0.55
	100	7.17×10^{11}	-0.14	26.99	3.94×10^{-1}	0.34	4.58×10^5	0.54
	0.01	1.20×10^{10}	-0.51	11.50	4.25×10^3	1.00	1.07×10^6	1.00

	0.1	1.28×10^7	0.61	11.32	4.92×10^3	1.00	3.40×10^6	1.00	
	1	7.68×10^6	0.78	11.65	5.04×10^3	1.00	6.68×10^6	1.00	
	10	1.74×10^7	0.68	11.84	5.05×10^3	1.00	7.74×10^6	1.00	
	100	1.94×10^7	0.67	11.87	5.05×10^3	1.00	7.87×10^6	1.00	
	R42	0.01	1.68×10^{10}	-0.49	14.18	3.66×10^2	0.09	5.18×10^5	0.48
	0.1	5.99×10^4	1.38	13.09	3.80×10^2	0.08	1.47×10^6	0.43	
	1	5.44×10^2	2.09	12.73	3.82×10^2	0.08	2.52×10^6	0.38	
	10	4.24×10^2	2.13	12.75	3.82×10^2	0.08	2.81×10^6	0.36	
	100	4.18×10^2	2.14	12.76	3.82×10^2	0.08	2.84×10^6	0.36	
	R43	0.01	3.43×10^{11}	-0.92	11.70	8.14×10^3	1.91	1.63×10^6	1.52
	0.1	7.75×10^8	0.11	11.65	9.47×10^3	1.92	5.33×10^6	1.57	
	1	1.06×10^9	0.17	12.11	9.69×10^3	1.92	1.08×10^7	1.62	
	10	2.97×10^9	0.05	12.33	9.72×10^3	1.92	1.27×10^7	1.64	
	100	3.39×10^9	0.03	12.36	9.72×10^3	1.92	1.29×10^7	1.64	
	1,6-H(s) rate rule								
R44	0.01	3.20×10^{22}	-4.04	21.21	1.83×10^2		5.60×10^5		
	0.1	2.58×10^{18}	-2.59	20.59	1.89×10^2		1.68×10^6		
	1	3.04×10^{18}	-2.55	20.87	1.90×10^2		2.75×10^6		
	10	4.09×10^{18}	-2.59	20.94	1.90×10^2		2.97×10^6		
	100	4.24×10^{18}	-2.59	20.95	1.90×10^2		3.00×10^6		
1,6-H(vt) rate rule		0.01	5.35×10^{-11}	5.84	43.72	2.92×10^{-15}	1.00	9.83×10^{-3}	1.00
	0.1	5.21×10^{-11}	5.84	43.72	2.92×10^{-15}	1.00	9.84×10^{-3}	1.00	
	1	5.20×10^{-11}	5.84	43.72	2.92×10^{-15}	1.00	9.84×10^{-3}	1.00	
	10	5.20×10^{-11}	5.84	43.72	2.92×10^{-15}	1.00	9.84×10^{-3}	1.00	
	100	5.20×10^{-11}	5.84	43.72	2.92×10^{-15}	1.00	9.84×10^{-3}	1.00	
	R45	0.01	2.33×10^{-14}	6.80	43.88	3.76×10^{-16}	0.13	2.33×10^{-3}	0.24
	0.1	2.12×10^{-14}	6.81	43.87	3.76×10^{-16}	0.13	2.34×10^{-3}	0.24	
	1	2.10×10^{-14}	6.81	43.87	3.76×10^{-16}	0.13	2.34×10^{-3}	0.24	
	10	2.10×10^{-14}	6.81	43.87	3.76×10^{-16}	0.13	2.34×10^{-3}	0.24	

R46	100	2.10×10^{-14}	6.81	43.87	3.76×10^{-16}	0.13	2.34×10^{-3}	0.24
	0.01	4.90×10^{-13}	6.50	44.30	8.79×10^{-16}	0.30	5.93×10^{-3}	0.60
	0.1	4.79×10^{-13}	6.50	44.29	8.79×10^{-16}	0.30	5.93×10^{-3}	0.60
	1	4.78×10^{-13}	6.50	44.29	8.79×10^{-16}	0.30	5.93×10^{-3}	0.60
	10	4.78×10^{-13}	6.50	44.29	8.79×10^{-16}	0.30	5.93×10^{-3}	0.60
R47	100	4.78×10^{-13}	6.50	44.29	8.79×10^{-16}	0.30	5.93×10^{-3}	0.60
	0.01	3.46×10^{-13}	6.49	43.33	1.56×10^{-15}	0.54	6.25×10^{-3}	0.64
	0.1	3.38×10^{-13}	6.49	43.33	1.56×10^{-15}	0.54	6.25×10^{-3}	0.64
	1	3.38×10^{-13}	6.49	43.33	1.56×10^{-15}	0.54	6.25×10^{-3}	0.64
	10	3.37×10^{-13}	6.49	43.33	1.56×10^{-15}	0.54	6.25×10^{-3}	0.64
R48	100	3.37×10^{-13}	6.49	43.33	1.56×10^{-15}	0.54	6.25×10^{-3}	0.64
	0.01	2.92×10^{-12}	6.33	42.77	1.04×10^{-14}	3.57	3.10×10^{-2}	3.15
	0.1	2.90×10^{-12}	6.33	42.77	1.04×10^{-14}	3.57	3.10×10^{-2}	3.15
	1	2.90×10^{-12}	6.33	42.77	1.04×10^{-14}	3.57	3.10×10^{-2}	3.15
	10	2.90×10^{-12}	6.33	42.77	1.04×10^{-14}	3.57	3.10×10^{-2}	3.15
R49	100	2.90×10^{-12}	6.33	42.77	1.04×10^{-14}	3.57	3.10×10^{-2}	3.15
	0.01	6.82×10^{-13}	6.26	42.60	1.35×10^{-15}	0.46	3.68×10^{-3}	0.37
	0.1	6.76×10^{-13}	6.26	42.60	1.35×10^{-15}	0.46	3.68×10^{-3}	0.37
	1	6.76×10^{-13}	6.26	42.60	1.35×10^{-15}	0.46	3.68×10^{-3}	0.37
	10	6.76×10^{-13}	6.26	42.60	1.35×10^{-15}	0.46	3.68×10^{-3}	0.37
1,6-H(vi) rate rule	100	6.76×10^{-13}	6.26	42.60	1.35×10^{-15}	0.46	3.68×10^{-3}	0.37
	0.01	1.05×10^{26}	-4.93	28.94	8.53×10^{-1}	1.00	9.34×10^4	1.00
	0.1	2.00×10^{19}	-2.71	27.28	8.59×10^{-1}	1.00	2.16×10^5	1.00
	1	1.59×10^{17}	-2.01	26.77	8.60×10^{-1}	1.00	2.94×10^5	1.00
	10	8.26×10^{16}	-1.92	26.71	8.60×10^{-1}	1.00	3.08×10^5	1.00
R50	100	7.72×10^{16}	-1.91	26.70	8.60×10^{-1}	1.00	3.10×10^5	1.00
	0.01	3.44×10^{22}	-4.82	28.98	5.29×10^{-1}	0.62	6.28×10^4	0.67
	0.1	5.27×10^{17}	-2.25	27.00	5.37×10^{-1}	0.63	1.50×10^5	0.70
	1	3.23×10^{13}	-0.87	25.89	5.38×10^{-1}	0.63	2.24×10^5	0.76

R51	10	7.23×10^{12}	-0.66	25.72	5.38×10^{-1}	0.63	2.42×10^5	0.79
	100	6.18×10^{12}	-0.64	25.71	5.38×10^{-1}	0.63	2.44×10^5	0.79
	0.01	4.53×10^{26}	-5.12	28.63	1.55	1.82	1.22×10^5	1.31
	0.1	8.95×10^{19}	-2.90	26.99	1.57	1.82	2.93×10^5	1.36
	1	2.32×10^{18}	-2.36	26.65	1.57	1.82	4.04×10^5	1.38
R52	10	1.66×10^{18}	-2.31	26.63	1.57	1.82	4.23×10^5	1.37
	100	1.60×10^{18}	-2.31	26.63	1.57	1.82	4.25×10^5	1.37
	0.01	4.27×10^{25}	-4.79	29.14	6.51×10^{-1}	0.76	8.98×10^4	0.96
	0.1	3.41×10^{19}	-2.78	27.64	6.54×10^{-1}	0.76	1.96×10^5	0.91
	1	2.57×10^{18}	-2.40	27.40	6.54×10^{-1}	0.76	2.50×10^5	0.85
R53	10	2.02×10^{18}	-2.36	27.39	6.54×10^{-1}	0.76	2.58×10^5	0.84
	100	1.97×10^{18}	-2.36	27.38	6.54×10^{-1}	0.76	2.59×10^5	0.84
	0.01	1.22×10^{28}	-5.51	30.33	6.78×10^{-1}	0.80	9.84×10^4	1.05
	0.1	3.72×10^{21}	-3.35	28.72	6.82×10^{-1}	0.79	2.25×10^5	1.04
	1	1.55×10^{20}	-2.89	28.42	6.82×10^{-1}	0.79	2.97×10^5	1.01
	10	1.15×10^{20}	-2.84	28.40	6.82×10^{-1}	0.79	3.09×10^5	1.00
	100	1.12×10^{20}	-2.84	28.40	6.82×10^{-1}	0.79	3.10×10^5	1.00

Table S21. Pressure-Dependent Rate Rules for Intramolecular H-Shift Reactions of Alkenyl

Peroxy Radicals

Reaction class	Pressure(atm)	Modified Arrhenius parameters			500K	1000K
		A(s ⁻¹)	n	E(kcal/mol)	f^a	f^a
1,4-H(as)	0.01	1.93×10^{-1}	2.90	15.04	85.01	7.81
	0.1	1.52×10^{-11}	6.21	12.38	85.49	12.44
	1	8.34×10^{-15}	7.28	11.57	85.71	18.13
	10	3.57×10^{-16}	7.73	11.19	85.71	20.08
	100	2.35×10^{-16}	7.78	11.14	85.71	20.31
1,4-H(s)	0.01	6.55×10^8	0.19	22.01	60.50	5.16
	0.1	6.30×10	2.50	20.25	60.50	7.01
	1	2.48×10^{-1}	3.30	19.65	60.50	8.07

1,4-H(vt)	10	1.05×10^{-1}	3.42	19.55	60.50	8.24
	100	9.61×10^{-2}	3.43	19.54	60.50	8.25
	0.01	9.15×10^{27}	-5.30	36.93	1.59	1.94
	0.1	3.82×10^{19}	-2.51	34.89	1.52	1.84
	1	6.98×10^{10}	0.32	32.48	1.50	1.72
1,4-H(vi)	10	1.65×10^4	2.44	30.53	1.50	1.63
	100	4.77×10	3.24	29.77	1.50	1.60
	0.01	3.22×10^{18}	-2.47	34.84	23.04	7.29
	0.1	7.22×10^9	0.36	32.57	23.27	8.21
	1	1.45×10^3	2.52	30.71	23.30	9.12
1,5-H(as)	10	1.23×10^{-3}	4.45	28.87	23.33	10.48
	100	7.17×10^{-5}	4.85	28.49	23.33	10.77
	0.01	9.53×10^9	-0.47	11.12	69.16	4.59
	0.1	4.94×10^7	0.47	11.28	91.39	5.51
	1	1.46×10^4	1.73	10.76	98.03	7.79
1,5-H(s)	10	4.92×10^3	1.93	10.83	98.91	9.96
	100	5.37×10^3	1.92	10.88	98.91	10.36
	0.01	1.14×10^{15}	-1.98	12.54	706.09	3.09
	0.1	1.43×10^{15}	-1.74	13.55	45.70	3.92
	1	1.47×10^{13}	-0.93	13.65	53.58	6.22
1,5-H(vt)	10	1.93×10^{11}	-0.24	13.47	55.10	11.18
	100	2.42×10^{11}	-0.24	13.60	55.23	13.59
	0.01	2.01×10^{28}	-5.60	31.26	31.93	6.87
	0.1	1.78×10^{20}	-2.93	29.30	29.30	6.97
	1	3.29×10^{12}	-0.42	27.16	28.88	6.77
1,5-H(vi)	10	9.99×10^8	0.71	26.15	28.73	6.27
	100	1.39×10^8	0.98	25.89	28.73	6.08
	0.01	9.39×10^{30}	-6.39	31.03	17.59	5.26
	0.1	3.08×10^{23}	-3.88	29.31	17.38	6.59

1,6-H(as)	1	4.14×10^{16}	-1.63	27.51	17.32	8.27
	10	3.16×10^{14}	-0.94	26.95	17.36	8.84
	100	1.66×10^{14}	-0.85	26.88	17.36	8.84
	0.01	1.20×10^{10}	-0.51	11.50	22.24	3.15
	0.1	1.28×10^7	0.61	11.32	24.92	3.63
1,6-H(s)	1	7.68×10^6	0.78	11.65	25.37	4.29
	10	1.74×10^7	0.68	11.84	25.45	4.52
	100	1.94×10^7	0.67	11.87	25.45	4.54
	0.01	3.20×10^{22}	-4.04	21.21	1.00	1.00
	0.1	2.58×10^{18}	-2.59	20.59	1.00	1.00
1,6-H(vt)	1	3.04×10^{18}	-2.55	20.87	1.00	1.00
	10	4.09×10^{18}	-2.59	20.94	1.00	1.00
	100	4.24×10^{18}	-2.59	20.95	1.00	1.00
	0.01	5.35×10^{-11}	5.84	43.72	27.81	13.30
	0.1	5.21×10^{-11}	5.84	43.72	27.81	13.25
1,6-H(vi)	1	5.20×10^{-11}	5.84	43.72	27.81	13.25
	10	5.20×10^{-11}	5.84	43.72	27.81	13.25
	100	5.20×10^{-11}	5.84	43.72	27.81	13.25
	0.01	1.05×10^{26}	-4.93	28.94	2.93	1.94
	0.1	2.00×10^{19}	-2.71	27.28	2.92	1.95
	1	1.59×10^{17}	-2.01	26.77	2.92	1.80
	10	8.26×10^{16}	-1.92	26.71	2.92	1.75
	100	7.72×10^{16}	-1.91	26.70	2.92	1.74

^a $f=k_{\max}/k_{\min}$ for each class.

Table S22. Pressure-Dependent Rate Constants, Rate Rules and Ratios of the Individually Calculated Rate constants for Concerted Elimination Reactions of Alkenyl Peroxy Radicals

Reaction	Pressure(atm)	modified Arrhenius parameters			500K		1000K	
		A(s ⁻¹)	n	E(kcal/mol)	k	k/k _{rule}	k	k/k _{rule}
Rate	0.01	2.60×10^{37}	-8.24	33.60	2.53	1.00	2.27×10^5	1.00

Rule-1	0.1	7.56×10^{30}	-5.99	32.33	2.68	1.00	8.36×10^5	1.00
	1	1.72×10^{24}	-3.78	30.73	2.71	1.00	2.07×10^6	1.00
	10	1.67×10^{21}	-2.79	29.98	2.71	1.00	3.03×10^6	1.00
	100	3.13×10^{20}	-2.55	29.78	2.71	1.00	3.24×10^6	1.00
R1	0.01	1.83×10^{33}	-7.07	31.81	1.51	0.60	1.27×10^5	0.56
	0.1	6.34×10^{26}	-4.84	30.57	1.68	0.63	4.63×10^5	0.55
	1	4.26×10^{18}	-2.15	28.49	1.72	0.63	1.13×10^6	0.54
	10	2.36×10^{11}	0.19	26.43	1.72	0.63	1.72×10^6	0.57
	100	4.03×10^8	1.07	25.61	1.72	0.63	1.91×10^6	0.59
R2	0.01	3.17×10^{33}	-7.10	32.13	1.49	0.59	1.58×10^5	0.70
	0.1	1.39×10^{26}	-4.61	30.53	1.56	0.58	5.35×10^5	0.64
	1	5.65×10^{17}	-1.87	28.31	1.57	0.58	1.19×10^6	0.57
	10	2.07×10^{13}	-0.43	27.08	1.57	0.58	1.64×10^6	0.54
	100	4.18×10^{12}	-0.21	26.90	1.57	0.58	1.73×10^6	0.53
R3	0.01	3.94×10^{39}	-8.89	33.70	6.28	2.48	3.33×10^5	1.47
	0.1	1.97×10^{33}	-6.70	32.57	6.74	2.51	1.33×10^6	1.59
	1	2.25×10^{25}	-4.07	30.63	6.82	2.52	3.73×10^6	1.80
	10	5.56×10^{21}	-2.87	29.75	6.83	2.52	6.13×10^6	2.02
	100	2.11×10^{21}	-2.72	29.67	6.83	2.52	6.75×10^6	2.08
R4	0.01	1.67×10^{42}	-9.63	35.05	6.83	2.69	4.15×10^5	1.83
	0.1	9.96×10^{35}	-7.43	33.93	7.23	2.69	1.71×10^6	2.05
	1	5.17×10^{29}	-5.35	32.56	7.30	2.69	4.93×10^6	2.37
	10	6.20×10^{28}	-5.01	32.48	7.30	2.69	7.49×10^6	2.47
	100	5.66×10^{28}	-4.99	32.49	7.30	2.69	7.97×10^6	2.46
R5	0.01	3.14×10^{34}	-7.36	32.91	1.33	0.52	1.84×10^5	0.81
	0.1	5.31×10^{26}	-4.75	31.13	1.36	0.51	5.97×10^5	0.71
	1	7.09×10^{20}	-2.81	29.65	1.36	0.50	1.21×10^6	0.58
	10	7.01×10^{19}	-2.47	29.43	1.36	0.50	1.47×10^6	0.48
	100	5.60×10^{19}	-2.44	29.41	1.36	0.50	1.50×10^6	0.46

R6	0.01	2.25×10^{38}	-8.44	35.17	1.13	0.45	2.27×10^5	1.00
	0.1	1.08×10^{31}	-5.98	33.55	1.15	0.43	7.63×10^5	0.91
	1	3.14×10^{28}	-5.10	33.09	1.15	0.42	1.48×10^6	0.71
	10	2.28×10^{28}	-5.04	33.11	1.15	0.42	1.69×10^6	0.56
	100	2.24×10^{28}	-5.04	33.12	1.15	0.42	1.72×10^6	0.53
R7	0.01	2.55×10^{35}	-7.56	35.86	1.95×10^{-1}	0.08	1.28×10^5	0.56
	0.1	5.45×10^{28}	-5.28	34.29	1.96×10^{-1}	0.07	3.66×10^5	0.44
	1	2.92×10^{27}	-4.83	34.09	1.96×10^{-1}	0.07	5.57×10^5	0.27
	10	2.40×10^{27}	-4.80	34.10	1.96×10^{-1}	0.07	5.94×10^5	0.20
	100	2.36×10^{27}	-4.80	34.10	1.96×10^{-1}	0.07	5.98×10^5	0.18
R8	0.01	4.92×10^{38}	-8.58	34.70	1.78	0.70	2.29×10^5	1.01
	0.1	2.78×10^{31}	-6.12	33.18	1.85	0.69	8.38×10^5	1.00
	1	5.80×10^{23}	-3.59	31.24	1.86	0.69	2.05×10^6	0.99
	10	2.72×10^{21}	-2.81	30.68	1.86	0.69	2.89×10^6	0.95
	100	1.54×10^{21}	-2.73	30.63	1.86	0.69	3.05×10^6	0.94
R9	0.01	1.30×10^{37}	-8.13	33.64	2.27	0.90	2.41×10^5	1.06
	0.1	1.12×10^{30}	-5.71	32.21	2.38	0.89	9.17×10^5	1.10
	1	7.34×10^{21}	-3.01	30.15	2.40	0.89	2.40×10^6	1.16
	10	4.03×10^{18}	-1.94	29.34	2.40	0.89	3.68×10^6	1.21
	100	1.69×10^{18}	-1.81	29.26	2.40	0.89	3.96×10^6	1.22
Rate	0.01	1.06×10^{35}	-7.40	36.18	1.09×10^{-1}	1.00	9.56×10^4	1.00
Rule-2	0.1	2.26×10^{27}	-4.85	34.36	1.10×10^{-1}	1.00	2.79×10^5	1.00
	1	5.10×10^{21}	-3.00	32.87	1.10×10^{-1}	1.00	4.95×10^5	1.00
	10	6.36×10^{19}	-2.38	32.36	1.10×10^{-1}	1.00	5.80×10^5	1.00
	100	3.35×10^{19}	-2.29	32.28	1.10×10^{-1}	1.00	5.93×10^5	1.00
R10	0.01	1.83×10^{36}	-7.80	36.59	1.14×10^{-1}	1.05	8.35×10^4	0.87
	0.1	1.04×10^{28}	-5.05	34.65	1.17×10^{-1}	1.06	2.64×10^5	0.95
	1	1.88×10^{19}	-2.21	32.27	1.18×10^{-1}	1.07	5.41×10^5	1.09
	10	9.37×10^{14}	-0.82	31.06	1.18×10^{-1}	1.07	7.05×10^5	1.22

R11	100	2.04×10^{14}	-0.60	30.87	1.18×10^{-1}	1.07	7.36×10^5	1.24
	0.01	2.19×10^{32}	-6.58	36.26	3.34×10^{-2}	0.31	5.89×10^4	0.62
	0.1	6.48×10^{23}	-3.79	34.06	3.36×10^{-2}	0.31	1.46×10^5	0.53
	1	3.36×10^{20}	-2.71	33.21	3.36×10^{-2}	0.31	2.14×10^5	0.43
	10	1.36×10^{20}	-2.58	33.12	3.36×10^{-2}	0.31	2.28×10^5	0.39
R12	100	1.24×10^{20}	-2.56	33.11	3.36×10^{-2}	0.31	2.29×10^5	0.39
	0.01	1.92×10^{33}	-6.91	34.83	1.70×10^{-1}	1.56	1.07×10^5	1.12
	0.1	3.40×10^{27}	-4.98	33.53	1.70×10^{-1}	1.55	2.78×10^5	1.00
	1	6.32×10^{26}	-4.71	33.46	1.71×10^{-1}	1.55	3.81×10^5	0.77
	10	5.67×10^{26}	-4.69	33.46	1.71×10^{-1}	1.55	3.98×10^5	0.69
R13	100	5.61×10^{26}	-4.69	33.46	1.71×10^{-1}	1.55	4.00×10^5	0.67
	0.01	7.79×10^{37}	-8.23	37.80	9.49×10^{-2}	0.87	1.03×10^5	1.07
	0.1	1.74×10^{29}	-5.36	35.70	9.63×10^{-2}	0.87	3.21×10^5	1.15
	1	5.14×10^{22}	-3.22	33.99	9.64×10^{-2}	0.87	6.29×10^5	1.27
	10	2.85×10^{21}	-2.80	33.69	9.65×10^{-2}	0.87	7.53×10^5	1.30
R14	100	2.12×10^{21}	-2.76	33.66	9.65×10^{-2}	0.87	7.70×10^5	1.30
	0.01	2.33×10^{33}	-6.87	36.65	3.94×10^{-2}	0.36	7.11×10^4	0.74
	0.1	2.38×10^{28}	-5.20	35.52	3.95×10^{-2}	0.36	1.65×10^5	0.59
	1	6.82×10^{27}	-5.00	35.46	3.95×10^{-2}	0.36	2.09×10^5	0.42
	10	6.19×10^{27}	-4.99	35.46	3.95×10^{-2}	0.36	2.15×10^5	0.37
R15	100	6.13×10^{27}	-4.98	35.46	3.95×10^{-2}	0.36	2.15×10^5	0.36
	0.01	2.41×10^{36}	-7.79	36.57	1.51×10^{-1}	1.39	1.23×10^5	1.28
	0.1	1.81×10^{29}	-5.41	34.92	1.52×10^{-1}	1.38	3.63×10^5	1.30
	1	5.80×10^{27}	-4.89	34.67	1.52×10^{-1}	1.38	5.76×10^5	1.16
	10	4.61×10^{27}	-4.85	34.68	1.52×10^{-1}	1.38	6.19×10^5	1.07
R16	100	4.52×10^{27}	-4.84	34.68	1.52×10^{-1}	1.38	6.24×10^5	1.05
	0.01	1.24×10^{37}	-8.02	36.82	1.53×10^{-1}	1.41	1.15×10^5	1.20
	0.1	3.80×10^{28}	-5.18	34.80	1.56×10^{-1}	1.41	3.70×10^5	1.33
	1	2.45×10^{21}	-2.83	32.91	1.56×10^{-1}	1.42	7.66×10^5	1.55

R17	10	5.80×10^{19}	-2.29	32.50	1.56×10^{-1}	1.42	9.51×10^5	1.64
	100	3.91×10^{19}	-2.23	32.46	1.56×10^{-1}	1.42	9.78×10^5	1.65
	0.01	3.47×10^{36}	-7.84	36.89	1.15×10^{-1}	1.06	1.04×10^5	1.09
	0.1	7.61×10^{27}	-4.97	34.80	1.17×10^{-1}	1.06	3.26×10^5	1.17
	1	1.65×10^{21}	-2.79	33.05	1.17×10^{-1}	1.06	6.43×10^5	1.30
rate	10	7.90×10^{19}	-2.35	32.72	1.17×10^{-1}	1.06	7.72×10^5	1.33
	100	5.77×10^{19}	-2.31	32.69	1.17×10^{-1}	1.06	7.90×10^5	1.33
	0.01	2.54×10^{33}	-6.73	45.11	2.21×10^{-5}	1.00	3.17×10^3	1.00
	0.1	5.06×10^{24}	-3.86	42.89	2.27×10^{-5}	1.00	7.80×10^3	1.00
	1	1.86×10^{16}	-1.14	40.52	2.28×10^{-5}	1.00	1.33×10^4	1.00
Rule-3	10	2.46×10^{10}	0.74	38.78	2.28×10^{-5}	1.00	1.66×10^4	1.00
	100	2.95×10^8	1.35	38.20	2.28×10^{-5}	1.00	1.75×10^4	1.00
	0.01	1.65×10^{29}	-5.52	44.91	3.30×10^{-6}	0.15	8.97×10^2	0.28
	0.1	2.64×10^{21}	-2.94	42.99	3.51×10^{-6}	0.16	2.20×10^3	0.28
	1	4.50×10^{13}	-0.42	40.84	3.55×10^{-6}	0.16	3.78×10^3	0.28
R18	10	5.87×10^7	1.46	39.11	3.56×10^{-6}	0.16	4.77×10^3	0.29
	100	2.56×10^6	1.89	39.69	3.56×10^{-6}	0.16	5.06×10^3	0.29
	0.01	3.53×10^{37}	-7.92	46.04	7.11×10^{-5}	3.21	7.37×10^3	2.33
	0.1	3.13×10^{28}	-4.93	43.76	7.31×10^{-5}	3.22	2.01×10^4	2.58
	1	1.75×10^{19}	-1.94	41.17	7.34×10^{-5}	3.22	3.71×10^4	2.78
R19	10	1.37×10^{12}	0.33	39.07	7.34×10^{-5}	3.22	4.82×10^4	2.89
	100	5.09×10^9	1.11	38.34	7.34×10^{-5}	3.22	5.11×10^4	2.92
	0.01	6.02×10^{29}	-5.60	44.39	1.13×10^{-5}	0.51	2.72×10^3	0.86
	0.1	2.56×10^{20}	-2.56	41.83	1.14×10^{-5}	0.50	5.60×10^3	0.72
	1	2.27×10^{12}	0.02	39.47	1.14×10^{-5}	0.50	7.93×10^3	0.59
R20	10	3.77×10^8	1.23	38.34	1.14×10^{-5}	0.50	8.74×10^3	0.53
	100	8.62×10^7	1.43	38.14	1.14×10^{-5}	0.50	8.86×10^3	0.51
	0.01	1.10×10^{29}	-5.33	45.73	2.84×10^{-6}	0.13	1.68×10^3	0.53
	0.1	4.43×10^{19}	-2.29	43.17	2.85×10^{-6}	0.13	3.30×10^3	0.42
R21								

1	6.36×10^{11}	0.22	40.83	2.86×10^{-6}	0.13	4.52×10^3	0.34
10	2.18×10^8	1.33	39.79	2.86×10^{-6}	0.13	4.92×10^3	0.30
100	5.99×10^7	1.50	39.62	2.86×10^{-6}	0.13	4.98×10^3	0.28

Table S23. Pressure-Dependent Rate Rules for Concerted Eliminations Reactions of Alkenyl

Peroxy Radicals

Reaction	Pressure(atm)	Modified Arrhenius parameters			500K	1000K
class		A(s ⁻¹)	n	E(kcal/mol)	f^a	f^a
Rate rules-1	0.01	2.60×10^{37}	-8.24	33.60	35.03	3.27
	0.1	7.56×10^{30}	-5.99	32.33	36.89	4.67
	1	1.72×10^{24}	-3.78	30.73	37.24	8.85
	10	1.67×10^{21}	-2.79	29.98	37.24	12.61
	100	3.13×10^{20}	-2.55	29.78	37.24	13.33
Rate rules-2	0.01	1.06×10^{35}	-7.40	36.18	5.09	2.09
	0.1	2.26×10^{27}	-4.85	34.36	5.06	2.53
	1	5.10×10^{21}	-3.00	32.87	5.09	3.67
	10	6.36×10^{19}	-2.38	32.36	5.09	4.42
	100	3.35×10^{19}	-2.29	32.28	5.09	4.55
Rate rules-3	0.01	2.54×10^{33}	-6.73	45.11	25.04	8.22
	0.1	5.06×10^{24}	-3.86	42.89	25.65	9.14
	1	1.86×10^{16}	-1.14	40.52	25.66	9.81
	10	2.46×10^{10}	0.74	38.78	25.66	10.15
	100	2.95×10^8	1.35	38.20	25.66	10.26

^a $f = k_{\max}/k_{\min}$ for each class.

6. Cartesian coordinates of reactants, products, and transition states

6.1 The optimized geometries of all the reactions at B3LYP/6-31G(2df,p) level for cycloaddition reactions of alkenyl peroxy radicals(TS_n is the transition state of the reaction R_n)

R1-C=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	2.32345800	0.13895400	-0.26716500
C	1.21630500	-0.36510100	0.26701700
H	2.35079200	1.14240800	-0.68233200
H	3.24886800	-0.42546200	-0.30275700
H	1.20908100	-1.37364800	0.67400400
C	-0.06793300	0.38738600	0.37541700
H	-0.41691200	0.48496100	1.40810800
H	-0.00908200	1.37950500	-0.08143600
O	-1.10257800	-0.37018700	-0.33678500
O	-2.29913800	0.09828700	-0.07161500

P1-YCC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.18652800	0.32753600	-0.10958800
C	-0.00001000	1.22291500	-0.00023100
H	-1.61078600	0.30883600	-1.13001200
H	-0.00014800	2.30220500	0.00089800
H	-1.99515200	0.55532000	0.59680100
O	-0.68146100	-0.95618600	0.25855800
O	0.68150700	-0.95620900	-0.25845400
C	1.18651500	0.32761400	0.10952300
H	1.61060100	0.30916900	1.13003200
H	1.99525900	0.55523200	-0.59677600

TS1

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.64970700	0.93508700	0.29576200
O	-1.20291900	-0.25910800	-0.28009800
C	1.40917700	-0.28592600	0.10927800
C	0.77682000	0.91415900	-0.18973000
H	-1.25081800	1.76492000	-0.08157800
H	-0.70582500	0.89719300	1.39286400
H	1.45947900	-0.65455200	1.12625700
H	2.19156100	-0.65846500	-0.54843800
H	1.04838400	1.50595600	-1.05746600
O	-0.29214600	-1.27026400	0.01466000

R2-C=CC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.37995800	-0.22114300	-0.16869600
C	1.20019100	-0.71744100	0.18629800
H	2.53311700	0.83529000	-0.36125500
H	3.25045500	-0.85979300	-0.27131900
H	1.09341300	-1.78418100	0.37129500

P2-YCC•C(C)OO

C	-0.05919300	0.07118500	0.39265200
H	-0.38771100	-0.00897800	1.43563200
O	-1.09639000	-0.65443900	-0.37746500
O	-2.30374000	-0.32057000	0.00979400
C	-0.04520100	1.52605400	-0.04315400
H	0.64555300	2.10264100	0.57831400
H	0.25887100	1.61961600	-1.08922500
H	-1.04718800	1.94354800	0.07532200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.49986100	0.58638300	0.24997000
C	0.18896700	1.17004300	-0.14564100
H	1.70063600	0.68714400	1.33235400
H	-0.05173700	2.21904900	-0.23342500
H	2.36339400	0.98604400	-0.29759400
O	1.38666700	-0.78846000	-0.12250600
O	-0.01443600	-1.09774300	0.11683400
C	-0.72738900	0.02391800	-0.42641800
H	-0.85497500	-0.11914000	-1.51609200
C	-2.09760100	0.06665000	0.24530200
H	-1.99099800	0.20298600	1.32414900
H	-2.64182200	-0.86319300	0.05786300
H	-2.68537600	0.89476300	-0.16115900

TS2

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.65803800	-0.07230400	0.37596100
O	0.12672000	1.12191500	-0.23953000
C	-1.61194800	-0.84104400	0.07969600
C	-0.27622000	-1.13663500	-0.15126400
H	0.55513700	0.01251000	1.46813200
H	-1.97540100	-0.62917800	1.07751000
H	-2.36944000	-1.20262000	-0.61241700
H	0.04210000	-1.72629400	-1.00603300
O	-1.24966100	1.08901100	-0.02592800
C	2.11274900	-0.19372200	-0.03606200
H	2.68382000	0.67353400	0.30430700
H	2.55212300	-1.09247200	0.40656600
H	2.19947600	-0.26065100	-1.12438800

R3-C=CC(CC)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.80371100	-1.50583000	-0.28707200

C	0.66185800	-1.34320000	0.37242500
H	2.21954400	-0.74208000	-0.93496000
H	2.37703900	-2.42218600	-0.19723700
H	0.29095700	-2.14655400	1.00552400
C	-0.22639200	-0.13281400	0.33317600
H	-0.49170500	0.17234200	1.35213400
O	-1.50148300	-0.62764200	-0.24741400
O	-2.50008100	0.17627600	0.02592000
C	0.24185900	1.08290700	-0.46031000
C	1.32966900	1.89089100	0.25625300
H	-0.64146700	1.71216700	-0.60753700
H	0.57727400	0.76875900	-1.45483200
H	1.60992800	2.76524800	-0.33820500
H	0.97364300	2.25061400	1.22756600
H	2.23306600	1.30089200	0.43267100

P3-YCC•C(CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.83354200	0.81677100	0.24627700
C	0.40722300	1.11341100	-0.06166800
H	2.06238800	0.90393200	1.32421100
H	-0.04242000	2.09183000	-0.13891100
H	2.55703500	1.42784700	-0.30873400
O	2.00844900	-0.52725100	-0.20456800
O	0.72391500	-1.15334200	0.06972700
C	-0.25050300	-0.19304700	-0.36350900
H	-0.41922900	-0.30610200	-1.45223600
C	-1.55457700	-0.50498200	0.37963000
C	-2.72712900	0.35651700	-0.09568700
H	-1.38488500	-0.37060000	1.45281500
H	-1.78313400	-1.56513500	0.22102800
H	-3.64654600	0.07878800	0.42733500
H	-2.54866400	1.42029500	0.09230900
H	-2.90478900	0.23186000	-1.16934500

TS3

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.18134000	-0.24930900	0.29029500
O	-0.15850700	0.99779400	-0.35700700
C	-2.21185200	-0.56286200	0.20721000
C	-0.98300300	-1.12895900	-0.10052000
H	0.19152500	-0.09458100	1.38057100
H	-2.44321100	-0.23735800	1.21374900
H	-3.07990000	-0.79768400	-0.40518900

R4-C=C(C)COO•

H	-0.85809100	-1.81044300	-0.93697000
O	-1.49075700	1.25032300	-0.03971700
C	1.54768800	-0.68392600	-0.21689100
C	2.67514400	0.27083200	0.18466600
H	1.49709300	-0.77418600	-1.30853200
H	1.74172500	-1.68954600	0.17586900
H	3.63697200	-0.07535600	-0.20440500
H	2.49091000	1.27564500	-0.20412400
H	2.76119800	0.34392500	1.27425900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.92007300	-1.04032200	-0.21007200
C	-1.01994500	-0.10321500	0.08284700
H	-1.67467400	-2.09701700	-0.18292400
H	-2.93948200	-0.78501900	-0.48089600
C	0.36913500	-0.49018500	0.49862300
H	0.64923200	-0.07634800	1.47263400
H	0.51753800	-1.57293500	0.50598900
O	1.31499100	0.07630800	-0.47122400
O	2.54671500	0.02566200	-0.02255000
C	-1.31369300	1.37263500	0.04701500
H	-0.63440100	1.88751200	-0.64099000
H	-2.34087000	1.56777900	-0.26874600
H	-1.16354400	1.82679200	1.03464100

P4-YCC•(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.16477600	1.18269200	-0.13592900
C	0.73445300	-0.01363400	-0.10635800
H	-0.23371800	1.63462400	-1.14223300
H	0.11535000	1.97093100	0.57645100
O	-1.43328000	0.68997700	0.29233000
O	-1.47050700	-0.67479000	-0.22254800
C	-0.17579100	-1.18343700	0.08373300
H	-0.13995300	-1.58632300	1.11421800
H	0.00335100	-2.01163300	-0.61486300
C	2.21124600	-0.00596100	0.03653200
H	2.53061200	0.09357500	1.08858600
H	2.65974700	-0.93145000	-0.34118300
H	2.66411800	0.83083100	-0.50710200

TS4

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	0.26424400	-0.96891300	0.63634900
O	1.19601700	-0.79852600	-0.43853100
C	-0.11720200	1.36283600	0.32940800
C	-0.74522700	0.12460000	0.35801500
H	-0.12855200	-1.98499400	0.54792200
H	0.75781600	-0.83642500	1.60890400
H	0.51498000	1.69066700	1.14423300
H	-0.53611200	2.16182300	-0.27908100
O	1.53447600	0.56191000	-0.41233200
C	-1.98712300	-0.21429200	-0.39575600
H	-2.67588800	-0.80267700	0.22448800
H	-2.51808300	0.67702200	-0.73825100
H	-1.74626000	-0.83787600	-1.26941200

R5-C=C(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.08432800	1.66380200	-0.20978300
C	0.47719100	0.52935900	0.13610100
H	0.54001500	2.60085900	-0.26602100
H	2.14162700	1.70667800	-0.44314700
C	-0.98303600	0.54065800	0.48654300
H	-1.18691300	0.10795200	1.47114000
H	-1.41793600	1.54173500	0.43161500
O	-1.69826200	-0.30039400	-0.48284000
O	-2.91675600	-0.56724500	-0.07664200
C	1.15061800	-0.82033900	0.23185800
C	2.63506200	-0.85867500	-0.12863300
H	0.59595300	-1.52133000	-0.40578400
H	1.00903600	-1.20049300	1.25456300
H	3.02294700	-1.87666100	-0.03332100
H	2.80458600	-0.53251600	-1.15965400
H	3.22585200	-0.21394500	0.52994500

P5-YCC•(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.92448500	1.16798400	-0.21340900
C	0.24300000	0.24485700	-0.04362900
H	-1.03844200	1.51842800	-1.25514300
H	-0.89573600	2.04719700	0.44460800
O	-2.05616500	0.40060700	0.19352800
O	-1.71909500	-0.95783400	-0.21689600
C	-0.36146100	-1.10475500	0.18778400
H	-0.29330200	-1.41911400	1.24736500
H	0.05640900	-1.90580500	-0.43506100

C	1.64207700	0.65466700	0.25626100
H	1.75947200	0.82895000	1.34247000
H	1.84256000	1.62704400	-0.21160800
C	2.70625800	-0.35982600	-0.19204500
H	3.71031900	-0.00224200	0.05375000
H	2.56888900	-1.32653900	0.30322600
H	2.65957800	-0.52766400	-1.27243300

TS5

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.49613000	-0.98257400	0.55377600
O	1.54659800	-0.95363300	-0.42012800
C	0.61177200	1.38907300	0.36543800
C	-0.24687100	0.30345300	0.25653200
H	-0.07471100	-1.89498600	0.36410900
H	0.90575800	-0.99791100	1.57303100
H	1.21188500	1.54504400	1.25249100
H	0.42134000	2.28305100	-0.22518200
O	2.14009600	0.30843200	-0.27731600
C	-1.46216600	0.26042100	-0.61460800
C	-2.71917400	-0.22843200	0.13146700
H	-1.26516000	-0.41893300	-1.45826700
H	-1.65200600	1.25202700	-1.03842500
H	-3.57273200	-0.27851800	-0.55056500
H	-2.57041600	-1.22729500	0.55416500
H	-2.97565300	0.44747700	0.95256600

R6-(cis)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.81928900	0.52831900	-0.14283600
C	-0.56610900	0.90860400	0.11292400
H	-2.52210200	1.30716100	-0.43526300
H	-0.30831800	1.95977100	0.00795100
C	0.56001300	0.03352500	0.54898100
H	1.01676500	0.37313300	1.48379400
H	0.29033500	-1.01949800	0.64871100
O	1.61586400	0.11465100	-0.47203600
O	2.72064500	-0.45673700	-0.05570200
C	-2.40944200	-0.84779300	-0.07087700
H	-3.20901100	-0.88536200	0.67918800
H	-2.87090700	-1.11345600	-1.02937900
H	-1.67987300	-1.62098400	0.17775200

P6-CYCC•COO

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.49986100	0.58638300	0.24997000
C	0.18896700	1.17004300	-0.14564100
H	1.70063600	0.68714400	1.33235400
H	-0.05173700	2.21904900	-0.23342500
H	2.36339400	0.98604400	-0.29759400
O	1.38666700	-0.78846000	-0.12250600
O	-0.01443600	-1.09774300	0.11683400
C	-0.72738900	0.02391800	-0.42641800
H	-0.85497500	-0.11914000	-1.51609200
C	-2.09760100	0.06665000	0.24530200
H	-1.99099800	0.20298600	1.32414900
H	-2.64182200	-0.86319300	0.05786300
H	-2.68537600	0.89476300	-0.16115900

TS6

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.16105300	0.63625000	0.57347500
O	-1.48189000	-0.63808100	-0.02614300
C	0.95627400	0.32377400	-0.55521400
C	-0.11610300	1.19400200	-0.35258900
H	-2.09400900	1.20285400	0.60011600
H	-0.78730600	0.49230800	1.59566500
H	-0.44373500	1.86101900	-1.14356300
O	-0.26465700	-1.22665500	-0.33368300
H	1.39789800	0.33442600	-1.55277600
C	1.89622700	-0.16948300	0.51024700
H	2.21996200	-1.19056000	0.29007700
H	2.78852000	0.46960300	0.53292500
H	1.43897100	-0.15902400	1.50065000

R7-(trans)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.64596500	0.32705700	-0.23290000
C	0.57009500	-0.08521700	0.43528500
H	1.53907800	1.15657900	-0.93220600
H	0.64662400	-0.91407500	1.13650200
C	-0.77700300	0.53559700	0.29539500
H	-1.20987600	0.84764600	1.25046200
H	-0.77429000	1.38456700	-0.39454400
O	-1.69668500	-0.47269400	-0.25403400
O	-2.94534600	-0.08550100	-0.14544400
C	3.02176600	-0.24897300	-0.10302700
H	3.73747100	0.51273400	0.22973900

P7-CYCC•COO

H	3.04809900	-1.07826500	0.60886800
H	3.38419900	-0.61440900	-1.07151600

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.49986100	0.58638300	0.24997000
C	0.18896700	1.17004300	-0.14564100
H	1.70063600	0.68714400	1.33235400
H	-0.05173700	2.21904900	-0.23342500
H	2.36339400	0.98604400	-0.29759400
O	1.38666700	-0.78846000	-0.12250600
O	-0.01443600	-1.09774300	0.11683400
C	-0.72738900	0.02391800	-0.42641800
H	-0.85497500	-0.11914000	-1.51609200
C	-2.09760100	0.06665000	0.24530200
H	-1.99099800	0.20298600	1.32414900
H	-2.64182200	-0.86319300	0.05786300
H	-2.68537600	0.89476300	-0.16115900

TS7

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.42454000	-0.73867800	0.16815500
O	1.52331800	0.58141400	-0.38576300
C	-0.90477200	-0.17250100	0.41818000
C	-0.01167400	-1.11589900	-0.08453400
H	2.15732300	-1.35086800	-0.36225000
H	1.65604000	-0.72677500	1.24306100
H	-0.81619400	0.11079300	1.46199700
H	-0.25526300	-1.71478400	-0.95729300
O	0.41428800	1.27062500	0.11516000
C	-2.24821400	0.08875700	-0.19838000
H	-2.29325700	-0.24957600	-1.23649000
H	-2.46910400	1.15998400	-0.17492300
H	-3.03967000	-0.41516600	0.37019000

R8-(cis)-CCC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.16294400	0.88458100	-0.22720700
C	0.08200600	1.03062400	0.23110500
H	-1.75059800	1.79276100	-0.36247800
H	0.45225400	2.03444000	0.42588200
C	1.05847200	-0.05914300	0.52090900
H	1.45740100	-0.00253100	1.53837400

P8-CCYCC•COO

H	0.66588400	-1.06295600	0.34902500
O	2.21119600	0.11366600	-0.37727200
O	3.19901000	-0.67855100	-0.03538200
C	-1.89854300	-0.38058200	-0.56356000
H	-2.23154000	-0.31787000	-1.60850300
H	-1.24102700	-1.25282700	-0.50365000
C	-3.12952100	-0.59594300	0.33432000
H	-3.81666400	0.25462500	0.27355300
H	-3.67876400	-1.49297700	0.03352800
H	-2.83541500	-0.71080900	1.38209400

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.83354200	0.81677100	0.24627700
C	0.40722300	1.11341100	-0.06166800
H	2.06238800	0.90393200	1.32421100
H	-0.04242000	2.09183000	-0.13891100
H	2.55703500	1.42784700	-0.30873400
O	2.00844900	-0.52725100	-0.20456800
O	0.72391500	-1.15334200	0.06972700
C	-0.25050300	-0.19304700	-0.36350900
H	-0.41922900	-0.30610200	-1.45223600
C	-1.55457700	-0.50498200	0.37963000
C	-2.72712900	0.35651700	-0.09568700
H	-1.38488500	-0.37060000	1.45281500
H	-1.78313400	-1.56513500	0.22102800
H	-3.64654600	0.07878800	0.42733500
H	-2.54866400	1.42029500	0.09230900
H	-2.90478900	0.23186000	-1.16934500

TS8

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.75001400	0.30558500	0.59583800
O	-1.65723200	-0.98949900	-0.03198500
C	0.34063800	0.71893800	-0.55896800
C	-0.95201700	1.18765700	-0.32440400
H	-2.81436000	0.54474000	0.64322200
H	-1.33389000	0.26832600	1.61112600
H	-1.48887600	1.73572100	-1.09218700
O	-0.31909900	-1.15695500	-0.35720800
H	0.73670800	0.89369200	-1.56183700
C	1.42339900	0.55445700	0.47986600
H	1.87405100	1.54750100	0.62758600
H	0.98479700	0.26463600	1.43834400

C	2.51578300	-0.43721400	0.06732300
H	3.30549500	-0.47650000	0.82328800
H	2.10288000	-1.44080700	-0.05214200
H	2.97710500	-0.14221300	-0.88178500

R9-(trans)-CCC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.05455100	0.81909700	-0.08678400
C	0.09831400	-0.00997100	0.32949000
H	0.77612600	1.84583500	-0.32693300
H	0.32532800	-1.04343100	0.57681500
C	-1.32371000	0.40220600	0.49954400
H	-1.71920700	0.18758900	1.49677800
H	-1.48179600	1.45966800	0.26791200
O	-2.14725400	-0.37887600	-0.43676900
O	-3.42314900	-0.26962900	-0.15191500
C	2.51291100	0.50293300	-0.26099900
H	3.09199600	1.20436900	0.35713000
H	2.79175600	0.75087500	-1.29542100
C	2.93224600	-0.93281500	0.05598800
H	2.72020700	-1.19072500	1.09858400
H	2.40736200	-1.65160100	-0.58112500
H	4.00558000	-1.06324600	-0.10770200

P9-CCYCC•OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.83354200	0.81677100	0.24627700
C	0.40722300	1.11341100	-0.06166800
H	2.06238800	0.90393200	1.32421100
H	-0.04242000	2.09183000	-0.13891100
H	2.55703500	1.42784700	-0.30873400
O	2.00844900	-0.52725100	-0.20456800
O	0.72391500	-1.15334200	0.06972700
C	-0.25050300	-0.19304700	-0.36350900
H	-0.41922900	-0.30610200	-1.45223600
C	-1.55457700	-0.50498200	0.37963000
C	-2.72712900	0.35651700	-0.09568700
H	-1.38488500	-0.37060000	1.45281500
H	-1.78313400	-1.56513500	0.22102800
H	-3.64654600	0.07878800	0.42733500
H	-2.54866400	1.42029500	0.09230900
H	-2.90478900	0.23186000	-1.16934500

TS9

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-1.84039100	0.86223600	0.20161900
O	-2.13752100	-0.46158100	-0.26679900
C	0.42368500	0.03583700	0.27969700
C	-0.39959800	1.05567400	-0.19230300
H	-2.54441000	1.53101500	-0.29861100
H	-1.97380500	0.92692600	1.29114700
H	0.40728000	-0.18833500	1.34236100
H	-0.17101900	1.58286000	-1.11425700
O	-1.07313000	-1.25272800	0.17616600
C	1.67388900	-0.39891700	-0.43568300
H	1.61266000	-0.12135300	-1.49332700
H	1.72388800	-1.49307300	-0.39987900
C	2.94538000	0.18912000	0.19908000
H	3.83853300	-0.17402900	-0.31800600
H	2.94550500	1.28253600	0.14796700
H	3.02878100	-0.09577100	1.25320400

R10-C=C(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.97928500	0.91330200	-0.35360800
C	1.13087500	-0.03302700	0.04406000
H	1.68314300	1.94687800	-0.48546800
H	3.01968200	0.68177800	-0.55735800
C	-0.31424800	0.26046200	0.37375900
H	-0.54465100	-0.10192900	1.38236000
O	-1.11173700	-0.61495200	-0.52210100
O	-2.32829200	-0.79227800	-0.06703100
C	1.54818800	-1.46941800	0.23123100
H	0.95778300	-2.13502000	-0.40689800
H	1.37916200	-1.79530900	1.26544500
C	-0.80609200	1.68747800	0.20596800
H	-0.29751900	2.35195800	0.90946900
H	-0.63266500	2.04850100	-0.81112800
H	-1.87820200	1.71795000	0.41199100
H	2.60544800	-1.60974900	-0.00382400

P10-YCC•(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.91457200	-1.22193100	0.30517000
C	0.42032700	-0.68853900	-0.09503300
H	-1.00807700	-1.37099600	1.39794200
H	-1.19108800	-2.16177700	-0.19178000
O	-1.83647500	-0.23593100	-0.15431800

O	-1.12475900	1.01748600	0.05006900
C	0.20527600	0.76013100	-0.41939400
H	0.24705500	0.92487000	-1.51352300
C	1.13003200	1.75830700	0.27505300
H	1.09198800	1.62627800	1.35940600
H	0.83276400	2.78290400	0.03479300
H	2.15982300	1.61434500	-0.06496300
C	1.71497400	-1.41292000	-0.06792200
H	2.43401000	-0.97719400	-0.77107000
H	2.19506000	-1.39050800	0.92498000
H	1.59210900	-2.47065400	-0.32903400

TS10

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.56580700	-0.49672800	0.45444700
O	0.05247500	-1.27575100	-0.58778500
C	1.56486100	0.57459900	0.54255100
C	0.21194600	0.80783100	0.34252700
H	-0.35202600	-0.96528000	1.42657000
H	1.91894000	0.01822500	1.40050300
H	2.29739900	1.23978500	0.09027400
O	1.43382100	-1.18521500	-0.35711500
C	-2.06071100	-0.46944900	0.19491400
H	-2.46721400	-1.48274500	0.24291800
H	-2.56345900	0.13714700	0.95394900
H	-2.28863100	-0.05687200	-0.79082300
C	-0.32034700	1.93546200	-0.47834300
H	-1.20569600	2.38721300	-0.01418000
H	0.42675600	2.72032800	-0.61675200
H	-0.63609400	1.57963100	-1.46983800

R11-C=C(CC)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.09075500	1.60731600	-0.37568100
C	0.62429600	0.43686800	0.05588100
H	0.44707200	2.46430900	-0.53136400
H	2.14275800	1.75894500	-0.58572600
C	-0.83863100	0.22753600	0.37853300
H	-0.93964700	-0.20709800	1.37959900
O	-1.29875200	-0.84894800	-0.53671700
O	-2.38680200	-1.42983700	-0.09249800
C	1.48839800	-0.78321100	0.29524100
H	1.07421500	-1.61405700	-0.28994900
H	1.36179600	-1.08924000	1.34439800

C	-1.77968900	1.41008700	0.22718400
H	-1.51720100	2.20030600	0.93545300
H	-1.74538100	1.81721600	-0.78669300
H	-2.79896000	1.07848400	0.43688300
C	2.97707800	-0.62987000	-0.01337800
H	3.43864400	0.15053000	0.60013000
H	3.50376100	-1.56678800	0.18890500
H	3.14413200	-0.37468100	-1.06460400

P11-YCC•(CC)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.09269300	-1.40184600	0.37140700
C	0.37225600	0.00902700	-0.03406400
H	0.10757000	-1.53922400	1.47013300
H	0.76385900	-2.14750000	-0.07365800
O	-1.20308000	-1.66851600	-0.15804800
O	-1.90115400	-0.40034000	-0.00948800
C	-0.95366300	0.58591800	-0.44067400
H	-1.01197800	0.69190300	-1.54100700
C	-1.35304400	1.90713100	0.21371900
H	-1.31609800	1.82314100	1.30289500
H	-2.36834400	2.18479000	-0.08282100
H	-0.67624000	2.70522700	-0.10514700
C	1.64571200	0.75665900	0.15230600
H	1.62271200	1.66834800	-0.45839800
H	1.73338900	1.11268200	1.19513800
C	2.90924100	-0.05262200	-0.18747000
H	3.80767300	0.55376900	-0.04012300
H	2.99933000	-0.93779700	0.45030800
H	2.89282200	-0.39008100	-1.22837800

TS11

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.60777800	0.73598900	0.43988300
O	-1.66803100	0.50162100	-0.50595000
C	-0.49624900	-1.64652000	0.49150200
C	0.25215400	-0.50704600	0.23243800
H	-1.02658300	0.71610400	1.45723700
H	-1.07141600	-1.75116200	1.40221200
H	-0.23193800	-2.58265900	0.00390900
O	-2.12779900	-0.79704700	-0.24723400
C	-0.02066000	2.10339500	0.14051100
H	-0.79468500	2.86751600	0.24897800
H	0.78562400	2.33317900	0.84231800

H	0.37092600	2.16063000	-0.87788900
C	1.46450600	-0.50232600	-0.64690900
H	1.57415200	-1.49207700	-1.10404700
H	1.33210400	0.21388900	-1.46806000
C	2.76493500	-0.16174100	0.11199400
H	3.61981900	-0.18487200	-0.57033000
H	2.71997900	0.83490900	0.56019100
H	2.94721300	-0.88256100	0.91444700

R12-C=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600
H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100
C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

P12-YCC•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.31794800	1.38384000	-0.11287300
C	-1.10189600	0.97206400	0.09618100
C	-1.27049800	-0.52328200	-0.21456800
C	1.38249900	0.36838500	0.13435700
H	-2.18560200	-0.93051000	0.22757900
H	-1.39758000	1.14301100	1.14678700
H	-1.78911500	1.56971100	-0.51478500
H	0.58580000	2.43225400	-0.18474900
H	1.64841200	0.29784300	1.20519400
H	2.30171200	0.58688600	-0.42243500
H	-1.28169200	-0.70728600	-1.29566900
O	0.98985400	-0.92388800	-0.32966700
O	-0.22113600	-1.27585600	0.38210400

TS12

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.31802400	1.38789500	0.19483500

C	1.55125900	-0.22435000	0.29004400
C	1.03420800	0.93661000	-0.25180800
H	-0.61673200	2.33583400	-0.26338300
H	-0.36172900	1.50580600	1.28346700
H	1.33054200	-0.49593800	1.31599900
H	2.45006200	-0.67032200	-0.12388000
H	1.40745400	1.28765500	-1.20946400
O	0.18119600	-1.40643100	-0.36526700
C	-1.34690700	0.28281800	-0.19706100
H	-2.32966300	0.48017800	0.24474700
H	-1.43377800	0.20330000	-1.28569800
O	-0.92736700	-0.96161200	0.34303500

R13-C=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.04555100	0.12476000	0.13592000
C	1.96013500	-0.39298900	-0.43011200
H	3.08603900	0.34352300	1.19929100
H	3.93983200	0.34291100	-0.43787900
H	1.96473200	-0.59864500	-1.50046700
C	0.68725200	-0.73697800	0.29058600
H	0.47162100	-1.80720800	0.17379000
H	0.79227500	-0.54311700	1.36385100
C	-0.51633400	0.03922700	-0.25228400
H	-0.62376300	-0.11705900	-1.33097300
O	-1.69106900	-0.60382300	0.35785600
O	-2.80695800	-0.22447000	-0.21852700
C	-0.52312600	1.52213300	0.07881600
H	-0.45860600	1.67507900	1.16079600
H	0.33373800	2.01257500	-0.39047400
H	-1.44251000	1.98136800	-0.29011900

P13-YCC•CC(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.24337900	1.18768100	-0.07005400
C	-0.24089800	1.31842100	0.02107100
C	-0.93410000	-0.00575600	-0.34924400
C	1.84722100	-0.14547700	0.21323300
H	-0.53941000	1.58220400	1.05272400
H	-0.61008200	2.13059700	-0.61731300
H	1.87559900	2.06876000	-0.08649100
H	1.98781600	-0.31737200	1.29647600
H	2.82269700	-0.27024800	-0.27224700
H	-0.87263000	-0.16277600	-1.43399100

TS13

O	1.04944600	-1.20088800	-0.32195900
O	-0.25597000	-1.09156400	0.29115000
C	-2.37954800	-0.08597400	0.11850800
H	-2.95816500	0.73355700	-0.31850200
H	-2.83249900	-1.03342700	-0.18372600
H	-2.43746300	-0.00505300	1.20845800

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.13658400	1.29728100	0.10954500
C	1.97962300	0.05227200	0.39029800
C	1.30639900	1.09459300	-0.21524900
H	-0.55446000	2.17709000	-0.38995100
H	-0.29381700	1.41219200	1.18887500
H	1.72493200	-0.25292700	1.39870900
H	2.97571500	-0.22400500	0.05940900
H	1.68929800	1.50359200	-1.14573800
O	0.89988200	-1.35559800	-0.35655600
C	-0.93763000	0.02911800	-0.33914700
H	-0.86662400	-0.07086000	-1.42836200
O	-0.32174200	-1.11632100	0.25407800
C	-2.38643500	0.04162800	0.12402300
H	-2.90269300	0.91808800	-0.27764200
H	-2.90761800	-0.85587700	-0.21843900
H	-2.44208900	0.07870600	1.21614700

R14-C=CCC(CC)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.11022800	0.01444400	-0.05704400
C	-2.05687600	-0.71971000	0.28696400
H	-3.12009100	0.60985400	-0.96572700
H	-4.00895700	0.04279900	0.54963400
H	-2.09479800	-1.30485100	1.20586700
C	-0.78148500	-0.82865900	-0.50003800
H	-0.63086200	-1.86761900	-0.82172900
H	-0.83924600	-0.22041200	-1.40775700
C	0.44435700	-0.42624700	0.32615900
H	0.52960200	-1.06529800	1.21161100
O	1.59904600	-0.77305200	-0.51926200
O	2.72066000	-0.76769200	0.16222000
C	0.53325400	1.04064900	0.74694600
H	-0.27900000	1.22897900	1.45808900
H	1.47173300	1.15412600	1.29894200
C	0.47511900	2.05183700	-0.40213800

H	-0.50032000	2.05222900	-0.89746200
H	0.65027800	3.06325200	-0.02469500
H	1.23918000	1.83901000	-1.15554200

P14-YCC•CC(CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.93259000	0.92636000	-0.15457600
C	0.53221700	1.42090400	-0.00283300
C	-0.48111900	0.29556100	-0.27715300
C	2.21123000	-0.50381100	0.16139800
H	0.36448000	1.78729600	1.02695900
H	0.33800300	2.27503700	-0.66335100
H	2.75815600	1.62489800	-0.23763100
H	2.37247000	-0.66764100	1.24308500
H	3.09597900	-0.87980900	-0.36659400
H	-0.52080900	0.08643300	-1.35494100
O	1.15061200	-1.35050800	-0.28077100
O	-0.04919800	-0.89704400	0.38723800
C	-1.88070000	0.59249400	0.25502700
H	-2.17288600	1.58299500	-0.11537700
H	-1.82404600	0.67326900	1.34772700
C	-2.92338500	-0.45439300	-0.14558800
H	-2.63461700	-1.44554000	0.21236100
H	-3.90425200	-0.21010400	0.27292600
H	-3.02879600	-0.50911400	-1.23454600

TS14

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.07216600	1.16740600	0.23666100
C	2.41069000	0.36444700	0.30243000
C	1.49786900	1.27340900	-0.19377200
H	-0.54030300	1.97223100	-0.17941500
H	-0.02197800	1.19621200	1.32918100
H	2.30019400	-0.03317500	1.30470400
H	3.41355800	0.31310100	-0.10951200
H	1.71940800	1.79357000	-1.12116800
O	1.57677400	-1.19518700	-0.45787000
C	-0.49535400	-0.21323800	-0.23584800
H	-0.49055600	-0.24591300	-1.33237100
O	0.38239700	-1.23445800	0.24514400
C	-1.88214100	-0.54270300	0.31356900
H	-2.11162900	-1.57560500	0.02947800
H	-1.84422900	-0.52136700	1.40934900
C	-2.98304000	0.39219600	-0.19692200

	H	-3.96136700	0.06725900	0.16848400
	H	-2.83428300	1.42330200	0.13804400
	H	-3.02331800	0.39843800	-1.29167300

R15-C=CC(C)COO•

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-2.78976800	-0.87830700	-0.25783400	
C	-1.81144100	-0.26221300	0.39677200	
H	-2.74671500	-1.03847300	-1.33161100	
H	-3.67567000	-1.24358600	0.25052800	
H	-1.89685600	-0.11737400	1.47429100	
C	-0.55327200	0.28307600	-0.22912200	
H	-0.60004800	0.11282700	-1.31184700	
C	0.64786500	-0.49848900	0.30635600	
H	0.80636500	-0.33704200	1.37753600	
H	0.55807800	-1.57090800	0.11287900	
O	1.83960200	-0.02719700	-0.38748900	
O	2.92589200	-0.59023000	0.08852600	
C	-0.40386100	1.79224700	0.03476700	
H	-0.38604900	1.99948200	1.11101100	
H	0.52363700	2.17518300	-0.39797300	
H	-1.24382900	2.34141600	-0.39875300	

P15-YCC•C(C)COO

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-0.17329600	1.25526100	0.04804800	
C	-1.00596300	0.05509500	0.36820600	
C	-0.25471800	-1.21034000	-0.08633400	
C	1.31175800	1.12083700	0.08049900	
H	-1.10152900	-0.02007800	1.46785400	
H	-0.62155500	2.24385300	0.03582100	
H	1.71462700	1.21210500	1.10588800	
H	1.80961100	1.87478000	-0.54102100	
H	-0.31407200	-1.33257600	-1.17574700	
O	1.73498000	-0.12612100	-0.47208300	
O	1.10795800	-1.16601600	0.31501500	
C	-2.41762600	0.12076400	-0.22662400	
H	-2.37921000	0.17246700	-1.31971900	
H	-3.00537700	-0.76038800	0.05233900	
H	-2.95180500	1.00598300	0.13234500	
H	-0.65512600	-2.10874400	0.39601300	

TS15

Cartesian Coordinates (Å)				
At.	X	Y	Z	

C	-0.96831600	0.08083400	0.35474000
C	1.12811000	1.40779300	0.26492500
C	-0.17587400	1.24258900	-0.15706700
H	-0.93379700	0.06492900	1.45168400
H	1.42261100	1.11421700	1.26577100
H	1.76773100	2.14565300	-0.20895800
H	-0.49682900	1.70529700	-1.08741000
O	1.81189400	-0.23911900	-0.46471800
C	-0.22298500	-1.21370800	-0.11166100
H	-0.65144400	-2.10253700	0.36560900
H	-0.27595100	-1.31203800	-1.20184600
O	1.13202500	-1.17329800	0.30440200
C	-2.42520300	0.06509500	-0.11561100
H	-2.95142500	-0.82357600	0.24730200
H	-2.96225200	0.94581000	0.24834300
H	-2.48438800	0.06595000	-1.20992100

R16-C=CC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.90555900	-0.96146300	-0.42145300
C	-1.93761800	-0.49734600	0.36131000
H	-2.81087800	-0.97192200	-1.50376100
H	-3.83399000	-1.34656400	-0.01338700
H	-2.07745400	-0.50189800	1.44285700
C	-0.62144700	0.06635900	-0.11803400
H	-0.61624900	0.05094200	-1.21577100
C	0.49499100	-0.86877100	0.35845000
H	0.69688900	-0.76558100	1.42969500
H	0.26174500	-1.91377900	0.13803000
O	1.72867300	-0.55341200	-0.35255600
O	2.71026800	-1.33705200	0.03030400
C	-0.46480500	1.52680100	0.36708600
H	-0.38790900	1.52473300	1.46318500
H	-1.39950100	2.04939900	0.13306400
C	0.70808400	2.30915300	-0.23405100
H	1.67434400	1.88284500	0.04298300
H	0.65529600	2.31900200	-1.32804700
H	0.68429800	3.34813700	0.10931500

P16-YCC•C(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.51390600	1.31802700	0.06273400
C	-0.53287400	0.28283500	0.32537800
C	-0.00144700	-1.09182100	-0.12782900

C	1.95038800	0.92382300	0.12138600
H	-0.68797300	0.21175800	1.41961300
H	0.24833900	2.37069600	0.06738700
H	2.33986400	0.92472900	1.15603800
H	2.58697000	1.58930100	-0.47422800
H	-0.05452600	-1.19131700	-1.22017800
O	2.15881800	-0.36818500	-0.44892400
O	1.33788200	-1.29045500	0.30478000
C	-1.88673300	0.63830700	-0.31569800
H	-1.76863200	0.65909400	-1.40669400
H	-2.14767600	1.66200200	-0.01979000
C	-3.03229600	-0.30485000	0.06707000
H	-3.97744200	0.03419100	-0.36758700
H	-2.85949600	-1.32619000	-0.28725500
H	-3.16285000	-0.34818700	1.15419900
H	-0.55584800	-1.91487800	0.33339800

TS16

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.50245700	0.30784400	0.25992200
C	1.81143500	1.21170800	0.36564900
C	0.53333800	1.30926500	-0.14553800
H	-0.55389100	0.25159100	1.35586800
H	1.97531000	0.83271600	1.36766900
H	2.60854600	1.83211300	-0.03180300
H	0.37224500	1.85769500	-1.07082100
O	2.22127100	-0.50902800	-0.39817000
C	0.01763400	-1.09082800	-0.21503700
H	-0.59150600	-1.90238300	0.19554100
H	0.02177900	-1.14213600	-1.30997300
O	1.32559200	-1.31968200	0.28462100
C	-1.89899200	0.62398000	-0.30062200
H	-2.15039600	1.65443000	-0.02268900
H	-1.85432400	0.60990500	-1.39801000
C	-3.00996700	-0.31308900	0.18411900
H	-3.98400400	0.01276100	-0.19296600
H	-2.85882600	-1.34315400	-0.15367500
H	-3.06578600	-0.32713800	1.27829700

R17-C=C(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.02080000	1.43505500	0.28599900
C	-1.36480300	0.17064600	0.04660700
H	-0.00227600	1.73792900	0.49635900

H	-1.76027000	2.22885400	0.26052100
C	-2.78209900	-0.22174900	-0.28300700
H	-2.83724200	-0.71168800	-1.26370500
H	-3.17536700	-0.94195500	0.44609800
H	-3.44648300	0.64524300	-0.29935100
C	-0.39203100	-0.98927300	0.07160000
H	-0.78845200	-1.77006200	0.73610200
H	-0.35600700	-1.45582800	-0.92336800
C	1.02766000	-0.69789800	0.52244200
H	1.60331600	-1.61839300	0.65436500
H	1.06868400	-0.11431500	1.44578400
O	1.69560200	0.07474700	-0.51836600
O	2.91521400	0.40269400	-0.15846500

P17-YCC•(C)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.98156300	0.03714200	-0.07833000
C	0.19624700	1.29597300	0.12465900
C	-1.28267600	1.08129300	-0.22631000
C	0.24848600	-1.24518700	0.16131200
H	-1.91932500	1.86276300	0.20143200
H	0.25992000	1.61701100	1.18082800
H	0.61220500	2.12130300	-0.46787600
H	0.21845100	-1.51268100	1.23461500
H	-1.43454300	1.04943700	-1.31210700
O	-1.08644200	-1.20122800	-0.34039500
O	-1.76160200	-0.12533500	0.35294600
H	0.71035800	-2.08386900	-0.37539300
C	2.47213500	0.05734800	-0.05433200
H	2.89813100	-0.86056600	-0.47525700
H	2.87064100	0.90862400	-0.61895800
H	2.87399100	0.15106200	0.97031100

TS17

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.14326700	1.20882400	0.59692700
C	0.46917100	-1.21655500	0.70350600
C	1.01396100	0.00825300	0.36042000
H	0.65621200	2.14670100	0.35782500
H	-0.19285300	1.26084200	1.63832200
H	-0.22095900	-1.29607500	1.53473800
H	0.98184200	-2.13527900	0.43396400
O	-0.98729200	-1.18935100	-0.55348600
C	-1.12134600	1.07625100	-0.30206200

H	-1.85780500	1.85238800	-0.06680900
H	-0.84850100	1.13297500	-1.36208400
O	-1.76975000	-0.15765100	-0.04007400
C	2.17572100	0.13498400	-0.57605100
H	2.92785200	0.82950400	-0.17941800
H	2.66238600	-0.82717100	-0.75535100
H	1.86352300	0.54158300	-1.54914500

R18-C=C(CC)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.41160800	1.67096100	0.01949900
C	-0.89414700	0.45780300	0.28659500
H	0.64844900	1.88075300	-0.05750500
H	-1.07812200	2.51015100	-0.15266500
C	-2.38446600	0.19891000	0.34248300
H	-2.63857600	-0.26319700	1.30714300
H	-2.91241700	1.15737400	0.30750600
C	-0.01925300	-0.74986600	0.55604400
H	-0.36896300	-1.23994700	1.47559600
H	-0.15782500	-1.49829700	-0.23580900
C	1.46979500	-0.50271800	0.72077800
H	1.98582000	-1.39431900	1.08800400
H	1.68981700	0.33861700	1.38284400
O	2.03645300	-0.19518000	-0.58758400
O	3.31734900	0.08050300	-0.49843400
C	-2.90532200	-0.70416000	-0.79001900
H	-2.67606500	-0.27132700	-1.76872000
H	-2.46202200	-1.70405800	-0.75357000
H	-3.99051800	-0.82392100	-0.71695600

P18-YCC•(CC)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.53162000	-0.12087600	0.30578700
C	-0.14851400	1.20632200	0.44001400
C	-1.50913500	1.19688000	-0.27251500
C	-0.36386100	-1.31707100	0.25130700
H	-2.15042100	2.01791000	0.06490500
H	-0.31825400	1.43680800	1.50777900
H	0.47529000	2.02035700	0.04977500
H	-0.69072600	-1.64024600	1.25737500
H	-1.38896400	1.25946100	-1.36106800
O	-1.52213100	-1.08218100	-0.55127500
O	-2.23636700	0.02039900	0.05608700
H	0.12663700	-2.17323100	-0.22887100

TS18

C	2.00557500	-0.26706600	0.52050600
H	2.24979400	-1.31839300	0.71848100
H	2.31384400	0.29140800	1.41849700
C	2.85645900	0.22595200	-0.67009500
H	2.66087400	1.28097000	-0.88624700
H	3.92452600	0.12098200	-0.45389600
H	2.63251500	-0.34661300	-1.57524900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.10176600	-1.12891600	0.57168000
C	0.20206100	1.31427600	0.69535000
C	-0.54130400	0.20620100	0.32813400
H	-0.55779700	-1.96351800	0.31129600
H	0.40123800	-1.24776700	1.61864700
H	0.87806800	1.26693800	1.54072300
H	-0.13624900	2.31029400	0.42461700
O	1.65417800	1.04436700	-0.53355100
C	1.38864000	-1.21197700	-0.30164500
H	1.97465100	-2.10546800	-0.05980200
H	1.13123500	-1.21436700	-1.36704800
O	2.23623100	-0.11084300	-0.01629300
C	-1.70320500	0.29639900	-0.62012500
H	-1.83795900	1.33518400	-0.94017200
H	-1.48320000	-0.28427000	-1.52864600
C	-3.01924600	-0.22482000	-0.01157800
H	-3.83258700	-0.16638600	-0.74126200
H	-2.92851700	-1.26941500	0.30363400
H	-3.30443100	0.36360200	0.86586400

R19-(cis)-CC=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.44545000	0.40357200	-0.26473500
C	-1.26639800	0.94827300	0.03924300
H	-3.19585100	1.05813000	-0.70576800
H	-1.12578500	2.00609800	-0.17936600
C	-2.89161000	-1.01525800	-0.06752800
H	-2.11964700	-1.65306700	0.36828700
H	-3.77066200	-1.05714400	0.58738600
H	-3.19618100	-1.46086600	-1.02250900
C	-0.07029400	0.27028700	0.65047200
H	-0.29225600	-0.75924000	0.94279400
H	0.23313100	0.80184600	1.56205800
C	1.11066900	0.27214600	-0.31462600

P19-CYCC•CCOO

H	1.38676700	1.28182600	-0.63403300
H	0.92669200	-0.34335600	-1.19938000
O	2.25418500	-0.29279400	0.38898400
O	3.31235100	-0.35074900	-0.38603700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.18514100	1.26580100	0.01863700
C	-1.30460400	1.17998800	0.04742400
C	-1.75924000	-0.23541000	-0.33765200
C	0.97985200	0.04567300	0.35995600
H	-2.78928500	-0.43186500	-0.02266700
H	-1.67976600	1.39892700	1.06312400
H	-1.76346700	1.92451400	-0.61431000
H	0.68159700	2.23025300	-0.00853700
H	1.02451500	-0.09270900	1.45625100
H	-1.67629100	-0.40110100	-1.41873400
O	0.35431500	-1.12496800	-0.19242500
O	-0.98355700	-1.20660000	0.35171100
C	2.39692300	0.05230200	-0.20524800
H	2.95335600	0.89985900	0.20540200
H	2.91951800	-0.86980400	0.06093000
H	2.37533500	0.14435000	-1.29444100

TS19

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.94270200	1.21896700	0.37166500
C	1.23325200	0.32617400	-0.49348000
C	0.18921000	1.23860400	-0.60269700
H	-1.65060000	2.03437900	0.19164800
H	-0.60513000	1.29191200	1.41035100
H	-0.01430500	1.65271300	-1.58638200
O	0.07779200	-1.21064600	-0.79635200
C	-1.68186800	-0.14316200	0.19739400
H	-2.42184700	-0.30416100	0.98926600
H	-2.16592600	-0.19403300	-0.78403000
O	-0.74710200	-1.20434300	0.32478000
H	1.87194200	0.23024900	-1.36975500
C	1.89024200	-0.10174000	0.79041300
H	2.42568700	-1.04227000	0.64489400
H	2.61700500	0.65917100	1.10114600
H	1.16884900	-0.24110600	1.59565900

R20-(trans)-CC=CCCCO•

Cartesian Coordinates (Å)

P20-CYCC•CCOO

At.	X	Y	Z
C	2.18039800	0.25134600	0.16956800
C	0.96255100	0.11084000	-0.34894500
H	2.42759200	1.18040000	0.68494900
H	0.70499300	-0.81239600	-0.86581600
C	3.27398900	-0.77212300	0.10336900
H	2.94976000	-1.67374300	-0.42398500
H	4.15778100	-0.37517800	-0.41150500
H	3.60471500	-1.06464700	1.10769900
C	-0.12554600	1.14631900	-0.27553400
H	0.23107500	2.03511100	0.25701400
H	-0.41235000	1.47438200	-1.28398100
C	-1.38506000	0.65537800	0.43175200
H	-2.13953800	1.44216900	0.52684700
H	-1.17373400	0.23086700	1.41680000
O	-1.96498300	-0.40359600	-0.38523800
O	-3.00855400	-0.94484300	0.19907800

TS20

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.18514100	1.26580100	0.01863700
C	-1.30460400	1.17998800	0.04742400
C	-1.75924000	-0.23541000	-0.33765200
C	0.97985200	0.04567300	0.35995600
H	-2.78928500	-0.43186500	-0.02266700
H	-1.67976600	1.39892700	1.06312400
H	-1.76346700	1.92451400	-0.61431000
H	0.68159700	2.23025300	-0.00853700
H	1.02451500	-0.09270900	1.45625100
H	-1.67629100	-0.40110100	-1.41873400
O	0.35431500	-1.12496800	-0.19242500
O	-0.98355700	-1.20660000	0.35171100
C	2.39692300	0.05230200	-0.20524800
H	2.95335600	0.89985900	0.20540200
H	2.91951800	-0.86980400	0.06093000
H	2.37533500	0.14435000	-1.29444100

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.14763100	1.25886200	-0.17660400
C	-1.09803800	0.21831800	-0.38385400
C	-0.29694100	1.19062900	0.19732000
H	1.66323500	2.09269400	0.31044100
H	1.27748700	1.36561200	-1.25966300

H	-0.86161300	-0.08901300	-1.39888000
H	-0.60939200	1.62703300	1.14293900
O	-0.11102200	-1.28102200	0.31623900
C	1.82607500	-0.07948000	0.24501600
H	2.84523400	-0.15058300	-0.15042200
H	1.83839300	-0.18044100	1.33557600
O	1.11504200	-1.16368600	-0.33005000
C	-2.50672300	-0.04655800	0.05837100
H	-3.21884900	0.46957500	-0.59618900
H	-2.72157500	-1.11719300	0.00051300
H	-2.67709700	0.28935600	1.08467000

R21-(cis)-CCC=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.90335400	0.86985500	-0.26185600
C	-0.63147100	1.27090200	-0.29330600
H	-2.60106400	1.37765900	-0.92817600
H	-0.37049100	2.07440900	-0.98124700
C	-2.52663700	-0.21117800	0.57551500
H	-1.78759600	-0.67936800	1.23271600
H	-3.27883700	0.24326400	1.23559600
C	0.52312300	0.74074600	0.51341600
H	0.19858000	0.00646000	1.25505100
H	0.99846200	1.56205900	1.06587400
C	1.57524800	0.10797100	-0.39127200
H	1.94413300	0.80293400	-1.15203200
H	1.21099700	-0.79788300	-0.88350000
O	2.70712300	-0.26635500	0.44574800
O	3.65569600	-0.83784700	-0.25949400
C	-3.21236500	-1.28926200	-0.28103800
H	-3.69688500	-2.04089200	0.34942900
H	-3.97873400	-0.84988700	-0.92840100
H	-2.48837200	-1.79934500	-0.92411100

P21-CCYCC•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.04647300	1.14356400	0.10268700
C	1.51944200	1.34170000	-0.03613400
C	2.25764700	0.02488600	0.24604300
C	-0.53341200	-0.18723000	-0.25436000
H	3.27927400	0.03743300	-0.14774400
H	1.76683300	1.66263600	-1.06380000
H	1.88231700	2.13535400	0.62780700
H	-0.60938100	1.99262500	0.25850900

H	-0.62786200	-0.29106500	-1.35190800
H	2.28907600	-0.19174500	1.32084000
O	0.33857300	-1.23867000	0.19815000
O	1.62474600	-1.04919100	-0.43609500
C	-1.89060500	-0.48834000	0.39023300
H	-2.09928000	-1.55219700	0.23398200
H	-1.81065400	-0.33395200	1.47187400
C	-3.03065200	0.35473400	-0.18799400
H	-3.98215500	0.08484300	0.27911700
H	-2.87579300	1.42538800	-0.02078300
H	-3.13229500	0.19768900	-1.26718100

TS21

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.63819300	0.89945600	-0.53524000
C	-0.60042300	0.79236900	0.58678200
C	0.67872100	1.33554500	0.52365700
H	2.57555500	1.46343300	-0.49336100
H	1.22732200	1.00664400	-1.54409000
H	1.10321300	1.72940600	1.44299900
O	0.06653400	-1.00556500	0.94852500
C	1.94401900	-0.60987300	-0.29282800
H	2.50690900	-1.04582300	-1.12563500
H	2.49662800	-0.74284700	0.64359100
O	0.72442400	-1.33568600	-0.23323300
H	-1.14217700	0.95702100	1.51788900
C	-1.49550300	0.51433600	-0.59561000
H	-1.82963400	1.48655400	-0.98584500
H	-0.92025900	0.03788100	-1.39277300
C	-2.71226000	-0.34480200	-0.24198600
H	-3.34774400	-0.49945900	-1.11882700
H	-2.39039300	-1.31839200	0.13322900
H	-3.32356600	0.13339500	0.53183200

R22-(trans)-CCC=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.55977300	0.30201100	0.34253300
C	0.37907400	0.13346200	-0.24868600
H	1.76362000	1.24585000	0.85216700
H	0.16769400	-0.80339300	-0.76213300
C	2.68012300	-0.69801100	0.35745200
H	2.36062500	-1.61745600	-0.14606400
H	2.90544500	-0.97382400	1.39731800
C	-0.72872100	1.15078800	-0.25967200

P22-CCYCC•CCOO

H	-0.41594100	2.05870500	0.26807300
H	-0.96643900	1.44799400	-1.29016900
C	-2.01585000	0.65549400	0.39282300
H	-2.78692700	1.43108600	0.42735400
H	-1.84973400	0.26010600	1.39840900
O	-2.53444200	-0.43392100	-0.42523200
O	-3.60027500	-0.97641800	0.11616000
C	3.96343700	-0.16062300	-0.29765400
H	4.30713600	0.75325600	0.19891900
H	4.77141600	-0.89639600	-0.23990700
H	3.79382700	0.07806400	-1.35216900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.04647300	1.14356400	0.10268700
C	1.51944200	1.34170000	-0.03613400
C	2.25764700	0.02488600	0.24604300
C	-0.53341200	-0.18723000	-0.25436000
H	3.27927400	0.03743300	-0.14774400
H	1.76683300	1.66263600	-1.06380000
H	1.88231700	2.13535400	0.62780700
H	-0.60938100	1.99262500	0.25850900
H	-0.62786200	-0.29106500	-1.35190800
H	2.28907600	-0.19174500	1.32084000
O	0.33857300	-1.23867000	0.19815000
O	1.62474600	-1.04919100	-0.43609500
C	-1.89060500	-0.48834000	0.39023300
H	-2.09928000	-1.55219700	0.23398200
H	-1.81065400	-0.33395200	1.47187400
C	-3.03065200	0.35473400	-0.18799400
H	-3.98215500	0.08484300	0.27911700
H	-2.87579300	1.42538800	-0.02078300
H	-3.13229500	0.19768900	-1.26718100

TS22

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.51687900	1.27825700	0.16109800
C	0.60031500	0.12066400	0.73247900
C	-0.03031400	1.16327100	0.06666900
H	-1.89834300	2.16533800	-0.35470300
H	-1.85192400	1.32064700	1.20381700
H	0.14691200	-0.21957300	1.65991300
H	0.46618000	1.63530400	-0.77534600
O	-0.27865200	-1.28641200	-0.24255600

C	-2.14606800	0.00404000	-0.47901400
H	-3.22597700	-0.03981600	-0.29986000
H	-1.94267600	-0.02937900	-1.55485400
O	-1.60684700	-1.14722500	0.14927900
C	2.05971400	-0.22567200	0.59065600
H	2.60436200	0.24886900	1.41914300
H	2.15073800	-1.30514000	0.75483800
C	2.70299600	0.15228300	-0.74583600
H	2.73892900	1.23682700	-0.88911500
H	3.73104100	-0.21818500	-0.79307900
H	2.14617000	-0.28285200	-1.58084300

R23-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000
C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100
H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900
H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

P23-YCC•C(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.74803600	1.38629000	0.18371700
C	-0.60337000	0.75853100	0.32037300
C	-0.57709700	-0.67224800	-0.26992900
C	1.95916300	0.52052300	0.20096900
H	-0.82740400	0.64065200	1.39816600
H	0.85713200	2.45966100	0.30496700
H	2.28598400	0.27928600	1.22931300
H	2.80730400	0.98468800	-0.31699800

H	-0.57228400	-0.61094400	-1.36699600
O	1.73082100	-0.69604500	-0.50839700
O	0.61668400	-1.34576100	0.14190900
C	-1.71632300	-1.56334200	0.20776100
H	-2.68173100	-1.14059600	-0.08177300
H	-1.69545800	-1.66495400	1.29731200
H	-1.62938200	-2.55929600	-0.23349100
C	-1.70579200	1.63098000	-0.29818600
H	-1.56522600	1.72810900	-1.37996900
H	-1.68504200	2.63761200	0.13135800
H	-2.70163200	1.21582200	-0.11820900

TS23

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.50383100	0.79515500	0.30758200
C	1.98357600	0.72386900	0.40864900
C	0.84177400	1.34237700	-0.05428500
H	-0.57134000	0.67241900	1.39693100
H	1.98961400	0.22544500	1.37092800
H	2.95768200	1.02103200	0.03315400
H	0.90540400	1.98487100	-0.92946100
O	1.68110900	-0.94549000	-0.50634100
C	-0.59576400	-0.66133100	-0.28382600
H	-0.56975100	-0.59737100	-1.37857500
O	0.54875600	-1.39989400	0.14932000
C	-1.65055500	1.68784100	-0.18256900
H	-2.62696800	1.31519000	0.13717800
H	-1.53794800	2.70324700	0.20890400
H	-1.65546200	1.75315400	-1.27679900
C	-1.80789400	-1.44852200	0.19591600
H	-1.82087300	-1.51309000	1.28840400
H	-2.73451000	-0.97445100	-0.13513100
H	-1.77860600	-2.46370300	-0.20815700

R24-C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800

P24-YCC•CCCOO

C	0.02912800	0.36494300	-0.07789300
H	0.13282400	0.90845700	0.86749900
H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.54544900	0.57588300	-0.18271000
C	1.31978900	-0.91189200	0.08197000
C	-0.89108100	1.27247400	-0.31412900
C	-1.69538000	0.04048000	-0.07932700
H	1.63929200	0.74072900	-1.26227800
H	1.37853000	-1.13939600	1.15380400
H	-2.18136400	-0.30407500	-1.00478200
H	2.50279500	0.86188900	0.27239000
H	2.07663400	-1.51336900	-0.43602100
H	-1.23798700	1.97883200	-1.06137700
H	-2.49761600	0.19581200	0.66329100
O	-0.94974000	-1.01644400	0.51142500
O	0.08665900	-1.40890600	-0.42641100
C	0.41781800	1.48430800	0.37348100
H	0.31855700	1.28531000	1.45072600
H	0.72623800	2.52955100	0.26842300

TS24

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.22556000	1.14633500	-0.21411500
C	1.00336500	-1.28990300	0.51297900
C	1.62966300	-0.30060500	-0.21365400
H	1.22960400	1.49657500	-1.25650800
H	1.99588400	1.75338300	0.28623700
H	0.45856900	-1.06467800	1.42132600
H	1.35988400	-2.31161000	0.43543900
H	2.35429800	-0.59471700	-0.96900300
C	-0.14799600	1.47119200	0.40307900
H	-0.15561200	1.25933500	1.47894700
H	-0.30894100	2.55219100	0.30666300
C	-1.35643600	0.77077200	-0.23345100
H	-2.27874000	1.26945900	0.08466000
H	-1.30254900	0.78694300	-1.32892700

O	-1.53414400	-0.57773000	0.20681200
O	-0.65052300	-1.41397300	-0.45529500

R25-C=CC(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.25621700	-1.07567800	0.32724700
C	-2.35204300	-0.39232300	-0.36581700
H	-3.18023300	-1.19384000	1.40483800
H	-4.10963800	-1.54453300	-0.15092800
H	-2.46689200	-0.29680000	-1.44644600
C	-1.14112700	0.29319000	0.21281600
H	-1.14509500	0.12775900	1.29870700
C	0.14294500	-0.34548600	-0.36417100
H	0.10418100	-1.42885400	-0.20696000
H	0.18144300	-0.18421200	-1.44872800
C	1.42019500	0.18496200	0.26712200
H	1.42622200	0.06588900	1.35574900
H	1.62772700	1.22928800	0.02250600
O	2.52451100	-0.60557100	-0.26277900
O	3.68106800	-0.17141700	0.18143400
C	-1.21042900	1.81005400	-0.04817600
H	-0.38152300	2.34551600	0.42458000
H	-1.17810300	2.02361400	-1.12291700
H	-2.14266600	2.22376200	0.34622700

P25-YCC•C(C)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.65621600	1.30557400	-0.64792800
C	0.61286500	1.57481400	0.16089100
C	-0.42805500	-1.20258200	-0.85352600
C	0.83793600	-1.55534300	-0.14930600
H	-0.41417400	1.40278200	-1.71250400
H	0.41139300	1.64396100	1.23622700
H	1.62271600	-1.83295900	-0.87021900
H	-1.38144900	2.09644900	-0.41165300
H	1.06324700	2.52291800	-0.15729300
H	-0.68376000	-1.78935300	-1.73046400
H	0.71630400	-2.41658600	0.53067100
O	1.31820300	-0.54951000	0.73296200
O	1.64712800	0.62158900	-0.05677200
C	-1.85301000	-0.24861500	1.02042700
H	-2.42658300	-1.17587700	1.11263300
H	-1.03596100	-0.28481500	1.74407000
H	-2.51398900	0.58315700	1.28930800

TS25

C	-1.32695500	-0.07905700	-0.42280400
H	-2.19977900	-0.09506500	-1.08681700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.25034100	-0.13783000	-0.38872700
C	0.37009600	1.64360700	0.48803300
C	-0.65615000	1.24537300	-0.34072300
H	-1.32354400	-0.40526800	-1.45445800
H	0.57673900	1.13068500	1.41916500
H	0.71757100	2.67054700	0.44582800
H	-0.97557000	1.92445000	-1.12816300
C	-0.39666500	-1.23248200	0.28427900
H	-0.35338400	-1.07982600	1.37020200
H	-0.91517200	-2.18887300	0.13660400
C	1.03657500	-1.40806800	-0.23659400
H	1.43019900	-2.37553300	0.09464700
H	1.07913300	-1.36303700	-1.33153800
O	1.96132400	-0.46349200	0.30705100
O	1.84274300	0.74873000	-0.35118800
C	-2.68854400	-0.13990400	0.17033400
H	-3.31147800	0.60323000	-0.33718100
H	-3.15776900	-1.12124000	0.03924100
H	-2.68908000	0.09879400	1.23913700

R26-C=CC(CC)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.65577400	-1.85424000	-0.39616400
C	1.88933700	-1.09063000	0.37546100
C	0.85147700	-0.11017500	-0.10766500
C	-0.54434300	-0.57001100	0.37558500
H	-0.60013400	-0.50388200	1.46916900
C	-1.69352900	0.21625500	-0.23597900
O	-2.92969500	-0.43632200	0.17896700
O	-3.98418700	0.21980800	-0.24634800
H	-1.75012300	1.25236000	0.10504300
H	1.98855500	-1.15998600	1.45995400
H	2.59165500	-1.81759600	-1.48026800
H	3.37774000	-2.54776900	0.02187800
H	0.85419400	-0.12586300	-1.20698800
H	-0.67881300	-1.62591200	0.11700900
H	-1.66858200	0.20222600	-1.33075000
C	1.18703400	1.32603900	0.35725300
C	2.50181100	1.86603900	-0.21158700

H	1.22296600	1.34005400	1.45519900
H	0.37211800	2.00109600	0.07172300
H	2.69597200	2.88083800	0.14837700
H	3.34868000	1.23569900	0.07367600
H	2.47146300	1.90118600	-1.30639000

P26-YCC•C(CC)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.33340200	1.07699500	0.98107300
C	-0.60288800	1.65572200	-0.07942300
C	-0.44393800	-1.31985600	0.88828000
C	-1.54272300	-1.35063000	-0.11944100
H	-0.15523100	1.16779900	1.95792100
H	-0.12433400	1.72292800	-1.06372100
H	-2.52196700	-1.46430500	0.37163200
H	1.23025800	1.70806200	1.02044600
H	-0.91419600	2.66669100	0.21074300
H	-0.52896100	-2.00302700	1.72789500
H	-1.44427300	-2.19553400	-0.82335500
O	-1.56418700	-0.23450600	-0.99844400
O	-1.83304200	0.95184200	-0.20961800
C	1.57580300	-0.66945100	-0.49979900
H	1.79760500	-1.74282900	-0.53812800
H	0.96300600	-0.45429900	-1.38024100
C	0.74752500	-0.40995800	0.78763300
H	1.40427500	-0.64629300	1.63518100
C	2.89228000	0.11198200	-0.57099600
H	3.50747500	-0.06247100	0.31932000
H	3.47792900	-0.19541400	-1.44317500
H	2.72948300	1.19117900	-0.65398200

TS26

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.81301800	-0.34001800	-0.28964000
C	0.60829400	1.62275700	0.54286200
C	-0.38208000	1.10444000	-0.26273800
H	-0.95180400	-0.60352600	-1.35021100
H	0.90850500	1.12932500	1.45915200
H	0.82367500	2.68525100	0.50340000
H	-0.78562900	1.74111800	-1.04562700
C	0.22578200	-1.32824600	0.28439400
H	0.31574100	-1.20870800	1.37162200
H	-0.16643000	-2.34132300	0.12646400
C	1.63684700	-1.28842800	-0.31780500

H	2.17146500	-2.20824400	-0.05542500
H	1.61389100	-1.18913800	-1.40945700
O	2.45689200	-0.25270500	0.22947600
O	2.15789600	0.95637700	-0.37173100
C	-2.18507000	-0.54821200	0.39979200
H	-2.42975500	-1.61768600	0.35997800
H	-2.08439000	-0.29314000	1.46253400
C	-3.33140200	0.25814500	-0.21649200
H	-4.27770200	0.03956400	0.28755600
H	-3.15337700	1.33478300	-0.13550300
H	-3.45861000	0.01972700	-1.27867700

R27-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393600	0.01912900	0.21624600
C	2.50767100	-0.37369400	-0.44139400
H	3.61461800	0.07695700	1.30107200
H	4.50795600	0.29247900	-0.30012900
H	2.53237300	-0.41673100	-1.53058100
C	1.20658100	-0.78156200	0.18939800
H	1.29137800	-0.72723600	1.28215600
C	0.00586100	0.07208200	-0.28137600
H	-0.03601000	0.02027100	-1.37829900
C	-1.28366200	-0.54535900	0.24668200
H	-1.38109900	-0.44387100	1.33248500
H	-1.38181400	-1.60131600	-0.02458500
O	-2.40657100	0.15928200	-0.35804800
O	-3.55264000	-0.24708400	0.13708900
H	1.00457700	-1.83346800	-0.05955400
C	0.13703600	1.54190200	0.13689500
H	-0.71143700	2.12975600	-0.22170500
H	0.17264800	1.63142600	1.22940800
H	1.05596300	1.97917100	-0.26129600

P27-YCC•CC(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.98932400	1.50607200	0.01548500
C	2.01985500	0.43581900	-0.12993800
C	-1.12393600	0.09652000	-0.33427800
C	-0.64253700	-1.27520000	0.16409900
H	2.59210800	0.29328400	0.80533600
H	-0.85605300	0.18289700	-1.39270100
H	-0.83741100	-2.04890700	-0.59182700
H	2.74975400	0.69388800	-0.91008200

H	-1.16916400	-1.55896100	1.08516000
O	0.71643600	-1.30747400	0.56863500
O	1.51204100	-0.82691500	-0.54435000
H	1.36579700	2.52440500	0.06655800
C	-0.43048600	1.25469300	0.41939300
H	-0.49849800	1.05252300	1.50452100
H	-1.00645900	2.17355100	0.25706800
C	-2.65102800	0.17701100	-0.21371100
H	-3.03648500	1.08708600	-0.68333900
H	-3.13548300	-0.67757200	-0.69882100
H	-2.96307500	0.18343300	0.83754700

TS27

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.53694000	1.35783100	-0.28296900
C	1.80855200	0.80931100	0.56880500
C	0.95025600	1.55159100	-0.21171500
H	-0.83554400	1.41022900	-1.34091500
H	-1.04623200	2.21320000	0.18935500
H	1.46863900	0.30873800	1.46680700
H	2.87157300	1.02410200	0.53935000
H	1.37884900	2.21845300	-0.95593200
C	-1.11024300	0.05294200	0.31180300
H	-0.88914200	0.01726200	1.38649600
C	-0.52368100	-1.23205800	-0.30493500
H	-1.15926700	-2.08465900	-0.03960600
H	-0.46440800	-1.16086300	-1.39825200
O	0.75649700	-1.59576400	0.21358400
O	1.75162100	-0.85121600	-0.39647700
C	-2.63753600	0.04338200	0.14097400
H	-3.08946400	-0.82298900	0.63377800
H	-3.08511900	0.94575500	0.56917900
H	-2.91727100	0.00860400	-0.91888300

R28-C=CCC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.72490700	-0.18739100	0.13810100
C	2.60479800	-0.51358800	-0.49921900
C	1.33971700	-0.99816400	0.15010500
C	0.09872500	-0.13192000	-0.18763600
H	0.02337700	-0.06662700	-1.28281200
C	-1.14828200	-0.86425500	0.30320600
O	-2.32556200	-0.31172600	-0.35749200
O	-3.42337200	-0.90541100	0.05062400

H	-1.12319300	-1.92895400	0.05166900
H	2.57270100	-0.44286900	-1.58682200
H	3.80253100	-0.24286500	1.22044500
H	4.61103800	0.14163900	-0.39418600
H	1.47509000	-1.04279900	1.23832600
H	-1.29920600	-0.75888000	1.38259700
H	1.14523000	-2.02702300	-0.18460800
C	0.24152900	1.29093100	0.38684200
C	-0.78430400	2.31632800	-0.10808200
H	1.24798100	1.64906500	0.14478100
H	0.20266600	1.22681100	1.48364200
H	-0.55737400	3.30708000	0.29809900
H	-0.76768200	2.39351800	-1.20073100
H	-1.80422800	2.05736000	0.18464400

P28-YCC•CC(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.60746600	1.39054500	-0.14930000
C	2.45915100	0.17652700	-0.31310800
C	-0.71610000	0.29770000	-0.14628600
C	-0.36921800	-1.10774000	0.37664200
H	3.10658900	0.01140100	0.56797900
H	-0.57934400	0.29694600	-1.23412300
H	-0.72912500	-1.88366300	-0.31075400
H	3.12563700	0.27393800	-1.18135700
H	-0.83018200	-1.28046500	1.35895900
O	1.00917800	-1.30435900	0.65096900
O	1.73611900	-1.02126000	-0.57134700
H	2.11541500	2.34710500	-0.23878700
C	0.23291300	1.36866500	0.44438700
H	0.28464700	1.22112400	1.53868800
H	-0.22286200	2.35551400	0.30211600
C	-2.18756200	0.64299200	0.14793900
H	-2.38688300	1.65145400	-0.23468700
H	-2.33228500	0.69686300	1.23623600
C	-3.20772200	-0.32803300	-0.45838800
H	-3.12304500	-1.33349300	-0.03423300
H	-4.22976300	0.01794000	-0.27565600
H	-3.07474400	-0.41364800	-1.54267600

TS28

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.34228800	1.14862100	0.48062500
C	-1.96356900	1.13450800	-0.62600400

C	-1.06586400	1.63555600	0.28994100
H	0.54124500	1.09890900	1.56206500
H	1.03938600	1.91195900	0.10495200
H	-1.63250500	0.62477200	-1.52204600
H	-2.95835400	1.56352700	-0.68301100
H	-1.43270900	2.33043900	1.04149300
C	0.70697800	-0.22175400	-0.13399100
H	0.60097700	-0.17063000	-1.22655400
C	-0.20281500	-1.37276900	0.34375700
H	0.27238700	-2.33231600	0.11006900
H	-0.38545600	-1.32118900	1.42409400
O	-1.45558100	-1.44605400	-0.33928800
O	-2.35710400	-0.55136900	0.20967800
C	2.17518900	-0.58791200	0.17556300
H	2.36981300	-1.58986700	-0.22620900
H	2.30541000	-0.66838900	1.26388200
C	3.22179000	0.37579200	-0.39364600
H	3.16872600	1.36752400	0.06466600
H	4.23164900	-0.00805500	-0.21884500
H	3.09692500	0.50044600	-1.47514300

R29-C=CCCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.77075500	-0.49856500	0.29660600
C	-2.75799800	0.05281400	-0.36369400
H	-3.72044300	-0.68680600	1.36564400
H	-4.69258600	-0.78050500	-0.20080500
H	-2.85101200	0.22245600	-1.43647200
C	-1.44897600	0.46940100	0.24559700
H	-1.47168300	0.29119800	1.32760700
C	-0.25360600	-0.27282400	-0.38025300
H	-0.21801900	-0.08026600	-1.45986500
C	1.08646700	0.11366900	0.23807500
H	1.09241200	-0.08905100	1.31455600
O	2.05530700	-0.83268700	-0.34395700
O	3.20355800	-0.80774300	0.28981400
H	-1.31507100	1.55069400	0.10659400
H	-0.39414500	-1.35215000	-0.25696600
C	1.55644700	1.53315600	-0.03898800
H	1.54303300	1.74518500	-1.11287800
H	0.91213500	2.25728800	0.46709300
H	2.57498600	1.65949400	0.33458400

P29-YCC•CCC(C)OO

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-0.61101500	1.33954500	0.04475900
C	-1.20038800	-0.03227500	-0.30272300
C	1.79394000	0.62624300	0.44806200
C	1.85224800	-0.83710000	0.17843600
H	-0.72990500	1.51565000	1.12109600
H	-1.19961000	-0.16871800	-1.39232200
H	1.97676500	-1.41375900	1.10754700
H	-1.20219000	2.10582200	-0.47335300
H	2.36090800	1.02317700	1.28378200
H	2.69202600	-1.11229600	-0.48369200
O	0.73045800	-1.31271500	-0.55444500
O	-0.44864100	-1.11259600	0.26472600
C	0.88253000	1.51064700	-0.33670400
H	0.98669800	1.30400100	-1.41177800
H	1.16087300	2.55866800	-0.18422500
C	-2.61569100	-0.21372400	0.23879900
H	-3.27183200	0.57088000	-0.14866100
H	-3.01778700	-1.18585800	-0.05624700
H	-2.62023100	-0.15510000	1.33182300

TS29

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.00654000	1.54636000	-0.21327000
C	1.87417400	-0.72918600	0.54458300
C	2.01499000	0.43348700	-0.18105500
H	0.88566500	1.86185200	-1.25974700
H	1.40982800	2.43414100	0.29851500
H	1.26167300	-0.76772000	1.43677000
H	2.64975800	-1.48596400	0.49004100
H	2.81464400	0.49118300	-0.91543700
C	-0.38628100	1.23121100	0.36442800
H	-0.32791900	1.02421700	1.44013000
H	-0.99347600	2.13902200	0.26484100
C	-1.16148900	0.07739500	-0.29902200
H	-1.02231200	0.10274200	-1.38741900
O	-0.70366800	-1.20749200	0.16541100
O	0.47480400	-1.56573600	-0.46320700
C	-2.64632100	0.11168500	0.05057000
H	-3.10660100	1.02787600	-0.32961200
H	-3.16046700	-0.74674600	-0.38857400
H	-2.78956200	0.07950900	1.13545300

R30-C=CCCC(CC)OO•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	4.11741700	-0.21427200	-0.41720600
C	3.09365600	0.22305900	0.30840100
C	1.71598600	0.50949900	-0.21930200
C	0.64329900	-0.36822900	0.45362100
H	0.64772400	-0.19875500	1.53765200
C	-0.76600300	-0.13452800	-0.09035800
O	-1.58805500	-1.22360800	0.46041200
O	-2.45849800	-1.68605400	-0.40827800
H	3.23044500	0.38825400	1.37716600
H	4.02511000	-0.39408700	-1.48489600
H	5.09006600	-0.40674400	0.02283400
H	1.69587300	0.35131800	-1.30439300
H	-0.79736100	-0.27173100	-1.17585900
H	1.48017100	1.56869200	-0.05008300
H	0.89753000	-1.42216500	0.29917700
C	-1.40229800	1.19613100	0.31217900
C	-2.78554500	1.44059000	-0.29671800
H	-0.72076900	1.99999300	0.01021000
H	-1.45729500	1.23071400	1.40755200
H	-3.18499400	2.40327300	0.03593900
H	-2.74028700	1.45477500	-1.39053300
H	-3.49286400	0.66024700	-0.00553700

P30-YCC•CCC(CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.16591900	1.53573700	-0.04160200
C	0.76114700	0.35043700	0.24594700
C	-2.32546300	0.24025100	-0.39464000
C	-2.00607900	-1.19549900	-0.16223100
H	-0.13219300	1.76355900	-1.11423300
H	0.83289400	0.19004200	1.33064000
H	-2.02354500	-1.76872600	-1.10163500
H	0.22852200	2.41372400	0.48607200
H	-3.00417100	0.49566900	-1.20180200
H	-2.72096500	-1.68331600	0.52356700
O	-0.77029200	-1.38880400	0.51435100
O	0.28074700	-0.86790800	-0.33732200
C	2.16366000	0.54751800	-0.33820100
C	3.16517100	-0.52408000	0.09937800
H	2.51586900	1.54197900	-0.03973900
H	2.08065100	0.56352900	-1.43219200
H	4.14181300	-0.36191300	-0.36652400
H	3.30713300	-0.51094600	1.18563100

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H	2.81141000	-1.51929300	-0.17976400
C	-1.64059300	1.31289800	0.38582800
H	-1.65172900	1.06766700	1.45787300
H	-2.18086500	2.25816400	0.26899500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.07884600	1.66120100	-0.13942600
C	2.45680900	-0.41844600	0.39322000
C	2.28700400	0.77773300	-0.26915100
H	0.79867700	2.00081900	-1.14691400
H	1.34392000	2.58359200	0.40067200
H	1.95756200	-0.62025600	1.33276000
H	3.35930600	-0.99598500	0.22241900
H	2.98053200	1.02875700	-1.06794600
C	-0.16162300	1.03560900	0.52651600
H	0.04109700	0.78154800	1.57418700
H	-0.93965000	1.80691900	0.54859000
C	-0.74717200	-0.21527300	-0.15285900
H	-0.70226100	-0.11590200	-1.24570200
O	-0.00045500	-1.39675300	0.20293600
O	1.16427600	-1.48413000	-0.53712700
C	-2.18493200	-0.51637000	0.28698000
H	-2.41033000	-1.54209600	-0.02301200
H	-2.23688900	-0.50364800	1.38278500
C	-3.22757000	0.43855900	-0.30189300
H	-4.23429300	0.14862200	0.01310400
H	-3.07167000	1.47342500	0.01924200
H	-3.20474000	0.42318600	-1.39698900

R31-C=C(C)CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.01898100	-1.06360200	0.42371800
C	2.21673900	-0.10961100	-0.04718700
H	2.72819400	-2.10947100	0.41816700
H	3.99913700	-0.83580600	0.83059500
C	0.85364600	-0.43853600	-0.61545300
H	0.75320300	-1.52576100	-0.70813400
C	-0.31454100	0.10631700	0.22959000
H	-0.26261100	1.19805800	0.29935000
C	-1.65728900	-0.28120100	-0.36508500
H	-1.81106800	-1.36460200	-0.38715200
O	-2.69732500	0.29035000	0.47917000
O	-3.89536200	-0.00189300	0.02816300

H	0.77361600	-0.02659800	-1.63206000
H	-0.24317700	-0.28346200	1.25103200
H	-1.79958300	0.11692000	-1.37488000
C	2.62176100	1.34248000	-0.05417500
H	2.58883800	1.75444600	-1.07105400
H	1.94533100	1.95676700	0.55211200
H	3.63383500	1.47676800	0.33491100

P31-YCC•(C)CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.81691600	-1.54955600	-0.12834500
C	-1.90349500	-0.47635700	-0.17138900
C	1.19584400	-0.01773300	0.10785600
C	0.64455900	1.36829100	0.19137200
H	-0.49514600	-1.77934000	-1.15087200
H	-2.37104400	-0.34484600	0.81265100
H	0.87300100	1.94148100	-0.72139900
H	-1.26053900	-2.46573000	0.28327900
H	-2.68759700	-0.74983200	-0.88776600
H	1.06426400	1.94127400	1.03846400
O	-0.74682600	1.41572600	0.47132500
O	-1.44689200	0.78893100	-0.63565600
C	0.42033600	-1.14843300	0.71414800
H	0.07723300	-0.88407300	1.72546200
H	1.07041100	-2.02434100	0.81844900
C	2.54611900	-0.23728300	-0.48959700
H	2.58824100	-1.17171100	-1.06440700
H	2.83454700	0.58106900	-1.15896100
H	3.33769600	-0.31477500	0.27548000

TS31

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.57101600	1.39352700	0.06827800
C	0.70799900	-0.98836100	0.90162700
C	1.28580200	0.07579500	0.23917900
H	0.72454400	1.72456600	-0.96997600
H	1.06520300	2.16449400	0.67975600
H	-0.06936700	-0.84032000	1.63955500
H	1.26624400	-1.91361600	1.00394000
C	-0.94033600	1.41258200	0.36156700
H	-1.13847600	1.21738000	1.42204300
H	-1.30158200	2.43069700	0.16954000
C	-1.80360200	0.45690700	-0.47525000
H	-2.85677600	0.74832200	-0.39279500

H	-1.51216300	0.47499800	-1.53306100
O	-1.78938600	-0.89147800	-0.00720900
O	-0.61166000	-1.51449700	-0.39612000
C	2.56539600	-0.08561200	-0.52560800
H	3.26557700	0.73026800	-0.30068000
H	3.06194200	-1.03278900	-0.30092200
H	2.38557900	-0.04522900	-1.60953000

R32-C=C(CC)CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.34931000	1.51560100	-0.47144000
C	1.69899400	0.51162500	0.11617600
H	1.89362800	2.49476100	-0.58157600
H	3.35382100	1.40902400	-0.86350900
C	0.29081900	0.70391600	0.64113600
H	0.06227200	1.77492800	0.67772700
C	-0.78415800	-0.00818800	-0.20414200
H	-0.60157500	-1.08769300	-0.23163700
C	-2.17750400	0.23734300	0.34838500
H	-2.45780300	1.29517400	0.32816400
O	-3.12209600	-0.48085800	-0.49618400
O	-4.35739100	-0.31392800	-0.08352400
H	0.22994000	0.33358700	1.67449900
H	-0.73471600	0.35069900	-1.23801000
H	-2.29734000	-0.14081500	1.36871700
C	2.29054500	-0.86704300	0.31822400
H	2.26043700	-1.09334700	1.39459800
H	1.62348800	-1.61066900	-0.13982400
C	3.71089700	-1.08279800	-0.20468000
H	4.42131600	-0.40109400	0.27317400
H	4.04082500	-2.10556400	-0.00062300
H	3.76817600	-0.92343300	-1.28599000

P32-YCC•(CC)CCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.16948600	1.57830700	0.11803100
C	-2.31480500	0.56743200	0.08886500
C	0.76376800	-0.06420600	-0.00289700
C	0.14338800	-1.41720200	-0.13704200
H	-0.89784400	1.78742300	1.15944300
H	-2.72986500	0.46691500	-0.92199100
H	0.28426200	-2.00949500	0.78110700
H	-1.53494100	2.51923000	-0.31414400
H	-3.12346400	0.88156300	0.75986500

H	0.57783700	-2.00632500	-0.96486900
O	-1.23005200	-1.38442000	-0.49932500
O	-1.95785200	-0.72342400	0.56948400
C	0.09277300	1.10925400	-0.65101500
H	-0.20285000	0.86826300	-1.68246900
H	0.79528300	1.94851500	-0.70954400
C	2.05756100	0.09159400	0.73377600
H	2.04738600	1.03065700	1.30581600
H	2.16866000	-0.71610100	1.46905400
C	3.30339000	0.09924000	-0.18269100
H	3.24670700	0.90902500	-0.91717400
H	4.21750300	0.23958300	0.40366300
H	3.39501900	-0.84300900	-0.73219200

TS32

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.32845500	1.26087400	0.10690000
C	0.10472000	-1.11948000	0.91930900
C	0.83711000	-0.15368300	0.25825900
H	0.56255900	1.59336000	-0.91561600
H	0.89991200	1.93936200	0.75772400
H	-0.64402400	-0.85721400	1.65571400
H	0.51566000	-2.11901100	1.02013000
C	-1.17413600	1.49071200	0.35805900
H	-1.42727100	1.32204000	1.41148500
H	-1.38193900	2.55058900	0.16446000
C	-2.14277100	0.66876900	-0.50434100
H	-3.14330000	1.11301900	-0.45455300
H	-1.82064700	0.63499600	-1.55267300
O	-2.34034200	-0.66308600	-0.03026700
O	-1.26177300	-1.45773100	-0.39071000
C	2.07391200	-0.52023200	-0.51686400
H	2.26467200	-1.59389000	-0.41687000
H	1.89791100	-0.33263700	-1.58695600
C	3.32925200	0.26245000	-0.08537900
H	4.19565100	-0.04384700	-0.67927700
H	3.19827700	1.34047900	-0.22087500
H	3.56020400	0.08283200	0.96945800

R33-(cis)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.09133200	0.32741800	0.27852900
C	1.94403300	0.92055200	-0.05449700
H	3.86711000	0.95386800	0.71666900

C	0.72028000	0.29337400	-0.66281700
H	0.89186800	-0.76308700	-0.89231900
C	-0.51411300	0.42785500	0.24929700
H	-0.68892900	1.48360400	0.48756100
C	-1.76018100	-0.14717000	-0.40110400
H	-1.67444000	-1.22008200	-0.59992200
O	-2.86982500	0.03713100	0.52399800
O	-3.98893500	-0.44240300	0.03225100
H	0.50277700	0.78532400	-1.62204500
H	-0.32926700	-0.08431600	1.19980100
H	-2.02137600	0.36519900	-1.33253400
H	1.85302100	1.98905000	0.13882600
C	3.46950300	-1.11671000	0.12234300
H	3.74790900	-1.55097900	1.09050300
H	2.66863300	-1.72753200	-0.29994600
H	4.34765000	-1.22078600	-0.52708900

P33-CYCC•CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.91000300	0.68882000	-0.01201400
C	1.76030400	-0.81058600	0.23796600
C	-0.52214100	1.18472000	-0.54290500
C	-1.27577900	-0.10060800	-0.41728400
H	2.16216800	0.85688000	-1.06537500
H	1.66733600	-1.02800600	1.30950500
H	-1.50573800	-0.49968000	-1.41751400
H	2.75596300	1.05315400	0.58559600
H	2.63186300	-1.35442100	-0.14611200
H	-0.78833800	1.85541000	-1.35392100
O	-0.53386400	-1.08554200	0.30647100
O	0.66258900	-1.40168900	-0.44833900
C	0.63798700	1.50277400	0.34236800
H	0.38437800	1.29807200	1.39280400
H	0.87428600	2.56968300	0.27327800
C	-2.58916300	0.02797200	0.37050500
H	-3.25705100	0.72732000	-0.13905600
H	-3.08487200	-0.94415800	0.44507200
H	-2.39705700	0.40504800	1.37884800

TS33

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.58195200	1.69884400	-0.11158200
C	1.50798100	0.19922000	-0.36370900
C	0.60708200	1.13504800	-0.84452800

H	-1.17655900	2.26587300	-0.83505700
H	-0.26380600	2.43307100	0.64209500
H	2.30053500	-0.08683800	-1.05140100
H	0.65236300	1.34549400	-1.90925400
C	-1.51560300	0.67056500	0.59490000
H	-1.19867000	0.51460900	1.63150000
H	-2.51724600	1.11417000	0.65131700
C	-1.65222100	-0.71554400	-0.04166700
H	-2.47996900	-1.25147700	0.43703500
H	-1.82988700	-0.67433700	-1.12127600
O	-0.50433100	-1.53841800	0.20374100
O	0.43812900	-1.35776300	-0.79342600
C	1.83902300	-0.02798500	1.08417600
H	0.97574500	0.09978000	1.73736200
H	2.23014300	-1.03714500	1.23082300
H	2.61111000	0.68536200	1.39879600

R34-(trans)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.92671400	0.14955200	0.39227800
C	-1.89216700	0.14419200	-0.44519400
C	-0.55620500	0.77713800	-0.17699900
H	-0.58162800	1.30008800	0.78674700
C	0.59407700	-0.24703000	-0.18284500
H	0.61321500	-0.78161700	-1.13995300
C	1.94134500	0.41711500	0.04114000
H	2.01038200	0.91076900	1.01553900
O	2.96064400	-0.62265900	0.00631900
O	4.15930700	-0.12635000	0.20891700
H	-0.34939600	1.54097100	-0.94105100
H	0.42397400	-0.99843100	0.59597000
H	2.18630800	1.14266400	-0.74114200
H	-1.99258100	-0.36129600	-1.40671800
H	-2.81993800	0.65527400	1.35258900
C	-4.25980000	-0.48498700	0.12990100
H	-4.28836200	-0.97161700	-0.84933900
H	-4.49784700	-1.23803100	0.89145800
H	-5.06694600	0.25740800	0.16432000

P34-CYCC•CCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.91000300	0.68882000	-0.01201400
C	1.76030400	-0.81058600	0.23796600
C	-0.52214100	1.18472000	-0.54290500

C	-1.27577900	-0.10060800	-0.41728400
H	2.16216800	0.85688000	-1.06537500
H	1.66733600	-1.02800600	1.30950500
H	-1.50573800	-0.49968000	-1.41751400
H	2.75596300	1.05315400	0.58559600
H	2.63186300	-1.35442100	-0.14611200
H	-0.78833800	1.85541000	-1.35392100
O	-0.53386400	-1.08554200	0.30647100
O	0.66258900	-1.40168900	-0.44833900
C	0.63798700	1.50277400	0.34236800
H	0.38437800	1.29807200	1.39280400
H	0.87428600	2.56968300	0.27327800
C	-2.58916300	0.02797200	0.37050500
H	-3.25705100	0.72732000	-0.13905600
H	-3.08487200	-0.94415800	0.44507200
H	-2.39705700	0.40504800	1.37884800

TS34

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.76197800	1.65873900	-0.20764900
C	1.26141600	0.18759800	0.35566100
C	0.67782300	1.24642700	-0.31757600
H	-1.13942700	1.83794000	-1.22512800
H	-0.83402900	2.63777200	0.29144100
H	0.80556300	-0.15707900	1.27821100
H	1.25259100	1.72221100	-1.11011000
C	-1.71252500	0.67105700	0.49462000
H	-1.44258000	0.55041000	1.55064000
H	-2.71669400	1.11318800	0.48674800
C	-1.82139100	-0.72224300	-0.13778100
H	-2.69201600	-1.24570300	0.27314200
H	-1.92488000	-0.66148000	-1.22847200
O	-0.72755500	-1.58189400	0.18243600
O	0.37779900	-1.24031600	-0.58577000
C	2.72184800	-0.13502300	0.20864500
H	3.30584900	0.35410600	0.99788600
H	2.88089500	-1.21262600	0.29373100
H	3.11161700	0.19960900	-0.75695000

R35-(cis)-CCC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.46997800	0.78037800	-0.33686200
C	-1.29912000	1.16853600	0.17088400
H	-3.16972800	1.56284800	-0.63153100

C	-0.16292600	0.30589800	0.64720000
H	-0.43051500	-0.75491800	0.61093700
C	1.12315700	0.54016800	-0.16821400
H	1.39142400	1.60294900	-0.14487600
C	2.28547600	-0.27791700	0.36677400
H	2.10377800	-1.35569700	0.30770200
O	3.45067600	0.01309700	-0.45706200
O	4.50236500	-0.66322400	-0.05616100
H	0.04472700	0.53618300	1.70239300
H	0.94794100	0.28141400	-1.21814000
H	2.54079400	-0.01852100	1.39917900
H	-1.11066600	2.23934400	0.24585600
C	-2.98605800	-0.61658500	-0.54195600
H	-3.19741700	-0.76196600	-1.61068100
H	-2.22890900	-1.36106500	-0.27712000
C	-4.27448200	-0.88588100	0.25398900
H	-5.05744500	-0.16685400	-0.00940500
H	-4.65939800	-1.88977600	0.05038400
H	-4.09531900	-0.80050800	1.33018400

P35-CCYCC•CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.43750200	0.33723300	0.03627500
C	1.96893500	-1.10234200	0.23876200
C	0.18125800	1.36709900	-0.51370000
C	-0.82078300	0.25862200	-0.47487100
H	2.73991000	0.47621900	-1.00805900
H	1.80709600	-1.32183900	1.30179700
H	-1.06901900	-0.06169900	-1.50012400
H	3.32998700	0.49578700	0.65583900
H	2.71503100	-1.80849600	-0.14544700
H	0.07040300	2.12539900	-1.28277900
O	-0.33036000	-0.87279200	0.24728300
O	0.78880700	-1.43234800	-0.48474800
C	1.36271200	1.39465600	0.39980900
H	1.04759900	1.21593500	1.43848800
H	1.82489300	2.38685100	0.37381400
C	-2.13424400	0.63879100	0.24043900
H	-2.49747900	1.56430700	-0.22018400
H	-1.89997100	0.88050800	1.28376200
C	-3.20917700	-0.44956700	0.16746600
H	-2.86416700	-1.37305000	0.63792300
H	-4.12458000	-0.12641300	0.67258500
H	-3.46448900	-0.67935300	-0.87297900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.64384200	1.74686900	0.24053800
C	-0.96475000	-0.20198100	0.79513400
C	-0.19486200	0.89205300	1.15668200
H	1.28427500	2.37223200	0.87111200
H	0.01442900	2.45178800	-0.32127400
H	-1.48647300	-0.69912200	1.61121700
H	-0.02600600	1.03394200	2.22049800
C	1.54541200	0.99773400	-0.78390100
H	1.00344200	0.82667500	-1.71994300
H	2.38140500	1.66118800	-1.03782500
C	2.13026900	-0.35122700	-0.35621400
H	2.89668600	-0.65652800	-1.07798600
H	2.57258900	-0.32731400	0.64529600
O	1.15722500	-1.40195900	-0.40473100
O	0.48140200	-1.48486600	0.80068300
C	-1.60821600	-0.41537900	-0.55056600
H	-1.01172300	0.03983200	-1.34393000
H	-1.63715100	-1.48946300	-0.75645900
C	-3.03460300	0.15978500	-0.58231900
H	-3.50347400	-0.02519100	-1.55371700
H	-3.66558400	-0.30074400	0.18545300
H	-3.03399400	1.24018600	-0.40618400

R36-(trans)-CCC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.34798700	-0.75741000	-0.32581100
C	-1.37793700	-0.19707400	0.39367400
C	0.01178100	-0.75148200	0.54014500
H	0.08227800	-1.71677200	0.02428000
C	1.08775200	0.20749000	-0.00309300
H	1.00864000	1.17949900	0.49802300
C	2.48859400	-0.34265900	0.20006400
H	2.65294800	-1.28348900	-0.33461900
O	3.43066800	0.63188000	-0.33311100
O	4.67115500	0.22221600	-0.20090300
H	0.22154700	-0.94810100	1.60186800
H	0.91756800	0.38670000	-1.07033100
H	2.73225100	-0.48955300	1.25714200
H	-1.56586600	0.73804400	0.91913500
H	-2.13160800	-1.69324300	-0.84309200
C	-3.74999700	-0.24366600	-0.51439700

H	-3.93729000	-0.13901200	-1.59312400
H	-4.45236900	-1.02368000	-0.18575500
C	-4.08318100	1.07194400	0.19040100
H	-3.96359700	0.98569900	1.27527500
H	-3.43491400	1.88427500	-0.15390000
H	-5.11830900	1.36401600	-0.00868100

P36-CCYCC•CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.43750200	0.33723300	0.03627500
C	1.96893500	-1.10234200	0.23876200
C	0.18125800	1.36709900	-0.51370000
C	-0.82078300	0.25862200	-0.47487100
H	2.73991000	0.47621900	-1.00805900
H	1.80709600	-1.32183900	1.30179700
H	-1.06901900	-0.06169900	-1.50012400
H	3.32998700	0.49578700	0.65583900
H	2.71503100	-1.80849600	-0.14544700
H	0.07040300	2.12539900	-1.28277900
O	-0.33036000	-0.87279200	0.24728300
O	0.78880700	-1.43234800	-0.48474800
C	1.36271200	1.39465600	0.39980900
H	1.04759900	1.21593500	1.43848800
H	1.82489300	2.38685100	0.37381400
C	-2.13424400	0.63879100	0.24043900
H	-2.49747900	1.56430700	-0.22018400
H	-1.89997100	0.88050800	1.28376200
C	-3.20917700	-0.44956700	0.16746600
H	-2.86416700	-1.37305000	0.63792300
H	-4.12458000	-0.12641300	0.67258500
H	-3.46448900	-0.67935300	-0.87297900

TS36

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.10525300	1.66764600	-0.20040500
C	0.79669900	0.15700300	0.60813000
C	0.33163700	1.23456100	-0.12579500
H	-1.34242200	1.86549800	-1.25615800
H	-1.22778900	2.64199300	0.29808100
H	0.20161800	-0.18044500	1.45103000
H	1.00463400	1.71358000	-0.83146600
C	-2.15639600	0.68896600	0.35572100
H	-2.03201200	0.55037400	1.43641400
H	-3.14307200	1.14997300	0.22130800

C	-2.20436600	-0.69365400	-0.30695300
H	-3.12858200	-1.20762900	-0.01942000
H	-2.16699800	-0.61590700	-1.40097500
O	-1.17498000	-1.57718300	0.13673400
O	0.02763300	-1.23785200	-0.47199400
C	2.25263900	-0.23250600	0.69691400
H	2.68954800	0.27561300	1.56882700
H	2.28722300	-1.30302500	0.92346700
C	3.09765400	0.05467200	-0.54681100
H	3.19086300	1.12738700	-0.74321400
H	4.10941600	-0.34106800	-0.41817500
H	2.66065600	-0.41619300	-1.43245300

R37-C=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.32345800	0.13895400	-0.26716500
C	1.21630500	-0.36510100	0.26701700
H	2.35079200	1.14240800	-0.68233200
H	3.24886800	-0.42546200	-0.30275700
H	1.20908100	-1.37364800	0.67400400
C	-0.06793300	0.38738600	0.37541700
H	-0.41691200	0.48496100	1.40810800
H	-0.00908200	1.37950500	-0.08143600
O	-1.10257800	-0.37018700	-0.33678500
O	-2.29913800	0.09828700	-0.07161500

P37-•CYCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.52617800	0.03964700	0.43325900
C	0.59916500	0.97834900	-0.04088400
H	-0.60903500	0.01469600	1.52651300
H	0.96166400	1.73139900	0.66445500
H	0.40735300	1.43074900	-1.02170500
O	0.32623400	-1.06948900	-0.02243000
O	1.48413400	-0.15102500	-0.13651500
C	-1.83813800	0.05956200	-0.21793000
H	-1.90029400	-0.06356000	-1.29321700
H	-2.75172400	0.18548400	0.34883700

TS37

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.67870200	0.20273100	0.51713100
C	0.56747600	0.98224400	0.10558000
H	-0.86458900	0.08199600	1.57945400

R38-C=CC(C)OO•

H	1.08193000	1.43831700	0.96131900
H	0.39772700	1.73927100	-0.66711800
O	1.30790100	-0.10916100	-0.44097700
O	0.52546200	-1.13519100	0.19186000
C	-1.72749700	-0.01509600	-0.35979600
H	-2.62246500	-0.53707700	-0.04289300
H	-1.62717100	0.21302400	-1.41531500

P38-•CYCC (C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.37995800	-0.22114300	-0.16869600
C	1.20019100	-0.71744100	0.18629800
H	2.53311700	0.83529000	-0.36125500
H	3.25045500	-0.85979300	-0.27131900
H	1.09341300	-1.78418100	0.37129500
C	-0.05919300	0.07118500	0.39265200
H	-0.38771100	-0.00897800	1.43563200
O	-1.09639000	-0.65443900	-0.37746500
O	-2.30374000	-0.32057000	0.00979400
C	-0.04520100	1.52605400	-0.04315400
H	0.64555300	2.10264100	0.57831400
H	0.25887100	1.61961600	-1.08922500
H	-1.04718800	1.94354800	0.07532200

TS38

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.70924300	-0.25266700	0.37533900
C	-0.62750700	-0.16516400	-0.39777600
H	0.54378300	-0.51192800	1.42980900
H	-0.48544500	-0.38181700	-1.46547000
O	0.79787000	1.20321300	0.22997600
O	-0.62508600	1.26385200	-0.17791900
C	1.86019400	-0.95875800	-0.19037100
H	2.34306400	-1.77042900	0.33875700
H	2.24105800	-0.66608100	-1.16212800
C	-1.85926000	-0.84699900	0.14721000
H	-2.75337400	-0.49451200	-0.37683600
H	-1.78787700	-1.92986800	-0.00120400
H	-1.97949500	-0.64035700	1.21420800

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.70345000	0.47932200	0.58501500
C	0.67519400	-0.18497200	0.46277700

H	-1.16569300	0.46346600	1.56718600
H	0.97146000	-0.59796700	1.43774600
O	0.27661200	-1.24751500	-0.41388000
O	-1.12002800	-1.17025000	-0.09407400
C	-1.20479900	1.37213300	-0.34656100
H	-2.16264100	1.85379100	-0.19047100
H	-0.73169700	1.50984200	-1.31148500
C	1.81686300	0.61323800	-0.13467600
H	2.09446700	1.43148500	0.53756800
H	2.69231500	-0.02895300	-0.26963500
H	1.54626600	1.03212700	-1.10660800

R39-C=CC(CC)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.80371100	-1.50583000	-0.28707200
C	0.66185800	-1.34320000	0.37242500
H	2.21954400	-0.74208000	-0.93496000
H	2.37703900	-2.42218600	-0.19723700
H	0.29095700	-2.14655400	1.00552400
C	-0.22639200	-0.13281400	0.33317600
H	-0.49170500	0.17234200	1.35213400
O	-1.50148300	-0.62764200	-0.24741400
O	-2.50008100	0.17627600	0.02592000
C	0.24185900	1.08290700	-0.46031000
C	1.32966900	1.89089100	0.25625300
H	-0.64146700	1.71216700	-0.60753700
H	0.57727400	0.76875900	-1.45483200
H	1.60992800	2.76524800	-0.33820500
H	0.97364300	2.25061400	1.22756600
H	2.23306600	1.30089200	0.43267100

P39-•CYCC (CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.21068500	-0.28565900	0.35789400
C	-0.18380000	-0.11497600	-0.28642200
H	1.13204400	-0.52358300	1.42715100
H	-0.17120500	-0.37060500	-1.35581100
O	1.38619500	1.15967200	0.18153700
O	-0.05512300	1.31737000	-0.11923200
C	2.25122800	-1.07462400	-0.30443900
H	2.55296000	-0.81930000	-1.31376600
H	2.72996500	-1.91022600	0.19007500
C	-1.40477800	-0.68559800	0.40171400
H	-1.36225500	-1.77970900	0.31837000

TS39

H	-1.35382000	-0.43985800	1.46871800
C	-2.71274000	-0.15740300	-0.19865500
H	-3.57864100	-0.57084100	0.32596700
H	-2.76043300	0.93291500	-0.12280700
H	-2.80076600	-0.42556800	-1.25689500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.24572400	0.43703700	0.55911300
C	0.18321800	-0.11988200	0.51993600
H	-1.76047800	0.38467900	1.51355600
H	0.46037600	-0.50063400	1.51474800
O	-0.08341200	-1.22080700	-0.36190700
O	-1.49939700	-1.23889300	-0.13403900
C	-1.76054300	1.29328300	-0.39942900
H	-2.75843500	1.70218700	-0.29461900
H	-1.24829200	1.46926500	-1.33759200
C	1.29522400	0.76102400	-0.02342600
H	1.37902100	1.63795900	0.63122700
H	1.01296600	1.12874800	-1.01531000
C	2.63527400	0.02178300	-0.10224200
H	2.55821300	-0.85284400	-0.75455400
H	3.41865500	0.67297700	-0.50005200
H	2.95575400	-0.32421100	0.88645900

R40-C=C(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.92007300	-1.04032200	-0.21007200
C	-1.01994500	-0.10321500	0.08284700
H	-1.67467400	-2.09701700	-0.18292400
H	-2.93948200	-0.78501900	-0.48089600
C	0.36913500	-0.49018500	0.49862300
H	0.64923200	-0.07634800	1.47263400
H	0.51753800	-1.57293500	0.50598900
O	1.31499100	0.07630800	-0.47122400
O	2.54671500	0.02566200	-0.02255000
C	-1.31369300	1.37263500	0.04701500
H	-0.63440100	1.88751200	-0.64099000
H	-2.34087000	1.56777900	-0.26874600
H	-1.16354400	1.82679200	1.03464100

P40-•CYC(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.42156600	-0.06672700	0.05192200

C	-0.81477900	-0.14948300	0.96874700
H	-0.90866500	0.61424600	1.74719700
H	-0.99054300	-1.14744700	1.38803900
O	-0.54219000	-0.15464600	-1.07963100
O	-1.66833700	0.11342900	-0.15636800
C	1.35235900	-1.20513500	0.04225300
H	0.96178700	-2.21509600	-0.00113900
H	2.42511400	-1.05878900	0.00722800
C	1.10307900	1.29424200	0.04228800
H	1.71807500	1.42091900	0.94012500
H	1.74997400	1.38866000	-0.83473200
H	0.35513700	2.08985600	0.01002200

TS40

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.53023000	0.10385600	0.18883600
C	0.72039800	-0.35482200	0.94693700
H	0.68379500	-1.42550600	1.19102300
H	0.95575300	0.21947000	1.84916200
O	1.67657900	-0.07676400	-0.07225000
O	0.72342400	-0.04893700	-1.14847100
C	-0.83244300	1.46119300	0.14769600
H	-1.71520400	1.81756500	-0.37043400
H	-0.12667300	2.20045400	0.50767900
C	-1.59194500	-0.91928500	-0.10232700
H	-2.10415600	-1.20130500	0.82624600
H	-2.34258500	-0.53034800	-0.79518600
H	-1.14563700	-1.82036200	-0.52957100

R41-C=C(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.08432800	1.66380200	-0.20978300
C	0.47719100	0.52935900	0.13610100
H	0.54001500	2.60085900	-0.26602100
H	2.14162700	1.70667800	-0.44314700
C	-0.98303600	0.54065800	0.48654300
H	-1.18691300	0.10795200	1.47114000
H	-1.41793600	1.54173500	0.43161500
O	-1.69826200	-0.30039400	-0.48284000
O	-2.91675600	-0.56724500	-0.07664200
C	1.15061800	-0.82033900	0.23185800
C	2.63506200	-0.85867500	-0.12863300
H	0.59595300	-1.52133000	-0.40578400
H	1.00903600	-1.20049300	1.25456300

P41-•CYC(CC)COO

H	3.02294700	-1.87666100	-0.03332100
H	2.80458600	-0.53251600	-1.15965400
H	3.22585200	-0.21394500	0.52994500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.07030900	0.34874800	-0.02873200
C	0.87432600	-0.48349700	0.98705800
H	0.39388200	-1.38067700	1.38992500
H	1.31463400	0.10832200	1.79862400
O	1.27393700	0.24802400	-0.90611400
O	1.84142900	-0.79881800	-0.02715300
C	-0.21091300	1.75407700	0.29956600
H	-1.11118800	2.24751200	-0.04644600
H	0.54763700	2.35160700	0.79181000
C	-1.09124800	-0.39709300	-0.68402200
H	-1.35885500	0.13505000	-1.60463000
H	-0.72310500	-1.38277600	-0.98628300
C	-2.31993700	-0.54210800	0.22032700
H	-2.73486000	0.42995900	0.50451900
H	-3.10795400	-1.10309300	-0.29009300
H	-2.07834000	-1.08031800	1.14352100

TS41

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.00870300	0.29610000	0.33083900
C	1.32925400	-0.19321100	0.89598400
H	1.22445000	-1.13519700	1.45199800
H	1.86854900	0.53608000	1.50950800
O	2.00695500	-0.38126600	-0.34392000
O	0.81851700	-0.40677800	-1.15368900
C	-0.12763800	1.63919500	-0.01266600
H	-1.04780700	2.04180200	-0.41584200
H	0.74383700	2.28320800	-0.02021500
C	-1.21569300	-0.57767600	0.57538600
H	-1.48304600	-0.48379900	1.63846900
H	-0.90254400	-1.61664900	0.43054200
C	-2.43589300	-0.27921800	-0.29795700
H	-3.22429600	-1.01291600	-0.10795900
H	-2.85474900	0.71085500	-0.09557400
H	-2.17612200	-0.33017000	-1.35957600

R42-(cis)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-1.81928900	0.52831900	-0.14283600
C	-0.56610900	0.90860400	0.11292400
H	-2.52210200	1.30716100	-0.43526300
H	-0.30831800	1.95977100	0.00795100
C	0.56001300	0.03352500	0.54898100
H	1.01676500	0.37313300	1.48379400
H	0.29033500	-1.01949800	0.64871100
O	1.61586400	0.11465100	-0.47203600
O	2.72064500	-0.45673700	-0.05570200
C	-2.40944200	-0.84779300	-0.07087700
H	-3.20901100	-0.88536200	0.67918800
H	-2.87090700	-1.11345600	-1.02937900
H	-1.67987300	-1.62098400	0.17775200

P42-CC•YCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.00185400	0.04726600	0.33623000
C	1.18440400	0.97079700	0.00994000
H	-0.20047400	-0.01485300	1.41292200
H	1.48482600	1.69786500	0.77000000
H	1.10154400	1.45636300	-0.97091400
O	0.88623700	-1.07270500	-0.05704300
O	2.06123200	-0.16797900	-0.03101400
C	-1.23590900	0.11334000	-0.44775900
H	-1.12767900	0.16766100	-1.52835700
C	-2.60112100	-0.00624800	0.13189500
H	-3.27006500	0.78088200	-0.24069700
H	-3.07667000	-0.96032700	-0.14508400
H	-2.58660700	0.04694400	1.22474800

TS42

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.03290100	0.86825100	0.43366000
C	-0.93195600	-0.24625400	0.96002300
H	-0.33848700	1.88900300	0.63907200
H	-1.78900600	0.15439200	1.51745100
H	-0.43084500	-1.01185100	1.56184000
O	-1.32875300	-0.79227400	-0.29405500
O	-1.04360300	0.40865200	-1.04549300
C	1.28488200	0.66026200	0.04924500
H	1.87249900	1.53298700	-0.22346200
C	1.91246000	-0.68154900	-0.14312500
H	2.55786100	-0.68767800	-1.02749000
H	2.55266700	-0.94794700	0.71102400

H	1.15924100	-1.46418700	-0.26086400
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R43-(trans)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.64596500	0.32705700	-0.23290000
C	0.57009500	-0.08521700	0.43528500
H	1.53907800	1.15657900	-0.93220600
H	0.64662400	-0.91407500	1.13650200
C	-0.77700300	0.53559700	0.29539500
H	-1.20987600	0.84764600	1.25046200
H	-0.77429000	1.38456700	-0.39454400
O	-1.69668500	-0.47269400	-0.25403400
O	-2.94534600	-0.08550100	-0.14544400
C	3.02176600	-0.24897300	-0.10302700
H	3.73747100	0.51273400	0.22973900
H	3.04809900	-1.07826500	0.60886800
H	3.38419900	-0.61440900	-1.07151600

P43-CC•YCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.00185400	0.04726600	0.33623000
C	1.18440400	0.97079700	0.00994000
H	-0.20047400	-0.01485300	1.41292200
H	1.48482600	1.69786500	0.77000000
H	1.10154400	1.45636300	-0.97091400
O	0.88623700	-1.07270500	-0.05704300
O	2.06123200	-0.16797900	-0.03101400
C	-1.23590900	0.11334000	-0.44775900
H	-1.12767900	0.16766100	-1.52835700
C	-2.60112100	-0.00624800	0.13189500
H	-3.27006500	0.78088200	-0.24069700
H	-3.07667000	-0.96032700	-0.14508400
H	-2.58660700	0.04694400	1.22474800

TS43

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.08615300	-0.35998600	0.51019600
C	-1.27864900	-0.90833400	0.11015400
H	0.30133300	-0.26661700	1.57083100
H	-1.85426600	-1.26138000	0.97636600
H	-1.24971000	-1.69398000	-0.65287900
O	-1.82760500	0.28381000	-0.44455400
O	-0.88718300	1.17501600	0.19092200
C	1.15340200	-0.33112600	-0.37221700

H	0.95840800	-0.56143200	-1.41772000
C	2.52098200	0.14681000	-0.01985900
H	2.63197900	0.30952800	1.05586300
H	3.28542400	-0.57205800	-0.34224600
H	2.75380600	1.09114100	-0.53079200

R44-(cis)-CCC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.16294400	0.88458100	-0.22720700
C	0.08200600	1.03062400	0.23110500
H	-1.75059800	1.79276100	-0.36247800
H	0.45225400	2.03444000	0.42588200
C	1.05847200	-0.05914300	0.52090900
H	1.45740100	-0.00253100	1.53837400
H	0.66588400	-1.06295600	0.34902500
O	2.21119600	0.11366600	-0.37727200
O	3.19901000	-0.67855100	-0.03538200
C	-1.89854300	-0.38058200	-0.56356000
H	-2.23154000	-0.31787000	-1.60850300
H	-1.24102700	-1.25282700	-0.50365000
C	-3.12952100	-0.59594300	0.33432000
H	-3.81666400	0.25462500	0.27355300
H	-3.67876400	-1.49297700	0.03352800
H	-2.83541500	-0.71080900	1.38209400

P44-CC•CYCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.55586200	-0.18648700	-0.34755100
C	1.86795100	-0.85499600	0.09048800
H	0.39004600	-0.25640500	-1.43009000
H	2.31883100	-1.58213900	-0.59110800
H	1.83307900	-1.25836600	1.11062900
O	1.21595700	1.10118400	-0.03881100
O	2.53105300	0.41981000	0.04322000
C	-0.68296400	-0.39925300	0.40792500
H	-0.61546600	-0.31290400	1.49076500
C	-2.02477700	-0.60972100	-0.20724200
H	-2.47201500	-1.53452300	0.18784900
H	-1.92221300	-0.75279800	-1.28938800
C	-3.00681600	0.55077100	0.06800800
H	-3.98627100	0.33908100	-0.37215100
H	-3.14340600	0.70019900	1.14358100
H	-2.63420000	1.48802600	-0.35511800

TS44

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.61204700	0.88573200	0.56625600
C	-1.14506100	-0.50674500	0.89558000
H	-1.22716200	1.71075400	0.91237000
H	-2.07108900	-0.43726400	1.48190000
H	-0.45000400	-1.18518800	1.39464100
O	-1.40359900	-0.95387200	-0.43030900
O	-1.46825100	0.37525300	-0.99919700
C	0.68507900	1.23046400	0.20294900
H	0.85802200	2.30027000	0.09344800
C	1.83470300	0.39156800	-0.26904500
H	1.91115100	0.54473600	-1.35788100
H	2.75234400	0.84645000	0.13148100
C	1.84220000	-1.11221400	0.02186400
H	1.85408000	-1.31395500	1.09785800
H	0.97462300	-1.60644800	-0.41990700
H	2.74358800	-1.56324200	-0.40349300

R45-(trans)-CCC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.05455100	0.81909700	-0.08678400
C	0.09831400	-0.00997100	0.32949000
H	0.77612600	1.84583500	-0.32693300
H	0.32532800	-1.04343100	0.57681500
C	-1.32371000	0.40220600	0.49954400
H	-1.71920700	0.18758900	1.49677800
H	-1.48179600	1.45966800	0.26791200
O	-2.14725400	-0.37887600	-0.43676900
O	-3.42314900	-0.26962900	-0.15191500
C	2.51291100	0.50293300	-0.26099900
H	3.09199600	1.20436900	0.35713000
H	2.79175600	0.75087500	-1.29542100
C	2.93224600	-0.93281500	0.05598800
H	2.72020700	-1.19072500	1.09858400
H	2.40736200	-1.65160100	-0.58112500
H	4.00558000	-1.06324600	-0.10770200

P45-CC•CYCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.55586200	-0.18648700	-0.34755100
C	1.86795100	-0.85499600	0.09048800
H	0.39004600	-0.25640500	-1.43009000
H	2.31883100	-1.58213900	-0.59110800

H	1.83307900	-1.25836600	1.11062900
O	1.21595700	1.10118400	-0.03881100
O	2.53105300	0.41981000	0.04322000
C	-0.68296400	-0.39925300	0.40792500
H	-0.61546600	-0.31290400	1.49076500
C	-2.02477700	-0.60972100	-0.20724200
H	-2.47201500	-1.53452300	0.18784900
H	-1.92221300	-0.75279800	-1.28938800
C	-3.00681600	0.55077100	0.06800800
H	-3.98627100	0.33908100	-0.37215100
H	-3.14340600	0.70019900	1.14358100
H	-2.63420000	1.48802600	-0.35511800

TS45

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.53370400	-0.63745600	0.45138800
C	-1.93602200	-0.71444900	-0.14045000
H	-0.42030600	-0.84440500	1.51175100
H	-2.67301500	-1.08735400	0.58344000
H	-2.01150600	-1.29165400	-1.06853200
O	-2.11629000	0.67212800	-0.41757800
O	-1.07513200	1.12459000	0.47401200
C	0.60103600	-0.67774100	-0.34304500
H	0.47213700	-0.61152300	-1.42254200
C	1.99826000	-0.60695300	0.17947700
H	1.99697800	-0.73723700	1.26769200
H	2.58404700	-1.43910500	-0.23785700
C	2.69796800	0.71761000	-0.18731700
H	3.71991200	0.73587400	0.20385600
H	2.74876400	0.84636500	-1.27340100
H	2.14913800	1.56923200	0.22379600

R46-C=C(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.97928500	0.91330200	-0.35360800
C	1.13087500	-0.03302700	0.04406000
H	1.68314300	1.94687800	-0.48546800
H	3.01968200	0.68177800	-0.55735800
C	-0.31424800	0.26046200	0.37375900
H	-0.54465100	-0.10192900	1.38236000
O	-1.11173700	-0.61495200	-0.52210100
O	-2.32829200	-0.79227800	-0.06703100
C	1.54818800	-1.46941800	0.23123100
H	0.95778300	-2.13502000	-0.40689800

H	1.37916200	-1.79530900	1.26544500
C	-0.80609200	1.68747800	0.20596800
H	-0.29751900	2.35195800	0.90946900
H	-0.63266500	2.04850100	-0.81112800
H	-1.87820200	1.71795000	0.41199100
H	2.60544800	-1.60974900	-0.00382400

P46-•CYC(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.65751800	0.09808200	0.07140100
C	-0.81081500	-0.13633300	0.51934700
H	-0.83182200	-0.50475400	1.55463000
O	0.58466300	-1.27270400	-0.49843200
O	-0.89167000	-1.25079300	-0.39278900
C	1.67639000	0.18101900	1.12827500
H	1.66152300	-0.53355800	1.94294300
H	2.48418500	0.90136300	1.08190900
C	0.86006000	1.10296600	-1.05421900
H	0.76883700	2.12958300	-0.68343100
H	1.85971200	0.98103900	-1.48140400
H	0.12757100	0.94396200	-1.84770200
C	-1.89574800	0.89193600	0.30065200
H	-2.87600600	0.43384200	0.46821800
H	-1.78582900	1.71423400	1.01540200
H	-1.87654300	1.29625400	-0.71353300

TS46

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.65123700	-0.28347100	0.07482100
C	0.75875900	-0.08843600	-0.51588000
H	0.68853500	-0.07506500	-1.61425800
O	0.96785600	1.24039900	-0.02862000
O	-0.42494800	1.54023200	0.15190200
C	-0.81043400	-0.58858400	1.42278200
H	-1.79850900	-0.75470100	1.83599100
H	0.01647600	-0.52365500	2.11853300
C	1.87452200	-1.01790900	-0.08053000
H	1.68071100	-2.03266000	-0.44305000
H	2.82704000	-0.68354400	-0.50255600
H	1.97173100	-1.04576300	1.00703600
C	-1.76894400	-0.55827200	-0.89251600
H	-1.63671300	-1.54936100	-1.34503500
H	-2.74353200	-0.54164000	-0.39810300
H	-1.76499100	0.18137200	-1.69688000

R47-C=C(CC)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.09075500	1.60731600	-0.37568100
C	0.62429600	0.43686800	0.05588100
H	0.44707200	2.46430900	-0.53136400
H	2.14275800	1.75894500	-0.58572600
C	-0.83863100	0.22753600	0.37853300
H	-0.93964700	-0.20709800	1.37959900
O	-1.29875200	-0.84894800	-0.53671700
O	-2.38680200	-1.42983700	-0.09249800
C	1.48839800	-0.78321100	0.29524100
H	1.07421500	-1.61405700	-0.28994900
H	1.36179600	-1.08924000	1.34439800
C	-1.77968900	1.41008700	0.22718400
H	-1.51720100	2.20030600	0.93545300
H	-1.74538100	1.81721600	-0.78669300
H	-2.79896000	1.07848400	0.43688300
C	2.97707800	-0.62987000	-0.01337800
H	3.43864400	0.15053000	0.60013000
H	3.50376100	-1.56678800	0.18890500
H	3.14413200	-0.37468100	-1.06460400

P47-•CYC (CC)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.20997400	-0.29285000	0.31843400
C	-1.33647500	-0.13135200	0.23943400
H	-1.82025500	-0.90091700	0.85713200
O	0.06968200	-1.11968000	-0.90614100
O	-1.28847000	-0.57469300	-1.13220500
C	0.73489300	-1.08228100	1.44221300
H	0.32474000	-2.06554900	1.64019200
H	1.52393300	-0.70925700	2.08292700
C	1.02280000	0.96193700	-0.00626800
H	1.01148100	1.62626700	0.86771400
H	0.51991200	1.49092800	-0.82097000
C	-2.03178600	1.19820900	0.41637600
H	-3.07346300	1.11229500	0.08997100
H	-2.03748100	1.48187400	1.47402400
H	-1.55739400	1.99272000	-0.16272100
C	2.46273300	0.64878400	-0.42697400
H	2.98205100	1.56202100	-0.73150100
H	3.03864000	0.19300400	0.38434700
H	2.46530300	-0.04308100	-1.27363300

TS47

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.23890800	-0.21364500	0.13478100
C	1.14338400	-0.13913600	-0.54400700
H	1.00779300	-0.13475500	-1.63646000
O	1.48631700	1.17487800	-0.09266400
O	0.13776300	1.58402400	0.18745900
C	-0.32312100	-0.50505100	1.49303600
H	-1.27967700	-0.58157100	1.99318700
H	0.56158300	-0.50968400	2.11693300
C	2.21075200	-1.14672400	-0.16386200
H	1.91979800	-2.14723700	-0.50012500
H	3.15744200	-0.88873600	-0.64815100
H	2.37432300	-1.17235500	0.91568400
C	-1.42469800	-0.38228600	-0.78589300
H	-1.36964400	-1.39496200	-1.21293500
H	-1.28434000	0.30701300	-1.62485000
C	-2.80145300	-0.15645400	-0.15835200
H	-3.57880700	-0.21446900	-0.92546300
H	-3.03596400	-0.90672300	0.60245000
H	-2.86088100	0.83203500	0.30714300

R48-C=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600
H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100
C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

P48-•CYCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.49899000	0.37790400	-0.11427000

C	0.24261300	1.23494300	0.10424100
C	-0.82110100	0.16454100	0.46915900
H	2.11044200	0.31758600	0.79561000
H	2.11795100	0.70309900	-0.95493200
H	0.37539100	1.97262500	0.89817400
H	-0.04660800	1.76222900	-0.80752400
H	-1.17965400	0.28043700	1.49568800
O	-0.05841300	-1.08613600	0.51386100
O	0.99387300	-0.90208800	-0.45996000
C	-1.94932300	0.06339100	-0.48599100
H	-1.74160400	0.01517000	-1.54944600
H	-2.94666800	-0.19002400	-0.14761600

TS48

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.94737200	0.05260200	-0.43112500
C	0.01021100	1.21262300	-0.15296000
H	0.89142400	-0.35350600	-1.43612700
H	-0.11766600	1.80542200	-1.06341100
H	0.42230800	1.87074900	0.61705600
O	-0.25658700	-1.27688700	0.20875700
C	2.15868200	-0.08372100	0.22959700
H	2.90303800	-0.79775700	-0.10279900
H	2.35698800	0.44616200	1.15563800
C	-1.35494800	0.63192400	0.30709500
H	-1.39894700	0.58357700	1.40071700
H	-2.21843300	1.18091200	-0.07857700
O	-1.41924000	-0.67512900	-0.23477600

R49-C=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.04555100	0.12476000	0.13592000
C	1.96013500	-0.39298900	-0.43011200
H	3.08603900	0.34352300	1.19929100
H	3.93983200	0.34291100	-0.43787900
H	1.96473200	-0.59864500	-1.50046700
C	0.68725200	-0.73697800	0.29058600
H	0.47162100	-1.80720800	0.17379000
H	0.79227500	-0.54311700	1.36385100
C	-0.51633400	0.03922700	-0.25228400
H	-0.62376300	-0.11705900	-1.33097300
O	-1.69106900	-0.60382300	0.35785600
O	-2.80695800	-0.22447000	-0.21852700

P49-•CYCCC(C)OO

C	-0.52312600	1.52213300	0.07881600
H	-0.45860600	1.67507900	1.16079600
H	0.33373800	2.01257500	-0.39047400
H	-1.44251000	1.98136800	-0.29011900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.11120100	0.05173000	-0.36467500
C	0.01802600	-1.02071700	-0.51963800
C	-1.28877300	-0.19571500	-0.41413700
H	1.38960700	0.44593300	-1.35272400
H	0.09469300	-1.55667300	-1.46812500
H	-1.84851800	-0.19219800	-1.35361400
O	-0.81764000	1.18970900	-0.29174000
O	0.45732500	1.08182300	0.37358200
C	-2.16144200	-0.55743000	0.72697100
H	-1.72568400	-0.66873900	1.71403500
H	-3.23983300	-0.48993000	0.64932800
H	0.07376400	-1.75288900	0.29082100
C	2.34763800	-0.36699300	0.41299900
H	2.87648800	-1.16011500	-0.12345300
H	3.03132000	0.47715900	0.53644900
H	2.07078200	-0.74004600	1.40343700

TS49

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.32162800	-0.25138700	0.43586200
C	0.09047500	-1.06681800	0.09606200
H	1.35772700	0.12713200	1.45252700
H	-0.24466900	-1.61388900	0.98373900
H	0.31227500	-1.80251600	-0.68235900
O	0.59052500	1.39273800	-0.18409100
C	2.53922600	-0.46802400	-0.19080200
H	3.45173200	-0.01808200	0.18249500
H	2.60028700	-1.00943200	-1.12931600
C	-1.03617400	-0.10435300	-0.38179600
H	-0.96897300	-0.00007300	-1.47173000
O	-0.71228000	1.15279400	0.20416400
C	-2.44048700	-0.48903400	0.04747700
H	-3.17135000	0.23888200	-0.31481500
H	-2.70166400	-1.46986500	-0.36041800
H	-2.50933600	-0.53871600	1.13846900

R50-C=CCC(CC)OO•

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-3.11022800	0.01444400	-0.05704400
C	-2.05687600	-0.71971000	0.28696400
H	-3.12009100	0.60985400	-0.96572700
H	-4.00895700	0.04279900	0.54963400
H	-2.09479800	-1.30485100	1.20586700
C	-0.78148500	-0.82865900	-0.50003800
H	-0.63086200	-1.86761900	-0.82172900
H	-0.83924600	-0.22041200	-1.40775700
C	0.44435700	-0.42624700	0.32615900
H	0.52960200	-1.06529800	1.21161100
O	1.59904600	-0.77305200	-0.51926200
O	2.72066000	-0.76769200	0.16222000
C	0.53325400	1.04064900	0.74694600
H	-0.27900000	1.22897900	1.45808900
H	1.47173300	1.15412600	1.29894200
C	0.47511900	2.05183700	-0.40213800
H	-0.50032000	2.05222900	-0.89746200
H	0.65027800	3.06325200	-0.02469500
H	1.23918000	1.83901000	-1.15554200

P50-•CYCCC(CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.61771700	0.17858900	-0.47048700
C	0.60510600	1.11263500	-0.46173000
C	1.79249700	0.12446100	-0.34401800
H	-0.87646200	-0.09160600	-1.50556900
H	0.66377300	1.72446000	-1.36443400
H	2.42279800	0.13260100	-1.23767200
O	1.15266200	-1.19601700	-0.38923500
O	-0.14502300	-0.98715700	0.20359500
C	2.60535400	0.27420600	0.88537700
H	2.10661000	0.35153100	1.84544300
H	3.67166000	0.08329700	0.87729900
H	0.57777600	1.78247200	0.40239400
C	-1.84819000	0.68908000	0.26955200
H	-2.13706600	1.64553800	-0.18261800
H	-1.56174000	0.90329100	1.30630000
C	-3.02727400	-0.28790400	0.23381600
H	-2.75863200	-1.24150200	0.69577300
H	-3.88932800	0.12053400	0.76944000
H	-3.33915700	-0.49162500	-0.79630600

TS50

Cartesian Coordinates (Å)

At.	X	Y	Z
C	1.67427000	-0.41791600	0.43572600
C	0.25375700	-0.90367200	0.22928800
H	1.86966000	0.03648400	1.40195900
H	-0.14685400	-1.27579000	1.17880100
H	0.22767000	-1.72961500	-0.48674900
O	1.36079800	1.29243900	-0.33834400
C	2.75140100	-1.01320700	-0.20142600
H	3.77087700	-0.79053600	0.09105300
H	2.61094500	-1.63953400	-1.07643000
C	-0.61801400	0.28272100	-0.28007400
H	-0.62656300	0.26585600	-1.37789500
O	0.07658700	1.45318400	0.14047600
C	-2.03626800	0.34654000	0.27111600
H	-2.48171000	1.29754400	-0.04173300
H	-1.98845600	0.36501900	1.36659800
C	-2.91083600	-0.81814900	-0.20365100
H	-2.51509200	-1.78363400	0.12797400
H	-3.92676300	-0.72502300	0.19014000
H	-2.97865100	-0.84365500	-1.29664300

R51-C=CC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.78976800	-0.87830700	-0.25783400
C	-1.81144100	-0.26221300	0.39677200
H	-2.74671500	-1.03847300	-1.33161100
H	-3.67567000	-1.24358600	0.25052800
H	-1.89685600	-0.11737400	1.47429100
C	-0.55327200	0.28307600	-0.22912200
H	-0.60004800	0.11282700	-1.31184700
C	0.64786500	-0.49848900	0.30635600
H	0.80636500	-0.33704200	1.37753600
H	0.55807800	-1.57090800	0.11287900
O	1.83960200	-0.02719700	-0.38748900
O	2.92589200	-0.59023000	0.08852600
C	-0.40386100	1.79224700	0.03476700
H	-0.38604900	1.99948200	1.11101100
H	0.52363700	2.17518300	-0.39797300
H	-1.24382900	2.34141600	-0.39875300

P51-•CYCC(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.19006200	1.45169500	-0.17054100
C	-0.73652100	0.42194600	0.52236700

C	0.19662500	-0.83883600	0.54217800
H	0.46766300	2.26449000	0.51231400
H	-0.24223400	1.87403000	-1.08319200
H	-0.89294700	0.73592800	1.55871600
H	0.15798600	-1.31294000	1.53011000
O	1.50813700	-0.26388800	0.46222600
O	1.34762100	0.72991500	-0.58277200
C	-0.01688700	-1.84177600	-0.53249300
H	0.45945900	-1.70003000	-1.49399600
H	-0.67018200	-2.69255400	-0.38401400
C	-2.09645900	0.23160900	-0.14833400
H	-2.68225500	-0.54578400	0.35260100
H	-2.67785900	1.15847500	-0.10920500
H	-1.98662100	-0.05766400	-1.19802700

TS51

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.49305000	-0.80507200	0.49644300
C	-0.35765900	0.71391400	0.49911900
H	-0.02428300	-1.28790300	1.34838600
H	-0.42410900	1.03507100	1.54539400
O	1.06704600	-1.10018400	-0.54527200
C	-1.55715800	-1.48448700	-0.07544500
H	-1.70983100	-2.53822500	0.12589400
H	-2.20799400	-1.02445000	-0.80919900
C	1.07590600	1.04021300	-0.02175300
H	1.02200100	1.35463900	-1.07153800
H	1.59103900	1.80472900	0.56695200
O	1.84215200	-0.14478400	0.08558400
C	-1.41470000	1.46942400	-0.31024700
H	-2.42117300	1.30312600	0.08357600
H	-1.21846000	2.54612800	-0.27926800
H	-1.40080600	1.16266700	-1.36139500

R52-C=CC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.90555900	-0.96146300	-0.42145300
C	-1.93761800	-0.49734600	0.36131000
H	-2.81087800	-0.97192200	-1.50376100
H	-3.83399000	-1.34656400	-0.01338700
H	-2.07745400	-0.50189800	1.44285700
C	-0.62144700	0.06635900	-0.11803400
H	-0.61624900	0.05094200	-1.21577100
C	0.49499100	-0.86877100	0.35845000

H	0.69688900	-0.76558100	1.42969500
H	0.26174500	-1.91377900	0.13803000
O	1.72867300	-0.55341200	-0.35255600
O	2.71026800	-1.33705200	0.03030400
C	-0.46480500	1.52680100	0.36708600
H	-0.38790900	1.52473300	1.46318500
H	-1.39950100	2.04939900	0.13306400
C	0.70808400	2.30915300	-0.23405100
H	1.67434400	1.88284500	0.04298300
H	0.65529600	2.31900200	-1.32804700
H	0.68429800	3.34813700	0.10931500

P52-•CYCC(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.06638700	-1.38991000	-0.15368600
C	0.39750200	-0.07633400	0.52390700
C	-0.94961600	0.72974900	0.54248500
H	-0.03527700	-2.23655500	0.54325200
H	0.50382400	-1.63935800	-1.05430100
H	0.67214500	-0.29539000	1.56126900
H	-1.10122300	1.17423500	1.53311600
O	-1.94301200	-0.30152300	0.44695400
O	-1.40207400	-1.15685400	-0.59179300
C	-1.13215100	1.74753500	-0.52418000
H	-1.49311100	1.43822900	-1.49658200
H	-0.87750000	2.78686800	-0.35857800
C	1.57603700	0.62838000	-0.15505600
H	1.69262100	1.62859200	0.28000300
H	1.34297900	0.78552300	-1.21512300
C	2.89687300	-0.13558900	-0.01610200
H	2.84053400	-1.12974000	-0.47290900
H	3.71534100	0.40334200	-0.50274000
H	3.16680600	-0.27172700	1.03710400

TS52

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.91905900	0.86309800	0.48749100
C	0.35412600	0.02197000	0.51950400
H	-1.57704300	0.69170500	1.33381200
H	0.63669300	-0.08114100	1.57512500
O	-1.91377800	-0.38173000	-0.55083200
C	-1.01010500	2.11173000	-0.10654700
H	-1.87031400	2.74520800	0.07519000
H	-0.29222700	2.45602500	-0.84101800

R53-C=C(C)CCOO•

C	-0.02851800	-1.39153600	-0.01959600
H	0.27378900	-1.47951000	-1.07099800
H	0.40003300	-2.21438700	0.55876700
O	-1.43473700	-1.51197200	0.08383600
C	1.55169200	0.61034500	-0.23941400
H	1.73731600	1.62997100	0.11576500
H	1.29939200	0.69139700	-1.30456200
C	2.83192700	-0.21652200	-0.07598200
H	2.71796100	-1.23138900	-0.47122000
H	3.66757600	0.24891400	-0.60692500
H	3.11456500	-0.30168600	0.97930600

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.02080000	1.43505500	0.28599900
C	-1.36480300	0.17064600	0.04660700
H	-0.00227600	1.73792900	0.49635900
H	-1.76027000	2.22885400	0.26052100
C	-2.78209900	-0.22174900	-0.28300700
H	-2.83724200	-0.71168800	-1.26370500
H	-3.17536700	-0.94195500	0.44609800
H	-3.44648300	0.64524300	-0.29935100
C	-0.39203100	-0.98927300	0.07160000
H	-0.78845200	-1.77006200	0.73610200
H	-0.35600700	-1.45582800	-0.92336800
C	1.02766000	-0.69789800	0.52244200
H	1.60331600	-1.61839300	0.65436500
H	1.06868400	-0.11431500	1.44578400
O	1.69560200	0.07474700	-0.51836600
O	2.91521400	0.40269400	-0.15846500

P53-•CYC(C)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.70096800	0.51154300	-0.17666800
C	0.38783900	0.81517000	-0.91315200
C	-0.65561600	-0.00388700	-0.09693500
H	1.94000700	1.28961200	0.56031700
H	0.15408200	1.88220000	-0.91467200
O	0.14426000	-0.53297600	1.02257800
O	1.46262900	-0.72895600	0.47264000
C	-1.22328400	-1.14381700	-0.86487900
H	-0.55975000	-1.78440800	-1.43441400
H	-2.22824500	-1.49749700	-0.66391700
H	0.41842700	0.47185400	-1.94919700

TS53

H	2.55871800	0.35570600	-0.83662100
C	-1.73147800	0.85225600	0.56596700
H	-2.39002100	1.28282600	-0.19399200
H	-2.34083400	0.24529800	1.24195400
H	-1.27806500	1.66227200	1.14280600

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.82725700	0.19047600	0.08758800
C	0.27033600	1.04006800	0.72007100
H	0.22908800	0.93222900	1.80819800
H	0.12929000	2.09850200	0.48694400
O	0.40996900	-0.74541000	-1.07934500
C	-1.72232400	0.78317200	-0.79641500
H	-2.60899700	0.25655000	-1.13140800
H	-1.50751800	1.74032200	-1.25849400
C	1.64764100	0.55899600	0.18805800
H	1.94352500	1.14789300	-0.68721800
H	2.43985800	0.58343000	0.94185400
O	1.46888300	-0.79318100	-0.18767600
C	-1.28054800	-0.99970500	0.90372500
H	-1.79042800	-0.65783300	1.81332100
H	-1.97221600	-1.62876300	0.33888900
H	-0.42050900	-1.60163800	1.20592600

R54-C=C(CC)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.41160800	1.67096100	0.01949900
C	-0.89414700	0.45780300	0.28659500
H	0.64844900	1.88075300	-0.05750500
H	-1.07812200	2.51015100	-0.15266500
C	-2.38446600	0.19891000	0.34248300
H	-2.63857600	-0.26319700	1.30714300
H	-2.91241700	1.15737400	0.30750600
C	-0.01925300	-0.74986600	0.55604400
H	-0.36896300	-1.23994700	1.47559600
H	-0.15782500	-1.49829700	-0.23580900
C	1.46979500	-0.50271800	0.72077800
H	1.98582000	-1.39431900	1.08800400
H	1.68981700	0.33861700	1.38284400
O	2.03645300	-0.19518000	-0.58758400
O	3.31734900	0.08050300	-0.49843400
C	-2.90532200	-0.70416000	-0.79001900
H	-2.67606500	-0.27132700	-1.76872000

H	-2.46202200	-1.70405800	-0.75357000
H	-3.99051800	-0.82392100	-0.71695600

P54-•CYC(CC)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.86323500	-0.93316200	0.12315000
C	0.46733600	-0.93199400	0.76463000
C	-0.22647100	0.27314700	0.06681100
H	1.91457400	-1.62406800	-0.72884800
H	-0.06346800	-1.86965900	0.58559900
O	0.78294800	0.70716800	-0.92064800
O	2.05435700	0.40419100	-0.31178300
C	-0.49413800	1.40662600	0.99024800
H	-1.27024600	2.12801200	0.75908700
H	0.24953400	1.68254900	1.72907600
H	0.52123700	-0.77375400	1.84358600
C	-1.44184000	-0.10656800	-0.78903000
H	-1.70765100	0.76362500	-1.40090800
H	-1.13300000	-0.89348900	-1.48545800
H	2.67580500	-1.15153500	0.82151500
C	-2.66021100	-0.56040600	0.02057700
H	-3.00140800	0.22022700	0.70693900
H	-3.49111600	-0.80686900	-0.64699200
H	-2.44017000	-1.45176200	0.61753800

TS54

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.29152600	0.64304800	0.09276500
C	1.04084500	0.89227600	0.79247900
H	0.92009900	0.73134100	1.86806200
H	1.37444100	1.92293200	0.64731900
O	0.45458000	-0.68422900	-1.11489300
C	-0.78331200	1.61305400	-0.77485500
H	-1.78831200	1.56399300	-1.17466000
H	-0.13416000	2.38855200	-1.16586400
C	2.09737100	-0.09261700	0.22397000
H	2.62930200	0.36318000	-0.61859400
H	2.81268300	-0.44401000	0.97316300
O	1.37302700	-1.22134400	-0.22543100
C	-1.23793400	-0.27463000	0.84999400
H	-1.54252100	0.24997400	1.76760800
H	-0.65461300	-1.14170800	1.17694700
C	-2.47173900	-0.74375800	0.07976700
H	-2.17097200	-1.23545400	-0.84881900

H	-3.04178600	-1.46023100	0.67875300
H	-3.14724200	0.08177100	-0.16603900

R55-(cis)-CC=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.44545000	0.40357200	-0.26473500
C	-1.26639800	0.94827300	0.03924300
H	-3.19585100	1.05813000	-0.70576800
H	-1.12578500	2.00609800	-0.17936600
C	-2.89161000	-1.01525800	-0.06752800
H	-2.11964700	-1.65306700	0.36828700
H	-3.77066200	-1.05714400	0.58738600
H	-3.19618100	-1.46086600	-1.02250900
C	-0.07029400	0.27028700	0.65047200
H	-0.29225600	-0.75924000	0.94279400
H	0.23313100	0.80184600	1.56205800
C	1.11066900	0.27214600	-0.31462600
H	1.38676700	1.28182600	-0.63403300
H	0.92669200	-0.34335600	-1.19938000
O	2.25418500	-0.29279400	0.38898400
O	3.31235100	-0.35074900	-0.38603700

P55-CC•YCCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.03850000	0.21902400	-0.12845000
C	0.89965800	1.22351100	0.10758600
C	-0.28367900	0.29447700	0.47642700
H	2.64820200	0.08084200	0.77427600
H	1.13316600	1.93312000	0.90390700
O	0.32042200	-1.04455800	0.51463800
O	1.37713400	-0.98806500	-0.47161900
C	-1.43173900	0.34427600	-0.46241300
H	-1.20330900	0.42840200	-1.52203200
H	0.66997700	1.79061900	-0.79739200
H	2.68377500	0.46937600	-0.97501900
H	-0.61838400	0.44209000	1.50927700
C	-2.79214800	-0.10777100	-0.05846600
H	-3.56788300	0.29919300	-0.71517300
H	-2.88307600	-1.20610600	-0.10293800
H	-3.02646500	0.18234200	0.97284000

TS55

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.36986200	-0.17638100	0.82609200

C	0.38138000	1.11181100	0.53977000
H	-0.04188500	-0.69493700	1.72075500
H	0.78637400	1.50381000	1.47705100
H	-0.27002600	1.88061200	0.11732900
O	0.74345000	-1.25730500	-0.31152900
C	-1.68446800	-0.41782800	0.44137500
C	1.54077700	0.79253100	-0.43866000
H	1.19828000	0.87299300	-1.47705500
H	2.42358400	1.42012600	-0.28543500
O	1.91953400	-0.53947400	-0.15737200
H	-2.18778600	-1.26483500	0.90170600
C	-2.42097200	0.25581900	-0.66754000
H	-3.41380300	0.59020500	-0.34002400
H	-1.88786200	1.11784400	-1.07430400
H	-2.59187600	-0.44730300	-1.49503800

R56-(trans)-CC=CCCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.18039800	0.25134600	0.16956800
C	0.96255100	0.11084000	-0.34894500
H	2.42759200	1.18040000	0.68494900
H	0.70499300	-0.81239600	-0.86581600
C	3.27398900	-0.77212300	0.10336900
H	2.94976000	-1.67374300	-0.42398500
H	4.15778100	-0.37517800	-0.41150500
H	3.60471500	-1.06464700	1.10769900
C	-0.12554600	1.14631900	-0.27553400
H	0.23107500	2.03511100	0.25701400
H	-0.41235000	1.47438200	-1.28398100
C	-1.38506000	0.65537800	0.43175200
H	-2.13953800	1.44216900	0.52684700
H	-1.17373400	0.23086700	1.41680000
O	-1.96498300	-0.40359600	-0.38523800
O	-3.00855400	-0.94484300	0.19907800

P56-CC•YCCCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.03850000	0.21902400	-0.12845000
C	0.89965800	1.22351100	0.10758600
C	-0.28367900	0.29447700	0.47642700
H	2.64820200	0.08084200	0.77427600
H	1.13316600	1.93312000	0.90390700
O	0.32042200	-1.04455800	0.51463800
O	1.37713400	-0.98806500	-0.47161900

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C	-1.43173900	0.34427600	-0.46241300
H	-1.20330900	0.42840200	-1.52203200
H	0.66997700	1.79061900	-0.79739200
H	2.68377500	0.46937600	-0.97501900
H	-0.61838400	0.44209000	1.50927700
C	-2.79214800	-0.10777100	-0.05846600
H	-3.56788300	0.29919300	-0.71517300
H	-2.88307600	-1.20610600	-0.10293800
H	-3.02646500	0.18234200	0.97284000

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.41200200	0.32670900	0.40776800
C	0.76936200	1.24676200	0.17581100
H	-0.48662700	-0.09215500	1.40708400
H	1.02118400	1.76441400	1.10609900
H	0.53252100	2.00678800	-0.57419800
O	0.48829700	-1.24741000	-0.21817100
C	-1.59701800	0.45686300	-0.30179200
H	-1.58940400	1.04218100	-1.21971800
C	1.97112600	0.38248600	-0.29552300
H	1.99715800	0.33406100	-1.39015500
H	2.93531000	0.72976500	0.08678200
O	1.75249100	-0.90825700	0.23858300
C	-2.85573900	-0.27013900	0.03058900
H	-3.71575800	0.41149000	0.06245500
H	-3.08960000	-1.02296000	-0.73567600
H	-2.78547400	-0.78432800	0.99291400

R57-(cis)-CCC=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.90335400	0.86985500	-0.26185600
C	-0.63147100	1.27090200	-0.29330600
H	-2.60106400	1.37765900	-0.92817600
H	-0.37049100	2.07440900	-0.98124700
C	-2.52663700	-0.21117800	0.57551500
H	-1.78759600	-0.67936800	1.23271600
H	-3.27883700	0.24326400	1.23559600
C	0.52312300	0.74074600	0.51341600
H	0.19858000	0.00646000	1.25505100
H	0.99846200	1.56205900	1.06587400
C	1.57524800	0.10797100	-0.39127200
H	1.94413300	0.80293400	-1.15203200
H	1.21099700	-0.79788300	-0.88350000

P57-CC•CYCCCOO

O	2.70712300	-0.26635500	0.44574800
O	3.65569600	-0.83784700	-0.25949400
C	-3.21236500	-1.28926200	-0.28103800
H	-3.69688500	-2.04089200	0.34942900
H	-3.97873400	-0.84988700	-0.92840100
H	-2.48837200	-1.79934500	-0.92411100

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.52105100	0.31072800	-0.28772900
C	1.38081100	1.22881800	0.18045200
C	0.29655300	0.20927700	0.60983000
H	3.25130000	0.13294100	0.51285200
H	1.68581800	1.88006000	1.00211700
O	0.95872400	-1.09315300	0.45520300
O	1.87368000	-0.89891600	-0.64840800
C	-0.96316200	0.27091500	-0.17202100
H	-0.87805500	0.45014900	-1.24216100
H	1.01088800	1.85692500	-0.63307700
H	3.03634500	0.66471400	-1.18489200
H	0.09122000	0.25369500	1.68520900
C	-2.24090900	-0.29160000	0.35404800
H	-2.18630400	-1.39508000	0.33935900
H	-2.35039300	-0.03021800	1.41674500
C	-3.48162700	0.15672500	-0.42769700
H	-4.39044300	-0.29479300	-0.01903700
H	-3.59819300	1.24463400	-0.39224600
H	-3.40771700	-0.13566300	-1.48053500

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.22856700	-0.73988700	-0.79554500
C	1.03439000	-1.19043300	0.40995500
H	0.71222200	-0.92284400	-1.74935900
H	1.73078300	-1.97478400	0.10031800
H	0.39847800	-1.60686800	1.19481800
O	0.85149300	1.08633200	-0.71689200
C	-1.16025500	-0.66773500	-0.82849100
C	1.82694000	0.02662800	0.95252700
H	1.22222300	0.58549600	1.67655100
H	2.78807500	-0.24566200	1.39838600
O	2.10197400	0.83479900	-0.17304600
H	-1.62617300	-0.55248600	-1.80544600
C	-2.06706300	-0.49759500	0.34767600

H	-1.56185000	-0.77761700	1.27743900
H	-2.93188600	-1.16720400	0.24561000
C	-2.57315200	0.95732100	0.46498900
H	-1.72923800	1.64450100	0.56611900
H	-3.13831200	1.24902000	-0.42590200
H	-3.22862300	1.06960000	1.33430300

R58-(trans)-CCC=CCCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.55977300	0.30201100	0.34253300
C	0.37907400	0.13346200	-0.24868600
H	1.76362000	1.24585000	0.85216700
H	0.16769400	-0.80339300	-0.76213300
C	2.68012300	-0.69801100	0.35745200
H	2.36062500	-1.61745600	-0.14606400
H	2.90544500	-0.97382400	1.39731800
C	-0.72872100	1.15078800	-0.25967200
H	-0.41594100	2.05870500	0.26807300
H	-0.96643900	1.44799400	-1.29016900
C	-2.01585000	0.65549400	0.39282300
H	-2.78692700	1.43108600	0.42735400
H	-1.84973400	0.26010600	1.39840900
O	-2.53444200	-0.43392100	-0.42523200
O	-3.60027500	-0.97641800	0.11616000
C	3.96343700	-0.16062300	-0.29765400
H	4.30713600	0.75325600	0.19891900
H	4.77141600	-0.89639600	-0.23990700
H	3.79382700	0.07806400	-1.35216900

P58-CC•CYCCCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.52105100	0.31072800	-0.28772900
C	1.38081100	1.22881800	0.18045200
C	0.29655300	0.20927700	0.60983000
H	3.25130000	0.13294100	0.51285200
H	1.68581800	1.88006000	1.00211700
O	0.95872400	-1.09315300	0.45520300
O	1.87368000	-0.89891600	-0.64840800
C	-0.96316200	0.27091500	-0.17202100
H	-0.87805500	0.45014900	-1.24216100
H	1.01088800	1.85692500	-0.63307700
H	3.03634500	0.66471400	-1.18489200
H	0.09122000	0.25369500	1.68520900
C	-2.24090900	-0.29160000	0.35404800

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H	-2.18630400	-1.39508000	0.33935900
H	-2.35039300	-0.03021800	1.41674500
C	-3.48162700	0.15672500	-0.42769700
H	-4.39044300	-0.29479300	-0.01903700
H	-3.59819300	1.24463400	-0.39224600
H	-3.40771700	-0.13566300	-1.48053500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.10536600	0.24021900	-0.40912700
C	-1.20139400	1.26155300	-0.17890900
H	-0.06043800	-0.17772300	-1.41057300
H	-1.41278200	1.79155900	-1.11224700
H	-0.89578300	2.00373100	0.56413500
O	-1.14525000	-1.25104300	0.20219300
C	1.08050400	0.25863200	0.31075800
H	1.12016600	0.84131100	1.23079300
C	-2.47028400	0.50797200	0.30422100
H	-2.48552800	0.45395200	1.39878900
H	-3.40361100	0.94476500	-0.06258700
O	-2.37667600	-0.79291700	-0.24096600
C	2.27983900	-0.57129700	-0.01169000
H	2.36958400	-1.37508700	0.73591400
H	2.13900400	-1.06953700	-0.97742000
C	3.58929100	0.23754700	-0.01655800
H	3.75313600	0.72720900	0.94929600
H	4.44738700	-0.41221900	-0.21256100
H	3.56873100	1.01596300	-0.78552500

R59-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000
C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100
H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900

H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

P59-•CYCC(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.27602000	-0.38139900	-0.53593500
C	-0.13761000	0.68374700	-0.59392500
C	1.05470700	-0.09161200	0.06947700
H	-1.50344000	-0.70987700	-1.55958900
H	0.12320700	0.82758300	-1.64765400
O	0.68508900	-1.46583200	-0.17610300
O	-0.71308600	-1.48991200	0.18067800
C	1.18816500	0.12931200	1.53976700
H	0.55171300	-0.42329000	2.21821000
H	1.89875300	0.84250400	1.93912000
C	-2.56711100	-0.01423200	0.17994100
H	-3.23260400	-0.88151100	0.21237000
H	-2.37538100	0.30906000	1.20589700
C	-0.43439400	2.05730000	0.00753500
H	-1.26058700	2.54587500	-0.51845600
H	-0.69037800	2.00071000	1.06837900
C	2.37800100	0.12876800	-0.66440700
H	2.67877500	1.17778100	-0.58374400
H	3.16883400	-0.48676100	-0.22785900
H	2.27543000	-0.12693300	-1.72205000
H	0.44001300	2.71038100	-0.08409800
H	-3.08479100	0.78913000	-0.35183900

R60-C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800
C	0.02912800	0.36494300	-0.07789300

P60-•CYCCCCOO

H	0.13282400	0.90845700	0.86749900
H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.25346400	1.28755000	0.13098000
C	1.24434700	1.14429900	-0.17239100
C	1.73697500	-0.23071900	0.28033900
C	-1.00255900	0.02829400	-0.32256100
H	2.74970700	-0.44077000	-0.08052600
H	1.41529700	1.23913900	-1.25150200
H	1.82148700	1.93417000	0.32075900
H	-0.41158900	1.40910600	1.20961000
H	-0.67238100	2.17018000	-0.36505400
H	-0.90013400	-0.08556100	-1.41678200
H	1.72537900	-0.32222200	1.37493800
O	-0.38731000	-1.13212800	0.27378300
O	0.94104500	-1.26100600	-0.29278100
C	-2.43193500	-0.01135300	0.07065300
H	-2.99404600	-0.93049900	-0.03987500
H	-2.92378800	0.86310300	0.47829600

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.37674100	1.27805000	0.18813600
C	2.47044500	-0.13837200	0.06247700
C	1.18980900	0.13393100	-0.38030200
H	0.79159500	2.22502500	-0.18139200
H	0.49440100	1.28615400	1.27807600
H	2.82554100	0.22937400	1.01995300
H	3.11893700	-0.81617500	-0.47953200
H	0.95779900	-0.13763100	-1.40740600
O	0.14130900	-1.30434400	0.31417600
C	-1.11242000	1.21081800	-0.18897300
H	-1.64628600	2.05211000	0.26780500
H	-1.21920200	1.31831400	-1.27569100
C	-1.78000100	-0.09047400	0.24269500
H	-2.80045700	-0.16608100	-0.14684000
H	-1.79999000	-0.19065200	1.33484700

	O	-1.09003200	-1.21617500	-0.30842800
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R61-C=CC(C)CCOO•

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-3.25621700	-1.07567800	0.32724700	
C	-2.35204300	-0.39232300	-0.36581700	
H	-3.18023300	-1.19384000	1.40483800	
H	-4.10963800	-1.54453300	-0.15092800	
H	-2.46689200	-0.29680000	-1.44644600	
C	-1.14112700	0.29319000	0.21281600	
H	-1.14509500	0.12775900	1.29870700	
C	0.14294500	-0.34548600	-0.36417100	
H	0.10418100	-1.42885400	-0.20696000	
H	0.18144300	-0.18421200	-1.44872800	
C	1.42019500	0.18496200	0.26712200	
H	1.42622200	0.06588900	1.35574900	
H	1.62772700	1.22928800	0.02250600	
O	2.52451100	-0.60557100	-0.26277900	
O	3.68106800	-0.17141700	0.18143400	
C	-1.21042900	1.81005400	-0.04817600	
H	-0.38152300	2.34551600	0.42458000	
H	-1.17810300	2.02361400	-1.12291700	
H	-2.14266600	2.22376200	0.34622700	

P61-•CYCC(C)CCOO

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-0.66317100	0.66754800	0.30893500	
C	0.62508800	1.44229800	-0.01746700	
C	1.86252300	0.59344800	0.26671600	
C	-0.56032700	-0.75237100	-0.27429000	
H	2.77400900	1.05841200	-0.12513400	
H	0.62407300	1.71646200	-1.08046500	
H	0.66471300	2.37538000	0.55701300	
H	-0.72919600	0.55099000	1.40017300	
H	-0.51367700	-0.70076700	-1.37326400	
H	1.99227400	0.41461000	1.34278600	
O	0.67017100	-1.37437700	0.17382400	
O	1.77791900	-0.64915000	-0.41748300	
C	-1.64458100	-1.67280700	0.15507800	
H	-1.77950200	-2.62305700	-0.34722900	
H	-2.20070600	-1.48984000	1.06757200	
C	-1.90874000	1.40417500	-0.19214000	
H	-1.88897200	1.50887900	-1.28327100	
H	-2.82768500	0.87311400	0.07401100	

TS61

H	-1.96480000	2.41028700	0.23608300
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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.76177200	-0.58303400	0.29490900
C	-1.53737100	1.82223000	0.09962000
C	-0.71919500	0.79802100	-0.33718300
H	-0.75379500	-0.44396600	1.38396200
H	-1.98791700	1.79978800	1.08707700
H	-1.66009700	2.72960000	-0.47944500
H	-0.42209300	0.81786500	-1.38362700
O	1.02208500	1.33849500	0.24921700
C	0.46057600	-1.43229100	-0.10248700
H	0.40037500	-2.40777300	0.39553600
H	0.42735900	-1.62720000	-1.18272500
C	1.80074000	-0.79162900	0.24120000
H	2.63631800	-1.37530800	-0.15902500
H	1.92596800	-0.67451100	1.32450800
O	1.91700100	0.49292000	-0.37518400
C	-2.06105300	-1.30985500	-0.09442800
H	-2.09832300	-2.30612200	0.35962000
H	-2.94079600	-0.74893600	0.23307200
H	-2.13124300	-1.43540800	-1.18101400

R62-C=CC(CC)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.65577400	-1.85424000	-0.39616400
C	1.88933700	-1.09063000	0.37546100
C	0.85147700	-0.11017500	-0.10766500
C	-0.54434300	-0.57001100	0.37558500
H	-0.60013400	-0.50388200	1.46916900
C	-1.69352900	0.21625500	-0.23597900
O	-2.92969500	-0.43632200	0.17896700
O	-3.98418700	0.21980800	-0.24634800
H	-1.75012300	1.25236000	0.10504300
H	1.98855500	-1.15998600	1.45995400
H	2.59165500	-1.81759600	-1.48026800
H	3.37774000	-2.54776900	0.02187800
H	0.85419400	-0.12586300	-1.20698800
H	-0.67881300	-1.62591200	0.11700900
H	-1.66858200	0.20222600	-1.33075000
C	1.18703400	1.32603900	0.35725300
C	2.50181100	1.86603900	-0.21158700
H	1.22296600	1.34005400	1.45519900

H	0.37211800	2.00109600	0.07172300
H	2.69597200	2.88083800	0.14837700
H	3.34868000	1.23569900	0.07367600
H	2.47146300	1.90118600	-1.30639000

P62-•CYCC(CC)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.55354400	0.01245600	-0.21081400
C	-0.08018200	-1.41615400	0.11164500
C	1.38799400	-1.60832000	-0.26323100
C	0.50770900	1.01721000	0.27570400
H	-0.69372900	-2.15710900	-0.41196000
H	-0.60665300	0.12102600	-1.30458600
H	1.53351900	-1.58438400	-1.35183100
O	1.80864200	0.65240200	-0.25036200
O	2.19387600	-0.61118600	0.34770900
C	0.28263700	2.41334500	-0.18159100
H	-0.26274900	2.61462500	-1.09691100
H	-0.19486000	-1.60153500	1.18789200
H	1.78434200	-2.55389000	0.12351700
H	0.58174200	0.97973800	1.37322200
H	0.80666100	3.23320100	0.29442000
C	-1.93557800	0.32816200	0.38409900
C	-3.07489800	-0.53353000	-0.17028900
H	-2.16496100	1.38515700	0.20160000
H	-1.88686200	0.21491100	1.47598000
H	-4.03698600	-0.22164100	0.24744500
H	-3.14218800	-0.44593400	-1.26058000
H	-2.94224800	-1.59290600	0.06988200

TS62

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.57839600	0.06912800	0.16970200
C	0.26275300	2.46180200	0.12983700
C	0.33899500	1.16627900	-0.34465400
H	-0.58324100	0.13366700	1.26677300
H	-0.19653200	2.68459000	1.08799100
H	0.76247400	3.27677900	-0.37987000
H	0.68356900	1.03864600	-1.36857400
O	2.00172700	0.53633900	0.36931900
C	-0.06981200	-1.32655000	-0.24030500
H	-0.72760100	-2.09795500	0.17408900
H	-0.12108400	-1.42041800	-1.33356700
C	1.35418700	-1.62932300	0.21560400

H	1.70741400	-2.58192300	-0.19310300
H	1.42815800	-1.65488100	1.30968800
O	2.26887700	-0.65099300	-0.28200400
C	-2.02099500	0.31842900	-0.33064600
H	-2.29306800	1.34912400	-0.07683200
H	-2.03428300	0.26569400	-1.42788000
C	-3.07465100	-0.63436600	0.24412400
H	-4.07712700	-0.33637800	-0.07807500
H	-2.92422500	-1.66798000	-0.08107500
H	-3.06177800	-0.62413300	1.33993900

R63-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393600	0.01912900	0.21624600
C	2.50767100	-0.37369400	-0.44139400
H	3.61461800	0.07695700	1.30107200
H	4.50795600	0.29247900	-0.30012900
H	2.53237300	-0.41673100	-1.53058100
C	1.20658100	-0.78156200	0.18939800
H	1.29137800	-0.72723600	1.28215600
C	0.00586100	0.07208200	-0.28137600
H	-0.03601000	0.02027100	-1.37829900
C	-1.28366200	-0.54535900	0.24668200
H	-1.38109900	-0.44387100	1.33248500
H	-1.38181400	-1.60131600	-0.02458500
O	-2.40657100	0.15928200	-0.35804800
O	-3.55264000	-0.24708400	0.13708900
H	1.00457700	-1.83346800	-0.05955400
C	0.13703600	1.54190200	0.13689500
H	-0.71143700	2.12975600	-0.22170500
H	0.17264800	1.63142600	1.22940800
H	1.05596300	1.97917100	-0.26129600

P63-•CYCCC(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.20318800	-1.05780800	0.61061100
C	-1.23883500	-0.51795300	0.50680900
C	-1.18219100	1.01591200	0.55932300
C	1.16168200	-0.28464600	-0.30413100
H	-2.15082000	1.46373000	0.30887100
H	-1.79758100	-0.86133600	1.38675500
H	0.56494000	-0.94952200	1.64021500
H	0.88076200	-0.43069200	-1.36077200
H	-0.87159200	1.37254600	1.55010800

TS63

O	1.04234500	1.12816400	-0.03453700
O	-0.29508400	1.52933300	-0.42722300
C	2.59264000	-0.62452000	-0.10879100
H	3.35605500	-0.04031900	-0.60802800
H	2.89243700	-1.42782900	0.55286600
H	0.23544500	-2.12519200	0.36282100
C	-1.97002600	-1.00839500	-0.75085900
H	-1.97252900	-2.10176800	-0.80522900
H	-3.01228600	-0.67182700	-0.75015900
H	-1.50166400	-0.62331000	-1.66114000

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.05362600	-1.13597400	0.06728200
C	-2.57808100	-0.98065900	0.11145700
C	-1.36778900	-0.53670700	-0.38508800
H	0.04066500	-2.14355100	-0.36142400
H	-0.07721000	-1.26120200	1.15709400
H	-2.63628200	-1.53425800	1.04323700
H	-3.51348600	-0.69650000	-0.35548000
H	-1.37188700	-0.12439700	-1.39112600
O	-1.14760400	1.19801300	0.39426800
C	1.18596600	-0.31893800	-0.34330900
H	1.20525300	-0.26608100	-1.44104500
C	1.11374600	1.11887700	0.17241800
H	1.93150900	1.72469000	-0.23283800
H	1.14957600	1.15001900	1.26917000
O	-0.07966200	1.76916100	-0.26920700
C	2.47709000	-0.99309900	0.13370200
H	2.55570200	-2.01085400	-0.26135800
H	3.36260700	-0.43800600	-0.19291600
H	2.50784400	-1.05825500	1.22742700

R64-C=CCC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.72490700	-0.18739100	0.13810100
C	2.60479800	-0.51358800	-0.49921900
C	1.33971700	-0.99816400	0.15010500
C	0.09872500	-0.13192000	-0.18763600
H	0.02337700	-0.06662700	-1.28281200
C	-1.14828200	-0.86425500	0.30320600
O	-2.32556200	-0.31172600	-0.35749200
O	-3.42337200	-0.90541100	0.05062400
H	-1.12319300	-1.92895400	0.05166900

H	2.57270100	-0.44286900	-1.58682200
H	3.80253100	-0.24286500	1.22044500
H	4.61103800	0.14163900	-0.39418600
H	1.47509000	-1.04279900	1.23832600
H	-1.29920600	-0.75888000	1.38259700
H	1.14523000	-2.02702300	-0.18460800
C	0.24152900	1.29093100	0.38684200
C	-0.78430400	2.31632800	-0.10808200
H	1.24798100	1.64906500	0.14478100
H	0.20266600	1.22681100	1.48364200
H	-0.55737400	3.30708000	0.29809900
H	-0.76768200	2.39351800	-1.20073100
H	-1.80422800	2.05736000	0.18464400

P64-•CYCCC(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.55024500	-1.00458000	0.69159800
C	-0.81871800	-0.29218900	0.67568300
C	-0.55940600	1.22211500	0.64945900
C	1.51095200	-0.40662500	-0.34413000
H	-1.47502600	1.79479000	0.46826200
H	-1.33728400	-0.52746200	1.61509400
H	1.01403700	-0.89082500	1.67902100
H	0.42985000	-2.07859000	0.50818200
H	1.11725400	-0.56230400	-1.36285600
H	-0.11249500	1.56577400	1.59148500
O	1.59783200	1.02012800	-0.14422200
O	0.29059100	1.57657700	-0.43476600
C	2.89936100	-0.92191200	-0.25243000
H	3.68171700	-0.46533000	-0.84639100
H	3.15474700	-1.72587800	0.42685000
C	-1.71465300	-0.75040300	-0.49251000
C	-3.18438200	-0.34159500	-0.34657400
H	-1.65797800	-1.84331700	-0.56935800
H	-1.31589000	-0.35356600	-1.43308400
H	-3.77943200	-0.71681400	-1.18478200
H	-3.61764100	-0.74484900	0.57577500
H	-3.30964100	0.74586200	-0.32286900

TS64

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.43951200	-1.11335200	0.10863600
C	-2.96702500	-1.10952600	0.02590600
C	-1.76219500	-0.59883400	-0.41569200

H	-0.26638300	-2.11757100	-0.30294400
H	-0.51181800	-1.23083200	1.19710300
H	-3.03879300	-1.65634400	0.96073800
H	-3.89307500	-0.88679000	-0.49041800
H	-1.74035200	-0.19564600	-1.42517300
O	-1.68211300	1.15285700	0.35555800
C	0.77510700	-0.23395500	-0.24850100
H	0.84903900	-0.19154800	-1.34532800
C	0.59159400	1.20249400	0.24637300
H	1.38284000	1.86098300	-0.12398200
H	0.56969900	1.24335300	1.34339500
O	-0.61595500	1.77584100	-0.26080600
C	2.07145600	-0.85911500	0.29697800
H	2.08719400	-1.91700400	0.00599200
H	2.03955800	-0.85060300	1.39510900
C	3.36361700	-0.19103500	-0.18629600
H	3.45582100	0.83949900	0.17033900
H	4.24053400	-0.73787000	0.17342400
H	3.41204200	-0.16927600	-1.28069000

R65-C=CCCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.77075500	-0.49856500	0.29660600
C	-2.75799800	0.05281400	-0.36369400
H	-3.72044300	-0.68680600	1.36564400
H	-4.69258600	-0.78050500	-0.20080500
H	-2.85101200	0.22245600	-1.43647200
C	-1.44897600	0.46940100	0.24559700
H	-1.47168300	0.29119800	1.32760700
C	-0.25360600	-0.27282400	-0.38025300
H	-0.21801900	-0.08026600	-1.45986500
C	1.08646700	0.11366900	0.23807500
H	1.09241200	-0.08905100	1.31455600
O	2.05530700	-0.83268700	-0.34395700
O	3.20355800	-0.80774300	0.28981400
H	-1.31507100	1.55069400	0.10659400
H	-0.39414500	-1.35215000	-0.25696600
C	1.55644700	1.53315600	-0.03898800
H	1.54303300	1.74518500	-1.11287800
H	0.91213500	2.25728800	0.46709300
H	2.57498600	1.65949400	0.33458400

P65-•CYCCCC(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-0.81516100	1.28545300	0.12979500
C	0.69745100	1.28730800	-0.12859500
C	1.32910600	-0.02482100	0.34916700
C	-1.42475500	-0.04284500	-0.33257800
H	1.17483400	2.13740100	0.37164100
H	-1.01730800	1.39933300	1.20175800
H	-1.27900000	-0.15208600	-1.42285600
H	1.24064200	-0.10533800	1.44220600
O	-0.71620900	-1.13034300	0.29187500
O	0.63214500	-1.13029100	-0.23490700
C	-2.85448300	-0.21880400	0.01997100
H	-3.31143800	-1.19732100	-0.06124700
H	-3.45431400	0.61967600	0.35127000
H	-1.30122700	2.12059600	-0.38709400
H	0.89205400	1.39095900	-1.20392600
C	2.78224200	-0.19221700	-0.07310400
H	3.38849000	0.61538600	0.34773100
H	3.17954300	-1.14719900	0.27997000
H	2.87383100	-0.16078700	-1.16312500

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.86793800	1.27157400	-0.18975000
C	-2.90403700	-0.21782600	0.00984500
C	-1.61805000	0.09851900	0.40354400
H	-1.30006300	2.20214400	0.20146200
H	-1.02993200	1.28142000	-1.27392800
H	-3.30898500	0.13937300	-0.93172600
H	-3.50640100	-0.92015400	0.57344400
H	-1.33525900	-0.17009100	1.41864000
O	-0.54090900	-1.29205700	-0.34266500
C	0.63666300	1.25982600	0.12732100
H	1.11274100	2.12784100	-0.34344500
H	0.78374500	1.36650500	1.21037900
C	1.35609300	-0.00692700	-0.33557900
H	1.28149300	-0.10160900	-1.42700600
O	0.70452900	-1.15836200	0.23529800
C	2.80874800	-0.07829500	0.11143600
H	3.26814900	-1.01264400	-0.22142400
H	3.37517300	0.75687800	-0.31067200
H	2.88150700	-0.02754600	1.20230800

R66-C=CCCC(CC)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	4.11741700	-0.21427200	-0.41720600
C	3.09365600	0.22305900	0.30840100
C	1.71598600	0.50949900	-0.21930200
C	0.64329900	-0.36822900	0.45362100
H	0.64772400	-0.19875500	1.53765200
C	-0.76600300	-0.13452800	-0.09035800
O	-1.58805500	-1.22360800	0.46041200
O	-2.45849800	-1.68605400	-0.40827800
H	3.23044500	0.38825400	1.37716600
H	4.02511000	-0.39408700	-1.48489600
H	5.09006600	-0.40674400	0.02283400
H	1.69587300	0.35131800	-1.30439300
H	-0.79736100	-0.27173100	-1.17585900
H	1.48017100	1.56869200	-0.05008300
H	0.89753000	-1.42216500	0.29917700
C	-1.40229800	1.19613100	0.31217900
C	-2.78554500	1.44059000	-0.29671800
H	-0.72076900	1.99999300	0.01021000
H	-1.45729500	1.23071400	1.40755200
H	-3.18499400	2.40327300	0.03593900
H	-2.74028700	1.45477500	-1.39053300
H	-3.49286400	0.66024700	-0.00553700

P66-•CYCCCC(CC)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.45311000	1.20719200	0.22244800
C	0.01741400	1.50531700	-0.10052100
C	0.90079600	0.30422500	0.25173500
C	-1.83981800	-0.17801000	-0.30835800
H	0.12946600	1.71394700	-1.17220300
H	0.35929000	2.39409000	0.44162700
H	-1.61052400	1.21275700	1.30783200
H	-2.11110800	1.96976000	-0.20929700
H	-1.74272800	-0.18848600	-1.40934600
H	0.88746800	0.13499300	1.33899000
O	-0.91096800	-1.15555800	0.19878300
O	0.38077700	-0.86708400	-0.38692400
C	-3.19081100	-0.63627000	0.09712400
H	-3.46986100	-1.67376000	-0.03950000
H	-3.90840200	0.05279400	0.52472600
C	2.34214900	0.43903200	-0.23648800
C	3.25475200	-0.70113000	0.22398400
H	2.72543700	1.40159000	0.12359500
H	2.33204700	0.49708600	-1.33189300

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H	4.27144900	-0.56705200	-0.15732600
H	3.31051200	-0.74372400	1.31723300
H	2.88026300	-1.66500400	-0.12885500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.15214000	1.30400700	-0.11678900
C	-3.35481800	0.05944800	-0.12185900
C	-2.06843700	0.19904900	0.36248700
H	-1.49785300	2.25700200	0.30525500
H	-1.24568400	1.39112500	-1.20559600
H	-3.65476300	0.51174300	-1.06189700
H	-4.06943200	-0.59424100	0.36369100
H	-1.88345500	-0.15432900	1.37402800
O	-1.11224700	-1.26716000	-0.40260000
C	0.32002900	1.10082100	0.27946200
H	0.91139100	1.93493600	-0.11323500
H	0.41340600	1.13196400	1.37343800
C	0.91772800	-0.21518800	-0.21759600
H	0.89870300	-0.24482700	-1.31597400
O	0.10167900	-1.30726500	0.25069500
C	2.32774700	-0.50659800	0.29388200
H	2.57172600	-1.53831900	0.01714300
H	2.32421500	-0.47097800	1.39012800
C	3.39267600	0.44401200	-0.26208400
H	3.22825300	1.47729400	0.05866100
H	4.38808500	0.14888500	0.08209900
H	3.40324700	0.43184200	-1.35751100

R67-C=C(C)CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.01898100	-1.06360200	0.42371800
C	2.21673900	-0.10961100	-0.04718700
H	2.72819400	-2.10947100	0.41816700
H	3.99913700	-0.83580600	0.83059500
C	0.85364600	-0.43853600	-0.61545300
H	0.75320300	-1.52576100	-0.70813400
C	-0.31454100	0.10631700	0.22959000
H	-0.26261100	1.19805800	0.29935000
C	-1.65728900	-0.28120100	-0.36508500
H	-1.81106800	-1.36460200	-0.38715200
O	-2.69732500	0.29035000	0.47917000
O	-3.89536200	-0.00189300	0.02816300
H	0.77361600	-0.02659800	-1.63206000

H	-0.24317700	-0.28346200	1.25103200
H	-1.79958300	0.11692000	-1.37488000
C	2.62176100	1.34248000	-0.05417500
H	2.58883800	1.75444600	-1.07105400
H	1.94533100	1.95676700	0.55211200
H	3.63383500	1.47676800	0.33491100

P67-•CYC(C)CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.02148300	1.33176500	-0.20711000
C	-1.41618800	1.10310500	0.28183000
C	-1.93756000	-0.22728400	-0.25642800
C	0.90429000	0.07250200	-0.03166100
H	-2.06239200	1.92461100	-0.04738400
H	0.00130200	1.57769300	-1.27549000
H	-2.06344200	-0.19816600	-1.34768000
O	0.18992300	-1.05593900	-0.62766800
O	-1.05231100	-1.28107700	0.09470900
C	2.13414000	0.16860200	-0.86868000
H	3.07849900	-0.22778200	-0.51586900
H	2.06600900	0.51078400	-1.89489800
H	0.48071000	2.18066200	0.31013600
H	-1.45401300	1.08322900	1.37665400
H	-2.89177000	-0.50981300	0.20179200
C	1.24801100	-0.23271600	1.42925400
H	1.85593700	-1.14006300	1.48371300
H	1.81564400	0.59444700	1.86690500
H	0.34756000	-0.39531500	2.02256100

TS67

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.13679800	1.32548500	-0.34892700
C	-2.18251700	-0.01664800	-0.84392900
C	-1.09018600	0.18506200	-0.00725800
H	-0.57270600	2.26068500	0.02805200
H	-0.08807400	1.41760800	-1.43928700
H	-2.19602500	0.37382000	-1.85570500
H	-3.00188000	-0.66137000	-0.54755800
O	0.04331200	-1.24425400	-0.61819700
C	1.28595100	1.18583700	0.21983600
H	1.89046200	2.03324400	-0.12392800
H	1.26421600	1.24068800	1.31415300
C	1.97115900	-0.10997700	-0.20030500
H	2.92603900	-0.24601800	0.31802000

H	2.13736200	-0.14552600	-1.28402500
O	1.17921400	-1.24032700	0.17611100
C	-1.23461000	-0.17336800	1.45369000
H	-1.50872000	0.71608600	2.03472100
H	-2.01153400	-0.92763600	1.59676500
H	-0.29735700	-0.56327700	1.85683700

R68-C=C(CC)CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.34931000	1.51560100	-0.47144000
C	1.69899400	0.51162500	0.11617600
H	1.89362800	2.49476100	-0.58157600
H	3.35382100	1.40902400	-0.86350900
C	0.29081900	0.70391600	0.64113600
H	0.06227200	1.77492800	0.67772700
C	-0.78415800	-0.00818800	-0.20414200
H	-0.60157500	-1.08769300	-0.23163700
C	-2.17750400	0.23734300	0.34838500
H	-2.45780300	1.29517400	0.32816400
O	-3.12209600	-0.48085800	-0.49618400
O	-4.35739100	-0.31392800	-0.08352400
H	0.22994000	0.33358700	1.67449900
H	-0.73471600	0.35069900	-1.23801000
H	-2.29734000	-0.14081500	1.36871700
C	2.29054500	-0.86704300	0.31822400
H	2.26043700	-1.09334700	1.39459800
H	1.62348800	-1.61066900	-0.13982400
C	3.71089700	-1.08279800	-0.20468000
H	4.42131600	-0.40109400	0.27317400
H	4.04082500	-2.10556400	-0.00062300
H	3.76817600	-0.92343300	-1.28599000

P68-•CYC(CC)CCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.17354000	0.46534000	1.23668200
C	1.35638700	1.22835500	0.62398500
C	2.24097100	0.25950200	-0.15776100
C	-0.50952100	-0.46901800	0.21333000
H	1.93818600	1.71977300	1.41191200
H	0.54208700	-0.16261900	2.05675800
H	2.74035800	-0.45468600	0.51176600
O	0.54076100	-1.29408100	-0.39071100
O	1.47153100	-0.44563400	-1.12086300
C	-1.36106400	-1.48269600	0.90004300

TS68

H	-2.18038900	-1.95799400	0.37327600
H	-1.07987000	-1.87103800	1.87206000
H	-0.55617000	1.15575600	1.67004800
H	1.00260200	2.01473300	-0.05241200
H	3.00188800	0.78152600	-0.74846300
C	-1.29028600	0.24949000	-0.90460900
H	-1.67352100	-0.53149500	-1.57143900
H	-0.58939300	0.83828900	-1.50049800
C	-2.44428500	1.13194400	-0.41782000
H	-2.08787000	1.99070500	0.15984600
H	-3.00925500	1.52417500	-1.26886500
H	-3.14143400	0.57309900	0.21550400

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.64042100	1.41101200	-0.36268600
C	1.42466000	1.32765800	1.01887300
C	0.62798500	0.68273100	0.07838200
H	-0.36681600	2.13107300	-1.14571000
H	-1.00831600	1.99703300	0.48643700
H	1.01796900	2.12040900	1.63706200
H	2.42890700	0.99383200	1.24390400
O	-0.22268800	-0.60461900	1.22931800
C	-1.77728100	0.52078300	-0.89548100
H	-2.64669400	1.15263400	-1.11172500
H	-1.48693500	0.05585000	-1.84404000
C	-2.19205100	-0.56850700	0.08732800
H	-2.90967400	-1.26281000	-0.36211100
H	-2.62108400	-0.14452900	1.00352800
O	-1.06605100	-1.37551300	0.44214000
C	1.26047600	-0.24406400	-0.94482500
H	1.46855800	0.34842100	-1.84769500
H	0.51231500	-0.98692300	-1.23520900
C	2.52662900	-0.97321000	-0.49082400
H	2.83632100	-1.69819100	-1.24928100
H	3.36650700	-0.28997600	-0.33207300
H	2.33887300	-1.51419000	0.44064700

R69-(cis)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.09133200	0.32741800	0.27852900
C	1.94403300	0.92055200	-0.05449700
H	3.86711000	0.95386800	0.71666900
C	0.72028000	0.29337400	-0.66281700

H	0.89186800	-0.76308700	-0.89231900
C	-0.51411300	0.42785500	0.24929700
H	-0.68892900	1.48360400	0.48756100
C	-1.76018100	-0.14717000	-0.40110400
H	-1.67444000	-1.22008200	-0.59992200
O	-2.86982500	0.03713100	0.52399800
O	-3.98893500	-0.44240300	0.03225100
H	0.50277700	0.78532400	-1.62204500
H	-0.32926700	-0.08431600	1.19980100
H	-2.02137600	0.36519900	-1.33253400
H	1.85302100	1.98905000	0.13882600
C	3.46950300	-1.11671000	0.12234300
H	3.74790900	-1.55097900	1.09050300
H	2.66863300	-1.72753200	-0.29994600
H	4.34765000	-1.22078600	-0.52708900

P69-CC•YCCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.48026100	1.37423700	0.11048400
C	1.89693000	0.92510000	-0.27404700
C	2.14422300	-0.50217200	0.21685100
C	-0.53363000	0.27961300	-0.23238500
H	2.64944900	1.60362100	0.14293300
H	0.42513700	1.56335100	1.18996000
H	2.19411200	-0.54703200	1.31350900
O	-0.11143000	-0.96174900	0.38813700
O	1.12552300	-1.37674800	-0.25090300
C	-1.91188800	0.53665800	0.26190800
H	-2.07015300	1.35504700	0.95752400
H	0.21282700	2.30607200	-0.40007100
H	2.00894000	0.94406300	-1.36488800
H	3.06953800	-0.92024800	-0.19472600
H	-0.54065100	0.09836300	-1.31994400
C	-3.06409400	-0.30130500	-0.17212600
H	-3.81211300	-0.40523800	0.62098300
H	-3.58683700	0.13869600	-1.03806600
H	-2.73380100	-1.30150500	-0.46919800

TS69

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.02318300	1.24670500	-0.00930500
C	1.99501300	-0.30457100	-0.53548000
C	0.66677300	0.05804500	-0.69148400
H	0.41695200	2.17330400	-0.44859000

H	0.29869700	1.25688600	1.05036700
H	0.21248800	-0.21964300	-1.63918800
O	-0.29982900	-1.31214200	0.24991200
C	-1.50918100	1.24110800	-0.14430700
H	-1.92677600	2.12304900	0.35521400
H	-1.78458000	1.31426400	-1.20401900
C	-2.15279300	-0.00924600	0.44796700
H	-3.22688200	-0.04349200	0.23695800
H	-1.99586000	-0.06244700	1.53286500
O	-1.62092100	-1.19168700	-0.15212700
H	2.39121900	-1.04138900	-1.22988800
C	2.89749400	0.09550600	0.58497900
H	3.88170600	0.39796000	0.20544300
H	2.49730200	0.91812200	1.18124600
H	3.07880100	-0.75126300	1.26309000

R70-(trans)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.92671400	0.14955200	0.39227800
C	-1.89216700	0.14419200	-0.44519400
C	-0.55620500	0.77713800	-0.17699900
H	-0.58162800	1.30008800	0.78674700
C	0.59407700	-0.24703000	-0.18284500
H	0.61321500	-0.78161700	-1.13995300
C	1.94134500	0.41711500	0.04114000
H	2.01038200	0.91076900	1.01553900
O	2.96064400	-0.62265900	0.00631900
O	4.15930700	-0.12635000	0.20891700
H	-0.34939600	1.54097100	-0.94105100
H	0.42397400	-0.99843100	0.59597000
H	2.18630800	1.14266400	-0.74114200
H	-1.99258100	-0.36129600	-1.40671800
H	-2.81993800	0.65527400	1.35258900
C	-4.25980000	-0.48498700	0.12990100
H	-4.28836200	-0.97161700	-0.84933900
H	-4.49784700	-1.23803100	0.89145800
H	-5.06694600	0.25740800	0.16432000

P70-CC•YCCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.48026100	1.37423700	0.11048400
C	1.89693000	0.92510000	-0.27404700
C	2.14422300	-0.50217200	0.21685100
C	-0.53363000	0.27961300	-0.23238500

H	2.64944900	1.60362100	0.14293300
H	0.42513700	1.56335100	1.18996000
H	2.19411200	-0.54703200	1.31350900
O	-0.11143000	-0.96174900	0.38813700
O	1.12552300	-1.37674800	-0.25090300
C	-1.91188800	0.53665800	0.26190800
H	-2.07015300	1.35504700	0.95752400
H	0.21282700	2.30607200	-0.40007100
H	2.00894000	0.94406300	-1.36488800
H	3.06953800	-0.92024800	-0.19472600
H	-0.54065100	0.09836300	-1.31994400
C	-3.06409400	-0.30130500	-0.17212600
H	-3.81211300	-0.40523800	0.62098300
H	-3.58683700	0.13869600	-1.03806600
H	-2.73380100	-1.30150500	-0.46919800

TS70

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.38183600	1.40203100	-0.18314400
C	-1.95604200	0.43494900	-0.31097400
C	-0.69432500	0.43158100	0.25295000
H	0.14334600	2.40033800	0.20763000
H	0.36534200	1.48027700	-1.27666900
H	-2.09377400	0.93062200	-1.27074200
H	-0.61644400	0.07230800	1.27713400
O	0.10422200	-1.18083200	-0.43870600
C	1.78778300	1.00817900	0.30089800
H	2.51902200	1.73988900	-0.06201600
H	1.81943300	1.04382300	1.39719400
C	2.21354200	-0.38351800	-0.15544400
H	3.16520600	-0.67787500	0.29961600
H	2.30158000	-0.43913500	-1.24768400
O	1.27373200	-1.36739900	0.28088600
C	-3.11911600	-0.32356500	0.23418400
H	-4.00178400	0.32060600	0.34357800
H	-3.41478000	-1.13623200	-0.44400700
H	-2.89284200	-0.76671400	1.20771600

R71-(cis)-CCC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.46997800	0.78037800	-0.33686200
C	-1.29912000	1.16853600	0.17088400
H	-3.16972800	1.56284800	-0.63153100
C	-0.16292600	0.30589800	0.64720000

H	-0.43051500	-0.75491800	0.61093700
C	1.12315700	0.54016800	-0.16821400
H	1.39142400	1.60294900	-0.14487600
C	2.28547600	-0.27791700	0.36677400
H	2.10377800	-1.35569700	0.30770200
O	3.45067600	0.01309700	-0.45706200
O	4.50236500	-0.66322400	-0.05616100
H	0.04472700	0.53618300	1.70239300
H	0.94794100	0.28141400	-1.21814000
H	2.54079400	-0.01852100	1.39917900
H	-1.11066600	2.23934400	0.24585600
C	-2.98605800	-0.61658500	-0.54195600
H	-3.19741700	-0.76196600	-1.61068100
H	-2.22890900	-1.36106500	-0.27712000
C	-4.27448200	-0.88588100	0.25398900
H	-5.05744500	-0.16685400	-0.00940500
H	-4.65939800	-1.88977600	0.05038400
H	-4.09531900	-0.80050800	1.33018400

P71-CCC•YCCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.92369300	1.36859600	-0.10967300
C	-2.36365500	1.00060600	0.27437200
C	-2.69005000	-0.40991000	-0.21782400
C	0.02944100	0.22090900	0.23746700
H	-3.07596200	1.72100500	-0.14303100
H	-0.85858500	1.55123900	-1.18973200
H	-2.73828000	-0.45158900	-1.31474900
O	-0.46157800	-0.99892700	-0.37868300
O	-1.72457600	-1.34069500	0.25378800
C	1.41779100	0.40152500	-0.26202500
H	1.57773900	1.06817500	-1.10663700
H	-0.60481100	2.28575700	0.39751400
H	-2.47526700	1.02517600	1.36513800
H	-3.63908300	-0.77511800	0.19014900
H	0.03438200	0.04554000	1.32465400
C	2.53486500	-0.48538900	0.17249600
H	2.36990300	-0.80185200	1.21132900
H	2.50827300	-1.41976400	-0.41452400
C	3.92184900	0.15519100	0.02557200
H	4.01047800	1.05282700	0.64572200
H	4.71047700	-0.54191600	0.32383100
H	4.11068800	0.44831500	-1.01280600

TS71

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.44972000	1.23101800	0.01930300
C	-1.46534700	-0.38212000	0.56547200
C	-0.14907100	0.02408000	0.71049400
H	0.03269700	2.14558400	0.46268400
H	0.16117300	1.23102500	-1.03682900
H	0.32492900	-0.24013700	1.65248700
O	0.84854000	-1.31739800	-0.24610400
C	1.98289600	1.27220900	0.13575900
H	2.36737400	2.16778500	-0.36605700
H	2.26908200	1.35035000	1.19224600
C	2.65646500	0.04373300	-0.46893600
H	3.73409400	0.04249900	-0.27385900
H	2.48507000	-0.01181300	-1.55153900
O	2.17086100	-1.15623800	0.13572600
H	-1.83173900	-1.13522200	1.26054600
C	-2.39098100	-0.01945400	-0.55315800
H	-2.06802000	0.90661800	-1.04005700
H	-2.33302100	-0.80063000	-1.32916600
C	-3.85298300	0.11331500	-0.09909300
H	-4.50785300	0.33654500	-0.94653000
H	-4.20659400	-0.81490800	0.36224300
H	-3.96660000	0.91470400	0.63780100

R72-(trans)-CCC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.34798700	-0.75741000	-0.32581100
C	-1.37793700	-0.19707400	0.39367400
C	0.01178100	-0.75148200	0.54014500
H	0.08227800	-1.71677200	0.02428000
C	1.08775200	0.20749000	-0.00309300
H	1.00864000	1.17949900	0.49802300
C	2.48859400	-0.34265900	0.20006400
H	2.65294800	-1.28348900	-0.33461900
O	3.43066800	0.63188000	-0.33311100
O	4.67115500	0.22221600	-0.20090300
H	0.22154700	-0.94810100	1.60186800
H	0.91756800	0.38670000	-1.07033100
H	2.73225100	-0.48955300	1.25714200
H	-1.56586600	0.73804400	0.91913500
H	-2.13160800	-1.69324300	-0.84309200
C	-3.74999700	-0.24366600	-0.51439700
H	-3.93729000	-0.13901200	-1.59312400

H	-4.45236900	-1.02368000	-0.18575500
C	-4.08318100	1.07194400	0.19040100
H	-3.96359700	0.98569900	1.27527500
H	-3.43491400	1.88427500	-0.15390000
H	-5.11830900	1.36401600	-0.00868100

P72-CCC•YCCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.92369300	1.36859600	-0.10967300
C	-2.36365500	1.00060600	0.27437200
C	-2.69005000	-0.40991000	-0.21782400
C	0.02944100	0.22090900	0.23746700
H	-3.07596200	1.72100500	-0.14303100
H	-0.85858500	1.55123900	-1.18973200
H	-2.73828000	-0.45158900	-1.31474900
O	-0.46157800	-0.99892700	-0.37868300
O	-1.72457600	-1.34069500	0.25378800
C	1.41779100	0.40152500	-0.26202500
H	1.57773900	1.06817500	-1.10663700
H	-0.60481100	2.28575700	0.39751400
H	-2.47526700	1.02517600	1.36513800
H	-3.63908300	-0.77511800	0.19014900
H	0.03438200	0.04554000	1.32465400
C	2.53486500	-0.48538900	0.17249600
H	2.36990300	-0.80185200	1.21132900
H	2.50827300	-1.41976400	-0.41452400
C	3.92184900	0.15519100	0.02557200
H	4.01047800	1.05282700	0.64572200
H	4.71047700	-0.54191600	0.32383100
H	4.11068800	0.44831500	-1.01280600

TS72

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.06351500	1.40647700	0.28776500
C	1.42602600	0.91823000	0.20726000
C	0.15195400	0.71536200	-0.28951400
H	-1.05525600	2.46116400	-0.01860700
H	-0.99138700	1.39607000	1.38168300
H	1.53352200	1.33457400	1.20866000
H	0.07626300	0.43471600	-1.33832600
O	-0.26158300	-1.07714700	0.29178400
C	-2.39057100	0.77350100	-0.16491600
H	-3.22870700	1.30781000	0.29745600
H	-2.49881600	0.89069800	-1.25057100

C	-2.50061400	-0.70843000	0.18004500
H	-3.40143800	-1.15275300	-0.25643500
H	-2.50750400	-0.86909800	1.26540200
O	-1.41397400	-1.44366000	-0.38665300
C	2.67037800	0.42299200	-0.45708500
H	3.42431400	1.22272700	-0.47245100
H	2.45614100	0.16823800	-1.50110900
C	3.26581500	-0.80822300	0.25798600
H	2.54412600	-1.62895500	0.25863700
H	4.18008600	-1.14176400	-0.24311900
H	3.51628000	-0.57643000	1.29848900

6.2 The optimized geometries of all the reactions at B3LYP/6-31G(2df,p) level for intramolecular H-shift reactions of alkenyl peroxy radicals(TS_n is the transition state of the reaction R_n)

R1-C=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600
H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100
C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

P1-C=CC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.10484100	-0.15441600	-0.19167600
C	-1.83811200	0.38719900	-0.10338000
H	-3.29482700	-1.18663400	0.08363000
H	-3.94767200	0.42969200	-0.53993600
H	-1.71210000	1.43032500	-0.39254300
C	-0.71037300	-0.28775000	0.33227100
H	-0.78701300	-1.33537200	0.61310700
C	0.63692700	0.33617700	0.45425200
H	1.00651900	0.29597400	1.48953500

TS1

H	0.62347600	1.38902900	0.13707300
O	1.52471800	-0.42509800	-0.36941600
O	2.86650000	0.02264500	-0.06394500
H	3.08027100	0.50934900	-0.87278000

R2-C=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.30140500	-0.77481700	0.16347100
C	0.65971500	0.18943600	1.00833000
C	-0.27114100	0.98309000	0.07807400
H	0.15139300	-0.37764900	1.79338100
H	1.40148000	0.86486300	1.45012800
H	-0.22275300	2.06726000	0.17883100
O	1.65254200	-0.03915200	-0.96422800
H	0.61788400	0.69555800	-0.88810100
C	-1.97709800	-0.82356000	-0.07626900
H	-2.96547600	-1.14951500	-0.37918600
H	-1.32622500	-1.57543300	0.35583200
C	-1.57965100	0.45603900	-0.24467300
H	-2.27882600	1.15664700	-0.69760000

P2-C=CC•C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.04555100	0.12476000	0.13592000
C	1.96013500	-0.39298900	-0.43011200
H	3.08603900	0.34352300	1.19929100
H	3.93983200	0.34291100	-0.43787900
H	1.96473200	-0.59864500	-1.50046700
C	0.68725200	-0.73697800	0.29058600
H	0.47162100	-1.80720800	0.17379000
H	0.79227500	-0.54311700	1.36385100
C	-0.51633400	0.03922700	-0.25228400
H	-0.62376300	-0.11705900	-1.33097300
O	-1.69106900	-0.60382300	0.35785600
O	-2.80695800	-0.22447000	-0.21852700
C	-0.52312600	1.52213300	0.07881600
H	-0.45860600	1.67507900	1.16079600
H	0.33373800	2.01257500	-0.39047400
H	-1.44251000	1.98136800	-0.29011900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.23938700	-0.36426600	-0.14242500
C	-1.98502200	0.20948500	-0.06619700

TS2

H	-3.38907200	-1.41800800	0.06907300
H	-4.11168700	0.21592400	-0.41698900
H	-1.90718500	1.27144400	-0.28899300
C	-0.82996200	-0.46952200	0.28114100
H	-0.89100500	-1.53362800	0.49724300
C	0.54257200	0.11596800	0.40735300
H	0.87683800	0.02196800	1.45333900
O	1.36970700	-0.77078000	-0.37036700
O	2.74502600	-0.54265500	0.02724100
H	3.10891100	-0.18621400	-0.79487900
C	0.70236300	1.56615500	-0.03724500
H	0.37812100	1.69702900	-1.07403500
H	0.12083300	2.23803700	0.60103200
H	1.75300600	1.85402100	0.04345400

R3-C=C(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	0.75585100	1.00842200	-0.63043000
C	0.59958700	-0.41900400	-0.45686600
C	-0.39003200	-0.54297600	0.72010600
H	0.17215700	-0.76290000	-1.40503600
H	-0.10587200	-1.25662200	1.49401300
O	0.89385000	1.49445600	0.66822100
H	0.09570300	0.62923100	1.14667800
C	-2.39410200	0.07745100	-0.62316800
H	-3.47247300	0.14777700	-0.70796600
H	-1.81265900	0.45349600	-1.45723700
C	1.93024900	-1.10872400	-0.17597900
H	1.78824700	-2.18732900	-0.05761100
H	2.62434300	-0.94024000	-1.00343500
H	2.37335000	-0.70858200	0.73940100
C	-1.81278900	-0.44215600	0.47962600
H	-2.45787900	-0.78539400	1.28654700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.02080000	1.43505500	0.28599900
C	-1.36480300	0.17064600	0.04660700
H	-0.00227600	1.73792900	0.49635900
H	-1.76027000	2.22885400	0.26052100
C	-2.78209900	-0.22174900	-0.28300700
H	-2.83724200	-0.71168800	-1.26370500
H	-3.17536700	-0.94195500	0.44609800
H	-3.44648300	0.64524300	-0.29935100

P3-C=C(C)C•COO

C	-0.39203100	-0.98927300	0.07160000
H	-0.78845200	-1.77006200	0.73610200
H	-0.35600700	-1.45582800	-0.92336800
C	1.02766000	-0.69789800	0.52244200
H	1.60331600	-1.61839300	0.65436500
H	1.06868400	-0.11431500	1.44578400
O	1.69560200	0.07474700	-0.51836600
O	2.91521400	0.40269400	-0.15846500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.76072000	-0.45119000	0.37669300
C	-1.50724800	-0.02566000	-0.01382900
H	-2.97527300	-1.50475900	0.52104400
H	-3.56952500	0.24813100	0.55333900
C	-0.48125000	-0.95099700	-0.22849500
H	-0.69379800	-2.00246300	-0.06041900
C	0.91268500	-0.58133100	-0.61606400
H	0.93596600	0.19500800	-1.39165600
O	1.55512000	-0.06483800	0.56290600
O	2.86861100	0.39474100	0.15827600
H	3.42631000	-0.29276000	0.54960300
H	1.46888800	-1.45254400	-0.98515800
C	-1.24214500	1.45347000	-0.21062200
H	-1.07144700	1.68594200	-1.26834100
H	-2.08936000	2.05386300	0.12798900
H	-0.34954000	1.76460700	0.33804100

TS3

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-1.92379300	0.48772200	-0.17262500
C	-1.17574400	0.13716000	0.99948200
C	0.05760100	-0.61833800	0.48366800
H	-0.95935700	1.07456600	1.51961300
H	-1.76597800	-0.52398800	1.64482700
H	0.27255500	-1.55860500	0.99342400
O	-1.89156600	-0.67372700	-0.94146300
H	-0.72418100	-0.97588400	-0.55266900
C	1.18967600	1.42702900	-0.28225200
H	2.06909200	1.94343300	-0.65122500
H	0.28129300	2.01075700	-0.19598400
C	1.23135700	0.11081700	0.03201900
C	2.50537100	-0.68551900	-0.12525700
H	2.35848200	-1.52462000	-0.81504500

H	3.32145500	-0.06946700	-0.50938400
H	2.81994800	-1.11504000	0.83319100

R4-(cis)-CC=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.44545000	0.40357200	-0.26473500
C	-1.26639800	0.94827300	0.03924300
H	-3.19585100	1.05813000	-0.70576800
H	-1.12578500	2.00609800	-0.17936600
C	-2.89161000	-1.01525800	-0.06752800
H	-2.11964700	-1.65306700	0.36828700
H	-3.77066200	-1.05714400	0.58738600
H	-3.19618100	-1.46086600	-1.02250900
C	-0.07029400	0.27028700	0.65047200
H	-0.29225600	-0.75924000	0.94279400
H	0.23313100	0.80184600	1.56205800
C	1.11066900	0.27214600	-0.31462600
H	1.38676700	1.28182600	-0.63403300
H	0.92669200	-0.34335600	-1.19938000
O	2.25418500	-0.29279400	0.38898400
O	3.31235100	-0.35074900	-0.38603700

P4-CC=CC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.53504700	0.51473200	-0.23231900
C	1.18658700	0.79680800	-0.07346600
H	3.17800500	1.32546100	-0.56537200
H	0.88167200	1.81996400	-0.29107500
C	0.18479700	-0.06565600	0.33527000
H	0.40386100	-1.10711000	0.55074200
C	-1.23666500	0.35256300	0.49667600
H	-1.36942600	1.42334300	0.29567900
O	-2.00795200	-0.41900700	-0.43134900
O	-3.39825700	-0.08721500	-0.19886800
H	-3.71110500	-0.90785200	0.20777900
C	3.20654500	-0.79993200	0.00015300
H	3.67492400	-1.16948000	-0.92204800
H	4.01629300	-0.70198800	0.73547800
H	2.52139000	-1.57105100	0.35799900
H	-1.60380400	0.14739900	1.51468200

TS4

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.46559500	-0.89654100	0.18963500

C	1.01841600	0.19461000	0.99984900
C	0.31341800	1.18687200	0.05057800
H	0.37977700	-0.23500900	1.77592800
H	1.87682900	0.70012000	1.45825500
O	1.92274300	-0.28752300	-0.98082300
H	1.03717600	0.64215800	-0.91968700
C	-2.00918400	0.16573300	-0.16023900
H	-3.05094100	0.43457700	-0.32878500
C	-1.11994000	1.19096800	-0.16917700
H	-1.53532800	2.17007200	-0.40245000
C	-1.76267700	-1.29787600	0.02221800
H	-0.70575300	-1.55501100	0.08924400
H	-2.28768600	-1.67297000	0.91119600
H	-2.18555400	-1.84823700	-0.82862900
H	0.72458600	2.19496900	0.11505700

R5-(trans)-CC=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.18039800	0.25134600	0.16956800
C	0.96255100	0.11084000	-0.34894500
H	2.42759200	1.18040000	0.68494900
H	0.70499300	-0.81239600	-0.86581600
C	3.27398900	-0.77212300	0.10336900
H	2.94976000	-1.67374300	-0.42398500
H	4.15778100	-0.37517800	-0.41150500
H	3.60471500	-1.06464700	1.10769900
C	-0.12554600	1.14631900	-0.27553400
H	0.23107500	2.03511100	0.25701400
H	-0.41235000	1.47438200	-1.28398100
C	-1.38506000	0.65537800	0.43175200
H	-2.13953800	1.44216900	0.52684700
H	-1.17373400	0.23086700	1.41680000
O	-1.96498300	-0.40359600	-0.38523800
O	-3.00855400	-0.94484300	0.19907800

P5-CC=CC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.53504700	0.51473200	-0.23231900
C	1.18658700	0.79680800	-0.07346600
H	3.17800500	1.32546100	-0.56537200
H	0.88167200	1.81996400	-0.29107500
C	0.18479700	-0.06565600	0.33527000
H	0.40386100	-1.10711000	0.55074200
C	-1.23666500	0.35256300	0.49667600

TS5

H	-1.36942600	1.42334300	0.29567900
O	-2.00795200	-0.41900700	-0.43134900
O	-3.39825700	-0.08721500	-0.19886800
H	-3.71110500	-0.90785200	0.20777900
C	3.20654500	-0.79993200	0.00015300
H	3.67492400	-1.16948000	-0.92204800
H	4.01629300	-0.70198800	0.73547800
H	2.52139000	-1.57105100	0.35799900
H	-1.60380400	0.14739900	1.51468200

R6-C=CC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.64248000	-0.92684800	0.29242900
C	1.31556200	0.30611800	0.94103100
C	0.51349800	1.10762600	-0.09890900
H	0.76122400	0.04339800	1.84702800
H	2.22761100	0.85552700	1.20275800
O	2.06438100	-0.52574400	-0.97555100
H	1.22454300	0.44584000	-1.01240100
C	-1.56579300	-0.24244600	0.15890800
C	-0.90366600	0.86363600	-0.25431100
H	-1.46969400	1.62457000	-0.79089100
H	0.81256200	2.14956700	-0.21470600
H	-1.01440700	-1.02113900	0.68107600
C	-3.02150500	-0.49387100	-0.06284700
H	-3.54815500	-0.64417900	0.88845200
H	-3.50163500	0.33257400	-0.59437000
H	-3.17551400	-1.41180200	-0.64519900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.78976800	-0.87830700	-0.25783400
C	-1.81144100	-0.26221300	0.39677200
H	-2.74671500	-1.03847300	-1.33161100
H	-3.67567000	-1.24358600	0.25052800
H	-1.89685600	-0.11737400	1.47429100
C	-0.55327200	0.28307600	-0.22912200
H	-0.60004800	0.11282700	-1.31184700
C	0.64786500	-0.49848900	0.30635600
H	0.80636500	-0.33704200	1.37753600
H	0.55807800	-1.57090800	0.11287900
O	1.83960200	-0.02719700	-0.38748900
O	2.92589200	-0.59023000	0.08852600
C	-0.40386100	1.79224700	0.03476700

P6-C=CC•(C)COO

H	-0.38604900	1.99948200	1.11101100
H	0.52363700	2.17518300	-0.39797300
H	-1.24382900	2.34141600	-0.39875300

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.95689400	-0.53099600	-0.24198800
C	1.63329900	-0.79123000	0.03721500
H	3.33703300	0.47570300	-0.36997400
H	3.67131200	-1.33880600	-0.34330700
H	1.35289300	-1.83659600	0.15915500
C	0.60542300	0.13688200	0.19480400
C	-0.76824900	-0.33235800	0.56889800
H	-1.14333700	0.20237200	1.45590600
H	-0.78841700	-1.40797600	0.78059500
C	0.78872000	1.61957400	0.04568300
H	0.94736400	2.10117800	1.02183900
H	1.64188000	1.87318200	-0.58732400
H	-0.10598700	2.07117900	-0.39310400
O	-1.62954000	-0.03936300	-0.53860200
O	-2.97661500	-0.36905400	-0.12499800
H	-3.36002100	0.51587100	-0.04266300

TS6

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.53931100	-0.79693500	0.23370900
C	0.69902900	0.08334800	0.98038100
C	-0.38526600	0.54950500	-0.01787100
H	0.32066200	-0.48809500	1.83352100
H	1.26918600	0.95248300	1.33059900
O	1.74021000	-0.10871900	-0.96381300
H	0.54025800	0.36630700	-0.95204600
C	-1.51815500	-1.68319500	0.01191400
H	-2.36576800	-2.29773200	-0.26975400
H	-0.70815700	-2.17955600	0.53337400
C	-1.47988200	-0.37241800	-0.29449200
H	-2.32491400	0.05324700	-0.83451300
C	-0.73122100	2.02435100	0.00951100
H	-1.24441600	2.29795300	0.94192300
H	0.16912800	2.64224900	-0.06284500
H	-1.39917400	2.28882900	-0.81608700

R7-C=CC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-2.90555900	-0.96146300	-0.42145300
C	-1.93761800	-0.49734600	0.36131000
H	-2.81087800	-0.97192200	-1.50376100
H	-3.83399000	-1.34656400	-0.01338700
H	-2.07745400	-0.50189800	1.44285700
C	-0.62144700	0.06635900	-0.11803400
H	-0.61624900	0.05094200	-1.21577100
C	0.49499100	-0.86877100	0.35845000
H	0.69688900	-0.76558100	1.42969500
H	0.26174500	-1.91377900	0.13803000
O	1.72867300	-0.55341200	-0.35255600
O	2.71026800	-1.33705200	0.03030400
C	-0.46480500	1.52680100	0.36708600
H	-0.38790900	1.52473300	1.46318500
H	-1.39950100	2.04939900	0.13306400
C	0.70808400	2.30915300	-0.23405100
H	1.67434400	1.88284500	0.04298300
H	0.65529600	2.31900200	-1.32804700
H	0.68429800	3.34813700	0.10931500

P7-C=CC•(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.79259800	-0.98902900	-0.28876000
C	1.44239400	-1.22225500	-0.14914400
H	3.45173600	-1.75632900	-0.67619500
H	3.24885000	-0.04351100	-0.01957200
H	1.07935400	-2.20563700	-0.44468200
C	0.48307700	-0.33310600	0.33717700
C	-0.94231800	-0.77962100	0.45727300
H	-1.06420600	-1.83706600	0.19391500
H	-1.31502000	-0.63324900	1.48373300
O	-1.72351300	0.03238200	-0.42969400
O	-3.10870300	-0.33528700	-0.22944700
H	-3.43508900	0.44369600	0.24358400
C	0.80663600	1.08077800	0.74410100
C	0.81542200	2.07175500	-0.43885000
H	1.78173700	1.11062700	1.24467800
H	0.06937500	1.41888600	1.48204400
H	1.04902000	3.08347500	-0.09165300
H	1.56451300	1.78330200	-1.18183100
H	-0.15938800	2.08791400	-0.93167400

TS7

Cartesian Coordinates (Å)			
At.	X	Y	Z

O	0.89694800	1.68459500	0.20609000
C	0.27795700	0.68418600	1.01679300
C	-0.06207400	-0.47125600	0.04726600
H	0.99959500	0.41984400	1.79582800
H	-0.63893500	1.07315400	1.47347300
O	0.07781500	1.73957200	-0.92257300
H	-0.14112700	0.46611200	-0.88979100
C	2.34795400	-1.13761600	-0.11259700
H	3.09243800	-1.84782300	-0.45444400
H	2.71633500	-0.24447600	0.37829900
C	1.03464900	-1.36110700	-0.31334700
H	0.74475000	-2.27578400	-0.82939800
C	-1.43569600	-1.11442800	0.19128700
H	-1.54282100	-1.49519400	1.21901500
H	-1.47697100	-2.00044200	-0.45304100
C	-2.62246500	-0.19830500	-0.13588400
H	-2.57987800	0.14319600	-1.17449500
H	-3.56618200	-0.73300400	0.00662100
H	-2.64726400	0.69224400	0.49868200

R8-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000
C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100
H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900
H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

P8-C=CC•(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	3.08720900	0.29908600	-0.34777000
C	1.76972600	0.64213300	-0.14034800
H	3.44026000	-0.72254200	-0.26988100
H	3.82336700	1.05157700	-0.60342200
C	0.73328700	-0.22776300	0.19713600
C	-0.68452500	0.24722700	0.39718800
O	-1.43870900	-0.46776000	-0.60646200
O	-2.84357000	-0.36797600	-0.26531500
H	-3.01864300	-1.27539400	0.02145700
H	-1.03479600	-0.11587300	1.37796200
H	1.51718500	1.69297500	-0.24949200
C	0.96306800	-1.70470300	0.36765100
H	1.06720400	-2.21067100	-0.60083100
H	1.87594300	-1.90906400	0.93763000
H	0.12506500	-2.17783300	0.88592600
C	-0.94650500	1.74459900	0.30005000
H	-2.01428000	1.92714400	0.43583900
H	-0.40131300	2.29060900	1.07586800
H	-0.65532600	2.13148200	-0.68028200

TS8

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.54528500	-0.28946800	-0.52404100
C	0.79899500	0.34270700	0.51900600
C	-0.63306000	0.50522900	-0.08660000
H	1.18992100	1.36083800	0.65432500
O	1.20356100	0.45657400	-1.65737300
H	-0.01414700	0.62862800	-1.24216800
C	-1.13383300	-1.94782100	-0.35859800
H	-1.87614700	-2.72852500	-0.48341600
H	-0.09319500	-2.24673200	-0.38901800
C	-1.50625000	-0.66261200	-0.20658000
H	-2.57294700	-0.44020500	-0.22713100
C	-1.32662900	1.80580400	0.26527700
H	-2.25196200	1.92891000	-0.30548600
H	-1.59665400	1.84050500	1.33040200
H	-0.68132100	2.66625700	0.06423400
C	0.95379700	-0.44945900	1.80644000
H	2.01163900	-0.51701500	2.07637200
H	0.43026400	0.06483100	2.61809300
H	0.54566200	-1.45742800	1.72143500

R9-C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

P9-C=CCC•COO

C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800
C	0.02912800	0.36494300	-0.07789300
H	0.13282400	0.90845700	0.86749900
H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.12743900	0.71131100	0.21250300
C	-1.84387500	0.57981700	-0.10636600
H	-3.82310900	-0.12046700	0.14014700
H	-3.53711700	1.65620800	0.55369700
H	-1.16526900	1.42472000	-0.01332900
C	-1.19710800	-0.70709700	-0.57622600
H	-1.97292900	-1.47847000	-0.67200400
H	-0.76472700	-0.55400400	-1.57449900
C	-0.12371100	-1.16105500	0.36467800
H	-0.41911400	-1.50683000	1.35050300
C	1.31271500	-0.88767200	0.09893700
H	1.59065600	-1.18076800	-0.92583700
H	1.97228800	-1.40992400	0.80114800
O	1.50380300	0.53491900	0.23410000
O	2.89422200	0.80777500	-0.06888800
H	2.81162200	1.21617100	-0.94266900

TS9

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.16571000	0.08836200	-0.58534400
C	1.59754000	-0.96233300	0.19793200
C	0.22311000	-0.42288800	0.60811900
H	1.56554900	-1.84831300	-0.44683600
H	2.20930900	-1.16391100	1.08578900
H	-0.11155400	-0.65070000	1.62072300

O	1.89900400	1.23420400	0.19671600
H	0.84249800	0.80527800	0.61798000
C	-0.86139000	-0.42179400	-0.44480700
H	-1.22576500	-1.45224300	-0.58509100
H	-0.41065600	-0.11898700	-1.40013500
C	-2.01768500	0.47793300	-0.10578800
C	-3.27333000	0.07928000	0.06721600
H	-1.76860500	1.53261200	0.00401200
H	-4.06623300	0.77809100	0.31113300
H	-3.56172800	-0.96353400	-0.03457200

R10-C=CC(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.25621700	-1.07567800	0.32724700
C	-2.35204300	-0.39232300	-0.36581700
H	-3.18023300	-1.19384000	1.40483800
H	-4.10963800	-1.54453300	-0.15092800
H	-2.46689200	-0.29680000	-1.44644600
C	-1.14112700	0.29319000	0.21281600
H	-1.14509500	0.12775900	1.29870700
C	0.14294500	-0.34548600	-0.36417100
H	0.10418100	-1.42885400	-0.20696000
H	0.18144300	-0.18421200	-1.44872800
C	1.42019500	0.18496200	0.26712200
H	1.42622200	0.06588900	1.35574900
H	1.62772700	1.22928800	0.02250600
O	2.52451100	-0.60557100	-0.26277900
O	3.68106800	-0.17141700	0.18143400
C	-1.21042900	1.81005400	-0.04817600
H	-0.38152300	2.34551600	0.42458000
H	-1.17810300	2.02361400	-1.12291700
H	-2.14266600	2.22376200	0.34622700

P10-C=CC(C)C•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.45188400	2.15082700	0.19185900
C	1.40196400	0.97044800	-0.41816400
H	1.49629700	2.23299600	1.27444000
H	1.45087300	3.08219800	-0.36431000
H	1.35147400	0.92299400	-1.50517900
C	1.38458700	-0.37396800	0.28378100
H	1.45969700	-0.17492800	1.36331000
C	0.07758800	-1.06312000	0.01446700
C	-1.21210400	-0.57400900	0.56697100

H	-1.78181000	-1.38918700	1.04185200
H	-1.05950200	0.21765400	1.31099600
O	-1.97771600	-0.06017100	-0.53277900
O	-3.25506700	0.36459800	0.00520800
H	-3.83552600	-0.32250300	-0.35212700
C	2.57990800	-1.24131100	-0.14388700
H	2.55859800	-2.21096800	0.36359500
H	2.55854900	-1.42699300	-1.22366700
H	3.52561700	-0.74597100	0.09250000
H	0.03503100	-1.83390700	-0.75100500

TS10

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.34328500	0.28019300	-0.08317900
C	1.59438500	-0.60702300	-0.91647500
C	0.25183000	-0.80684700	-0.20050900
H	1.52394000	-0.12272300	-1.89727000
H	2.10567900	-1.57287900	-1.01498000
O	2.08853500	-0.20716000	1.21779900
H	0.96465100	-0.57848300	0.95643000
C	-0.86744400	0.20115700	-0.38648400
H	-1.19838300	0.10918500	-1.43640000
C	-2.04202400	-0.14947600	0.49377700
C	-3.24704300	-0.50689500	0.06397700
H	-1.84983900	-0.08705700	1.56508200
H	-4.05295600	-0.74168300	0.75111500
H	-3.47906100	-0.57672900	-0.99544200
C	-0.42659600	1.66015100	-0.15235000
H	-0.09400900	1.79971400	0.88088400
H	0.40524400	1.94260500	-0.80164500
H	-1.26366900	2.33760000	-0.34081600
H	-0.09479900	-1.84021500	-0.15553300

R11-C=CCCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.77075500	-0.49856500	0.29660600
C	-2.75799800	0.05281400	-0.36369400
H	-3.72044300	-0.68680600	1.36564400
H	-4.69258600	-0.78050500	-0.20080500
H	-2.85101200	0.22245600	-1.43647200
C	-1.44897600	0.46940100	0.24559700
H	-1.47168300	0.29119800	1.32760700
C	-0.25360600	-0.27282400	-0.38025300
H	-0.21801900	-0.08026600	-1.45986500

C	1.08646700	0.11366900	0.23807500
H	1.09241200	-0.08905100	1.31455600
O	2.05530700	-0.83268700	-0.34395700
O	3.20355800	-0.80774300	0.28981400
H	-1.31507100	1.55069400	0.10659400
H	-0.39414500	-1.35215000	-0.25696600
C	1.55644700	1.53315600	-0.03898800
H	1.54303300	1.74518500	-1.11287800
H	0.91213500	2.25728800	0.46709300
H	2.57498600	1.65949400	0.33458400

P11-C=CCC•C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.98975200	0.71594600	0.72594400
C	1.98648700	0.49044100	-0.11602900
H	3.60215100	-0.09249600	1.11695700
H	3.24470600	1.71774900	1.05525000
H	1.38786900	1.32076000	-0.48348000
C	1.58917400	-0.86621400	-0.63235900
H	2.26141900	-1.63378200	-0.21655500
C	0.16330200	-1.25674300	-0.38502500
C	-0.83680200	-0.37732200	0.28123000
H	-0.36883900	0.16094800	1.11703700
O	-1.17571200	0.62299800	-0.71689200
O	-1.90668500	1.68739200	-0.04776000
H	-2.78737900	1.56247400	-0.42746700
H	-0.18256300	-2.19604300	-0.80828600
H	1.77019400	-0.89988500	-1.72162500
C	-2.07690700	-1.12211000	0.76343400
H	-1.80983700	-1.84431400	1.54098000
H	-2.80010600	-0.41996500	1.18537200
H	-2.54847400	-1.66255600	-0.06413900

TS11

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-1.68064600	0.87053200	0.67572300
C	-1.35445300	-0.50883200	0.41763500
C	0.02041200	-0.41528500	-0.26622000
H	-1.29331300	-0.96568700	1.41429600
O	-1.35481700	1.51452200	-0.54229000
H	-0.42570900	0.77007700	-0.78505800
C	1.21432500	-0.13223700	0.61606300
H	1.46739700	-1.04370000	1.18137600
H	0.91918800	0.62224800	1.35827900

C	2.42151600	0.33493400	-0.14965000
C	3.59143300	-0.29354800	-0.19298100
H	2.28873900	1.26246400	-0.70514400
H	4.42773400	0.09414000	-0.76469900
H	3.76284300	-1.22010700	0.34828800
H	0.20510000	-1.10805000	-1.08852100
C	-2.40430000	-1.20889000	-0.43774400
H	-2.12824100	-2.25466600	-0.60638300
H	-3.37589100	-1.18451200	0.06257600
H	-2.49774400	-0.70949500	-1.40509100

R12-C=C(C)CCCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.01898100	-1.06360200	0.42371800
C	2.21673900	-0.10961100	-0.04718700
H	2.72819400	-2.10947100	0.41816700
H	3.99913700	-0.83580600	0.83059500
C	0.85364600	-0.43853600	-0.61545300
H	0.75320300	-1.52576100	-0.70813400
C	-0.31454100	0.10631700	0.22959000
H	-0.26261100	1.19805800	0.29935000
C	-1.65728900	-0.28120100	-0.36508500
H	-1.81106800	-1.36460200	-0.38715200
O	-2.69732500	0.29035000	0.47917000
O	-3.89536200	-0.00189300	0.02816300
H	0.77361600	-0.02659800	-1.63206000
H	-0.24317700	-0.28346200	1.25103200
H	-1.79958300	0.11692000	-1.37488000
C	2.62176100	1.34248000	-0.05417500
H	2.58883800	1.75444600	-1.07105400
H	1.94533100	1.95676700	0.55211200
H	3.63383500	1.47676800	0.33491100

P12-C=C(C)CC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.36253900	-0.54855400	-1.15881700
C	1.72065900	-0.22268200	-0.03724500
H	2.60121600	0.19059700	-1.91740600
H	2.67765100	-1.56782500	-1.35864700
C	1.29817800	1.20836800	0.24420500
H	1.69305200	1.85359300	-0.55850700
C	-0.18202800	1.41413500	0.38108200
C	-1.18839400	0.71415700	-0.45948500
H	-1.92159600	1.41689200	-0.88484600

H	-0.72004200	0.15682800	-1.27816200
O	-1.88737100	-0.20583900	0.40252700
O	-2.87028700	-0.88798100	-0.41519300
H	-3.68609900	-0.48316900	-0.08740200
H	-0.54846700	2.11366800	1.12598500
H	1.78376200	1.55617600	1.16661600
C	1.37740600	-1.23466500	1.02500700
H	0.29244000	-1.29584900	1.16563100
H	1.75125000	-2.22850800	0.76671700
H	1.80794100	-0.94639200	1.99286900

TS12

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.36978900	0.28610800	-0.51399300
C	1.97159200	-0.96951600	0.03862200
C	0.53087100	-0.73222100	0.50563500
H	2.07528100	-1.70919900	-0.76374800
H	2.60887500	-1.24335600	0.88850100
O	1.93040300	1.20581600	0.46591900
H	0.95590000	0.54257300	0.77054300
C	-0.54585200	-0.71036600	-0.55736100
H	-0.77052200	-1.75122900	-0.83740300
C	-1.82140900	-0.02078400	-0.11605300
C	-2.89092800	-0.71542200	0.26868400
H	-3.80001200	-0.22475400	0.60130500
H	-2.90117200	-1.80112000	0.26226300
H	0.23686700	-1.19510500	1.44840900
C	-1.79784600	1.48538900	-0.14530100
H	-1.71046600	1.84800400	-1.17770900
H	-2.70475300	1.91174100	0.28991900
H	-0.93092800	1.88793900	0.39043300
H	-0.13917800	-0.22336800	-1.45327900

R13-(cis)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.09133200	0.32741800	0.27852900
C	1.94403300	0.92055200	-0.05449700
H	3.86711000	0.95386800	0.71666900
C	0.72028000	0.29337400	-0.66281700
H	0.89186800	-0.76308700	-0.89231900
C	-0.51411300	0.42785500	0.24929700
H	-0.68892900	1.48360400	0.48756100
C	-1.76018100	-0.14717000	-0.40110400
H	-1.67444000	-1.22008200	-0.59992200

O	-2.86982500	0.03713100	0.52399800
O	-3.98893500	-0.44240300	0.03225100
H	0.50277700	0.78532400	-1.62204500
H	-0.32926700	-0.08431600	1.19980100
H	-2.02137600	0.36519900	-1.33253400
H	1.85302100	1.98905000	0.13882600
C	3.46950300	-1.11671000	0.12234300
H	3.74790900	-1.55097900	1.09050300
H	2.66863300	-1.72753200	-0.29994600
H	4.34765000	-1.22078600	-0.52708900

P13-CC=CCC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.54367600	-0.87509600	-0.13993400
C	-1.27025200	-0.64290000	0.18331300
H	-2.79989900	-1.88799200	-0.44850100
H	-0.55675400	-1.45950700	0.10404200
C	-0.65136500	0.66826500	0.62578800
H	-1.42674400	1.43567200	0.73466200
H	-0.19463800	0.53385400	1.61584400
C	0.39451900	1.12872000	-0.34337600
H	0.07359500	1.43875200	-1.33326800
C	1.84206500	0.89801600	-0.09960800
H	2.12452200	1.18922500	0.92427100
H	2.47511300	1.44796000	-0.80531200
O	2.07817200	-0.51632800	-0.25370500
O	3.48286000	-0.74514800	0.02077500
H	3.43030700	-1.16124400	0.89319100
C	-3.69761000	0.08461000	-0.12983500
H	-4.15240700	0.15561400	-1.12590600
H	-4.48825700	-0.26362100	0.54658000
H	-3.41518600	1.09339200	0.17975300

TS13

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.68748300	-0.06922500	-0.58178400
C	2.00321700	-1.05151100	0.19708300
C	0.69652700	-0.36291700	0.60578400
H	1.87446000	-1.92670900	-0.45057800
H	2.58639800	-1.32314600	1.08567000
H	0.33784900	-0.55191600	1.61813600
O	2.54641100	1.09870300	0.20125700
H	1.44664200	0.78780800	0.61902000
C	-0.37985400	-0.23635800	-0.44768600

H	-0.85885800	-1.21730300	-0.58214000
H	0.10594300	-0.00090100	-1.40492900
C	-1.40019100	0.82006200	-0.11805300
C	-2.71066300	0.66428600	0.07472500
H	-0.98745400	1.82360500	-0.02722500
H	-3.28868900	1.55780100	0.30635100
C	-3.51627000	-0.59997800	0.00589800
H	-4.03279900	-0.78321400	0.95629900
H	-4.29734000	-0.52108500	-0.76043900
H	-2.91390900	-1.48226500	-0.22245400

R14-(trans)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.92671400	0.14955200	0.39227800
C	-1.89216700	0.14419200	-0.44519400
C	-0.55620500	0.77713800	-0.17699900
H	-0.58162800	1.30008800	0.78674700
C	0.59407700	-0.24703000	-0.18284500
H	0.61321500	-0.78161700	-1.13995300
C	1.94134500	0.41711500	0.04114000
H	2.01038200	0.91076900	1.01553900
O	2.96064400	-0.62265900	0.00631900
O	4.15930700	-0.12635000	0.20891700
H	-0.34939600	1.54097100	-0.94105100
H	0.42397400	-0.99843100	0.59597000
H	2.18630800	1.14266400	-0.74114200
H	-1.99258100	-0.36129600	-1.40671800
H	-2.81993800	0.65527400	1.35258900
C	-4.25980000	-0.48498700	0.12990100
H	-4.28836200	-0.97161700	-0.84933900
H	-4.49784700	-1.23803100	0.89145800
H	-5.06694600	0.25740800	0.16432000

P14-CC=CCC•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.67487100	0.11859200	-0.03077300
C	1.37610900	0.02513000	-0.30838200
H	0.89770900	-0.95183000	-0.35062900
C	0.45321100	1.20342200	-0.54102500
H	1.04676500	2.12745600	-0.52332700
H	0.00216100	1.12742500	-1.54002100
C	-0.63294600	1.26426800	0.48889900
H	-0.35357100	1.49380300	1.51284400
C	-1.99596200	0.73646900	0.22095100

H	-2.37516300	1.08763300	-0.75150100
H	-2.71304800	1.02295500	0.99870700
O	-1.89218300	-0.70150300	0.17887100
O	-3.21551000	-1.21542100	-0.11328100
H	-3.10536600	-1.48201000	-1.03732400
C	3.59177300	-1.04184200	0.21813600
H	4.41880700	-1.05853200	-0.50279700
H	4.04897100	-0.98014400	1.21387400
H	3.06074200	-1.99544100	0.14791200
H	3.13119600	1.10784600	0.02071400

TS14

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.76416600	0.20039000	-0.54324700
C	2.27656100	-0.84525400	0.29891500
C	0.83582800	-0.43060500	0.61670100
H	2.36751500	-1.77452100	-0.27568900
H	2.86732500	-0.91329800	1.22076600
H	0.48490400	-0.61514900	1.63266300
O	2.34142700	1.36536300	0.13547100
H	1.31793200	0.85442700	0.55030400
C	-0.19854000	-0.62663400	-0.46761300
H	-0.44832300	-1.69805400	-0.53330800
H	0.25996400	-0.35712200	-1.42931800
C	-1.45431700	0.16960900	-0.24190600
C	-2.66966600	-0.34521600	-0.07004200
H	-1.32518700	1.25181200	-0.21670000
H	-2.78831800	-1.42903800	-0.09750400
C	-3.92270700	0.44636600	0.15691200
H	-3.72230200	1.52149500	0.17243600
H	-4.66422400	0.24956700	-0.62738500
H	-4.39698800	0.17426700	1.10815100

R15-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393600	0.01912900	0.21624600
C	2.50767100	-0.37369400	-0.44139400
H	3.61461800	0.07695700	1.30107200
H	4.50795600	0.29247900	-0.30012900
H	2.53237300	-0.41673100	-1.53058100
C	1.20658100	-0.78156200	0.18939800
H	1.29137800	-0.72723600	1.28215600
C	0.00586100	0.07208200	-0.28137600
H	-0.03601000	0.02027100	-1.37829900

C	-1.28366200	-0.54535900	0.24668200
H	-1.38109900	-0.44387100	1.33248500
H	-1.38181400	-1.60131600	-0.02458500
O	-2.40657100	0.15928200	-0.35804800
O	-3.55264000	-0.24708400	0.13708900
H	1.00457700	-1.83346800	-0.05955400
C	0.13703600	1.54190200	0.13689500
H	-0.71143700	2.12975600	-0.22170500
H	0.17264800	1.63142600	1.22940800
H	1.05596300	1.97917100	-0.26129600

P15-C=CCC•(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.41839200	-1.62684100	-0.03436800
C	-1.88113000	-0.49900400	-0.48897600
H	-2.66713700	-1.75783700	1.01539100
H	-2.63304100	-2.46347500	-0.69058800
H	-1.63615700	-0.40666200	-1.54541300
C	-1.54161300	0.70135500	0.36564400
H	-2.13632600	1.56497900	0.03991500
H	-1.84210100	0.48460200	1.40169500
C	-0.08039500	1.06099000	0.31021500
C	0.36524200	2.30850400	-0.37988900
H	-0.26015700	3.16700800	-0.10267700
H	1.40724800	2.55065900	-0.14837900
H	0.29664700	2.21918700	-1.47640100
C	0.93431100	0.05930600	0.74185500
H	1.75071600	0.53168200	1.31071300
H	0.49169800	-0.73453300	1.35507500
O	1.48456700	-0.52094100	-0.45512000
O	2.47411200	-1.49771500	-0.04173100
H	3.29104000	-1.03222700	-0.27140100

TS15

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-2.14392600	-0.82562500	-0.35268100
C	-1.64774700	0.46114700	-0.70673900
C	-0.26318500	0.53135800	-0.03575800
H	-1.62539900	0.50102600	-1.80247900
H	-2.29753700	1.25402600	-0.31371200
O	-1.87315000	-0.88897800	1.03380800
H	-0.82959700	-0.23141700	0.93385700
C	0.79461400	-0.34301800	-0.69475200
H	1.18388700	0.17783400	-1.58419300

H	0.29977000	-1.25534700	-1.05234700
C	1.93621900	-0.70911300	0.21294900
C	3.21345300	-0.40553200	0.00486300
H	1.65720100	-1.27378500	1.10203500
H	3.99315600	-0.70966900	0.69497000
H	3.53273300	0.15282400	-0.87103600
C	0.18410400	1.86931600	0.48752200
H	1.09711200	1.77769700	1.08217400
H	0.41293300	2.55569000	-0.34295000
H	-0.59239900	2.34299300	1.09616200

R16-C=CCC(CC)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.72490700	-0.18739100	0.13810100
C	2.60479800	-0.51358800	-0.49921900
C	1.33971700	-0.99816400	0.15010500
C	0.09872500	-0.13192000	-0.18763600
H	0.02337700	-0.06662700	-1.28281200
C	-1.14828200	-0.86425500	0.30320600
O	-2.32556200	-0.31172600	-0.35749200
O	-3.42337200	-0.90541100	0.05062400
H	-1.12319300	-1.92895400	0.05166900
H	2.57270100	-0.44286900	-1.58682200
H	3.80253100	-0.24286500	1.22044500
H	4.61103800	0.14163900	-0.39418600
H	1.47509000	-1.04279900	1.23832600
H	-1.29920600	-0.75888000	1.38259700
H	1.14523000	-2.02702300	-0.18460800
C	0.24152900	1.29093100	0.38684200
C	-0.78430400	2.31632800	-0.10808200
H	1.24798100	1.64906500	0.14478100
H	0.20266600	1.22681100	1.48364200
H	-0.55737400	3.30708000	0.29809900
H	-0.76768200	2.39351800	-1.20073100
H	-1.80422800	2.05736000	0.18464400

P16-C=CCC•(CC)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.93323500	-1.14564000	-0.63523600
C	-1.64891900	-1.19476600	-0.29398300
H	-3.28194500	-1.49828700	-1.60028300
H	-3.68990800	-0.75607100	0.04060000
H	-0.91140600	-1.58130200	-0.99426200
C	-1.08357400	-0.71694100	1.02831600

H	-1.91259800	-0.37163100	1.66072300
H	-0.61541400	-1.56805700	1.54234700
C	-0.06829000	0.38141800	0.86266700
C	1.37973100	0.03185300	0.81480200
H	1.63990800	-0.72145100	1.57374400
H	2.02018100	0.91067000	0.95985300
O	1.64184400	-0.52349200	-0.49183000
O	3.05424200	-0.85296400	-0.54435200
H	3.01606100	-1.81808100	-0.48116800
C	-0.50328000	1.77238800	0.51253900
C	-0.37118200	2.10928200	-0.99151300
H	0.10232800	2.49338600	1.08070700
H	-1.54407900	1.92260000	0.82254800
H	-0.64148800	3.15446200	-1.17448200
H	0.65237900	1.94830100	-1.33998600
H	-1.03021700	1.47154200	-1.58643600

TS16

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-1.78693300	-1.59317700	-0.08313800
C	-1.48072600	-0.48251200	-0.92238200
C	-0.19528800	0.10974900	-0.31305600
H	-1.35226500	-0.88079200	-1.93618000
H	-2.29467300	0.25125500	-0.90949000
O	-1.63006400	-1.05348900	1.21554000
H	-0.70103300	-0.31148300	0.87451700
C	1.04203000	-0.74184400	-0.57052400
H	1.42539000	-0.51925900	-1.57916300
H	0.72798000	-1.79374600	-0.57574600
C	2.14018200	-0.55183900	0.43903100
C	3.37326100	-0.13523100	0.16846200
H	1.86940400	-0.79279000	1.46659900
H	4.12489100	-0.03245700	0.94387300
H	3.68421600	0.11070100	-0.84331800
C	-0.00217900	1.60935200	-0.34581300
H	0.98632100	1.84035900	0.06590500
H	0.03850200	1.93081500	-1.40084200
C	-1.06941300	2.43062700	0.39151200
H	-2.06674600	2.29917200	-0.03780400
H	-1.12480700	2.14522200	1.44642700
H	-0.82841400	3.49652000	0.34262500

R17-(trans)-CC=COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	1.05261700	0.43130200	0.00003800
C	-0.10024300	-0.23364200	0.00003600
H	-0.23844800	-1.30847100	0.00030100
O	-1.28983900	0.46700100	0.00001200
O	-2.35125000	-0.32131300	-0.00005100
H	1.01514000	1.51778700	-0.00000400
C	2.39504100	-0.22943600	-0.00002900
H	2.97876300	0.06797500	-0.87946300
H	2.97856200	0.06727500	0.87976300
H	2.31020400	-1.31941700	-0.00055500

P17-C•C=COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.13311200	-0.25253900	-0.12948400
C	0.04518300	0.20241200	0.22042200
H	0.21934400	1.18806700	0.65938500
O	1.17697100	-0.57213000	0.12034000
O	2.26881900	0.31483300	-0.26451000
H	2.90713900	0.08838500	0.42681400
C	-2.55538700	0.08728400	-0.06006400
H	-3.02367900	0.06908900	-1.05105800
H	-3.11157500	-0.60894500	0.57918400
H	-2.69765400	1.09884400	0.35379200

TS17

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.48522900	0.46516800	0.00126900
C	0.20151300	0.87552500	-0.01926500
C	-0.72024300	-0.08375200	0.16158600
H	0.09909000	1.95703600	-0.03530300
O	1.44611800	-0.94763800	-0.06038000
H	0.30933000	-1.01638600	0.30428700
C	-2.17415300	-0.19371300	-0.04818700
H	-2.39259400	-0.75158800	-0.96896000
H	-2.67413000	-0.71500300	0.77416600
H	-2.63518100	0.79733900	-0.16610300

R18-(trans)-CCC=COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.44834000	0.21281600	0.44939300
C	-0.70541500	-0.28196400	0.00758500
H	-0.86849800	-1.24059300	-0.47077000
O	-1.86310600	0.45767500	0.14796000
O	-2.92938900	-0.15925600	-0.33234000

H	0.44115800	1.20007800	0.90663100
C	1.76348300	-0.49870400	0.33906200
H	2.16595400	-0.66338700	1.34791800
H	1.61290400	-1.49082400	-0.10083500
C	2.79577200	0.29017100	-0.48437100
H	2.97475400	1.27880200	-0.04914700
H	3.75176100	-0.24065800	-0.51707100
H	2.44884600	0.43532600	-1.51170200

P18-CC•C=COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.68626200	-0.34043100	0.24207200
H	-0.91926000	-0.58362100	1.28184500
O	-1.79576000	-0.15846900	-0.54976600
O	-2.78995300	0.53588800	0.25993500
H	-3.54216400	-0.05931600	0.13113400
C	0.52772800	-0.28605500	-0.24988300
C	1.92375400	-0.55182600	0.11588200
C	2.84369600	0.67314500	-0.03314800
H	2.31799800	-1.37942900	-0.48986700
H	1.95197700	-0.90940900	1.16039400
H	3.86869300	0.42029600	0.25392800
H	2.85469000	1.02686400	-1.06784300
H	2.50027000	1.49626800	0.59950900

TS18

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	2.08262300	0.25164700	0.20967300
C	0.91018500	0.91065800	0.12172600
C	-0.17875000	0.14427100	-0.04940300
H	0.99841100	1.97051100	0.34356000
O	1.81478600	-1.08065100	-0.18405000
H	0.63539600	-0.98844900	0.00335400
C	-1.57738100	0.37400800	-0.45921400
H	-1.67738300	0.13699800	-1.52937500
H	-1.79644800	1.45201500	-0.38729000
C	-2.60926500	-0.43283300	0.34184600
H	-2.56468700	-0.17821800	1.40462800
H	-3.62292300	-0.23126300	-0.01706100
H	-2.42037300	-1.50618600	0.24747300

R19-C=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.32345800	0.13895400	-0.26716500

C	1.21630500	-0.36510100	0.26701700
H	2.35079200	1.14240800	-0.68233200
H	3.24886800	-0.42546200	-0.30275700
H	1.20908100	-1.37364800	0.67400400
C	-0.06793300	0.38738600	0.37541700
H	-0.41691200	0.48496100	1.40810800
H	-0.00908200	1.37950500	-0.08143600
O	-1.10257800	-0.37018700	-0.33678500
O	-2.29913800	0.09828700	-0.07161500

P19-C=C•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.50233600	-0.05684000	0.19949100
C	-1.30297200	-0.14941400	-0.31210500
H	-2.72773600	0.63031200	1.02139000
H	-3.33806600	-0.65263300	-0.15981300
C	0.01924000	0.47578100	-0.18533800
H	0.27805900	1.04012500	-1.09201100
H	0.03463300	1.18179600	0.66645100
O	0.97700100	-0.56121300	0.01842900
O	2.26767400	0.08684600	0.03044500
H	2.51211800	-0.02182300	0.96070100

TS19

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	1.37062400	0.36833000	0.34945400
C	0.18831800	0.93487500	-0.20420300
C	-0.85664800	-0.14592900	-0.03926400
H	-0.01728000	1.85920500	0.34640400
H	0.31812200	1.15052700	-1.27374200
O	1.36773100	-0.95361800	-0.13856200
H	0.19957000	-1.07704800	-0.08752600
C	-2.15639100	-0.23864000	0.08449300
H	-2.79711400	0.64469300	0.11371100
H	-2.66180700	-1.19691800	0.16785600

R20C=CC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.37995800	-0.22114300	-0.16869600
C	1.20019100	-0.71744100	0.18629800
H	2.53311700	0.83529000	-0.36125500
H	3.25045500	-0.85979300	-0.27131900
H	1.09341300	-1.78418100	0.37129500
C	-0.05919300	0.07118500	0.39265200

P20-C=C•C(C)OO

H	-0.38771100	-0.00897800	1.43563200
O	-1.09639000	-0.65443900	-0.37746500
O	-2.30374000	-0.32057000	0.00979400
C	-0.04520100	1.52605400	-0.04315400
H	0.64555300	2.10264100	0.57831400
H	0.25887100	1.61961600	-1.08922500
H	-1.04718800	1.94354800	0.07532200

TS20

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.52725500	-0.37048700	-0.10069400
C	1.27734500	-0.63101100	0.18019100
H	2.87661600	0.64296900	-0.31997100
H	3.28894000	-1.14645200	-0.13031500
C	-0.01465600	0.05359100	0.37278600
H	-0.29705000	0.00079900	1.43542300
C	0.00173900	1.52076400	-0.07832900
H	-0.99672200	1.94599000	0.04336700
H	0.70666100	2.09808400	0.52688300
H	0.29297800	1.58839500	-1.12944800
O	-0.96924800	-0.71589200	-0.37837000
O	-2.28211500	-0.23168900	-0.01689400
H	-2.61062100	-0.98627700	0.49245400

R21-(cis)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.81928900	0.52831900	-0.14283600
C	-0.56610900	0.90860400	0.11292400

H	-2.52210200	1.30716100	-0.43526300
H	-0.30831800	1.95977100	0.00795100
C	0.56001300	0.03352500	0.54898100
H	1.01676500	0.37313300	1.48379400
H	0.29033500	-1.01949800	0.64871100
O	1.61586400	0.11465100	-0.47203600
O	2.72064500	-0.45673700	-0.05570200
C	-2.40944200	-0.84779300	-0.07087700
H	-3.20901100	-0.88536200	0.67918800
H	-2.87090700	-1.11345600	-1.02937900
H	-1.67987300	-1.62098400	0.17775200

P21-CC=C•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.91388400	0.59199200	-0.09967900
C	0.64005300	0.78716000	0.13988000
H	2.54147800	1.45524400	-0.33041200
C	2.63436100	-0.73994500	-0.09313400
H	1.95646000	-1.57122500	0.11314700
H	3.11436100	-0.91903700	-1.06203600
H	3.42710700	-0.74510100	0.66431500
C	-0.56787900	0.04993800	0.52886500
H	-0.95982500	0.41032700	1.49200900
H	-0.36075400	-1.02941700	0.63936300
O	-1.54737600	0.24418900	-0.49238400
O	-2.71755600	-0.49094500	-0.07027700
H	-3.32188900	0.23838600	0.12930900

TS21

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-1.85928500	0.53015500	-0.35502100
C	-0.60896300	0.87690200	0.23114600
C	0.23823900	-0.36452600	0.06434000
H	-0.24126100	1.76193900	-0.30004400
H	-0.72514800	1.10107600	1.30084100
O	-2.09118100	-0.78386900	0.10362300
H	-0.95873100	-1.10115600	0.06892900
C	1.50365600	-0.69452500	-0.04064100
H	1.76025500	-1.75024100	-0.13252900
C	2.67080700	0.26603600	-0.04991600
H	3.26807800	0.13445200	-0.95909400
H	2.34548000	1.30778400	0.00111800
H	3.33262100	0.07253600	0.80239300

R22-(trans)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.64596500	0.32705700	-0.23290000
C	0.57009500	-0.08521700	0.43528500
H	1.53907800	1.15657900	-0.93220600
H	0.64662400	-0.91407500	1.13650200
C	-0.77700300	0.53559700	0.29539500
H	-1.20987600	0.84764600	1.25046200
H	-0.77429000	1.38456700	-0.39454400
O	-1.69668500	-0.47269400	-0.25403400
O	-2.94534600	-0.08550100	-0.14544400
C	3.02176600	-0.24897300	-0.10302700
H	3.73747100	0.51273400	0.22973900
H	3.04809900	-1.07826500	0.60886800
H	3.38419900	-0.61440900	-1.07151600

P22-CC=C•COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.79818800	0.31945500	-0.27015900
C	0.64680700	0.05194100	0.29651000
H	1.82390300	1.08958200	-1.05286500
C	3.11649900	-0.33380900	0.04368500
H	3.00970000	-1.08968500	0.82429800
H	3.53272200	-0.81271000	-0.85052500
H	3.85026300	0.41001400	0.37626500
C	-0.73891100	0.53262100	0.25258800
H	-1.06673300	0.90358600	1.23525900
H	-0.83779000	1.36454300	-0.46800700
O	-1.57139900	-0.55508400	-0.15130500
O	-2.92164400	-0.04107800	-0.17123500
H	-3.30321700	-0.51727800	0.58015300

TS22

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	-1.98025400	0.06217000	-0.39079000
C	-1.04039000	0.96662700	0.18117100
C	0.27780300	0.23406600	0.09179100
H	-1.08882400	1.89476300	-0.39942400
H	-1.28224400	1.16637400	1.23430300
O	-1.61800100	-1.18432200	0.16163500
H	-0.46118900	-0.96286700	0.15670100
C	1.55256800	0.51962700	-0.02546800
H	1.83970800	1.57312500	-0.11501400
C	2.68199300	-0.47394800	-0.05567300

R23-C=CCCCOO•

H	3.25155300	-0.38371500	-0.98777100
H	3.38301300	-0.29039800	0.76669700
H	2.31217900	-1.49829100	0.02682800

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800
C	0.02912800	0.36494300	-0.07789300
H	0.13282400	0.90845700	0.86749900
H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

P23-C=CC•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.68701300	-0.44161100	-0.14213200
C	-2.46182200	0.15737400	-0.36090800
H	-3.86950100	-1.04071500	0.74412900
H	-4.50438900	-0.33341100	-0.84420700
H	-2.34380300	0.74815600	-1.26952200
C	-1.36626400	0.07530200	0.48233300
H	-1.45768300	-0.51051200	1.39601900
C	-0.04606200	0.72888200	0.22501800
H	0.22179300	1.39943400	1.05382400
H	-0.08990200	1.34175900	-0.68156400
C	1.08365200	-0.30037200	0.08564800
H	0.91957200	-0.94559800	-0.78886600
H	1.14420400	-0.93807400	0.97704100
O	2.28505300	0.44137200	-0.06062600
O	3.36866100	-0.51288200	-0.10072900
H	3.61505800	-0.46640500	-1.03577300

TS23

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-0.40088600	1.24066000	-0.01717000
H	-0.28454600	1.49972100	-1.07490900
H	-0.29658200	2.16807800	0.56152400
C	-1.82586600	0.69128300	0.19493700
H	-2.57985700	1.35065600	-0.24507900
H	-2.04154600	0.53551100	1.25862900
O	-1.15081700	-1.46982600	0.18348100
O	-1.93863400	-0.54391200	-0.49858100
H	-0.05209400	-0.85947600	0.20992600
C	0.65835000	0.22716000	0.38758900
H	0.82171100	0.15921500	1.46702100
C	1.87266700	0.10814700	-0.40730500
C	3.06718600	-0.29330400	0.05836800
H	1.77404800	0.33679700	-1.46819500
H	3.92820700	-0.38932200	-0.59303200
H	3.21756000	-0.53495400	1.10640300

R24-(cis)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.09133200	0.32741800	0.27852900
C	1.94403300	0.92055200	-0.05449700
H	3.86711000	0.95386800	0.71666900
C	0.72028000	0.29337400	-0.66281700
H	0.89186800	-0.76308700	-0.89231900
C	-0.51411300	0.42785500	0.24929700
H	-0.68892900	1.48360400	0.48756100
C	-1.76018100	-0.14717000	-0.40110400
H	-1.67444000	-1.22008200	-0.59992200
O	-2.86982500	0.03713100	0.52399800
O	-3.98893500	-0.44240300	0.03225100
H	0.50277700	0.78532400	-1.62204500
H	-0.32926700	-0.08431600	1.19980100
H	-2.02137600	0.36519900	-1.33253400
H	1.85302100	1.98905000	0.13882600
C	3.46950300	-1.11671000	0.12234300
H	3.74790900	-1.55097900	1.09050300
H	2.66863300	-1.72753200	-0.29994600
H	4.34765000	-1.22078600	-0.52708900

P24-CC=CC•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.14160000	-0.32313700	-0.46043200
C	1.83156900	-0.74631100	-0.28824700
H	3.79509700	-0.95279100	-1.05876400

H	1.56551400	-1.68464400	-0.77548800
C	0.82454400	-0.12644600	0.43073900
H	1.02476000	0.81333700	0.93997700
C	-0.56724700	-0.66446000	0.55170300
H	-0.84221400	-0.79609600	1.60777800
H	-0.64213400	-1.64827100	0.07626100
C	-1.60157300	0.27853800	-0.07700100
H	-1.43531800	0.37506600	-1.15921900
H	-1.54262800	1.27936600	0.37023700
O	-2.87561200	-0.29200500	0.18220200
O	-3.86474300	0.62962800	-0.32691700
H	-4.16773200	0.15251400	-1.11286400
C	3.76055700	0.91750500	0.09948100
H	3.05259000	1.52915900	0.66281300
H	4.59711200	0.67429100	0.76881700
H	4.18109500	1.54295800	-0.69927600

TS24

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.00359000	-1.24225100	0.22272000
H	1.06423400	-1.73861900	-0.75184300
H	0.91244200	-2.02746500	0.98515800
C	2.32139500	-0.47970100	0.46215400
H	3.19209000	-1.11578300	0.27617400
H	2.36987600	-0.07095600	1.47867500
O	1.44345700	1.52372700	-0.12342700
O	2.40718900	0.58033300	-0.48015900
H	0.41126400	0.79049700	-0.08572100
C	-0.19965300	-0.30986000	0.25560800
H	-0.50371400	-0.03208700	1.26742800
C	-1.28991000	-0.54404800	-0.68047200
C	-2.58240100	-0.17972000	-0.54804300
H	-1.00627900	-1.04053400	-1.60767700
C	-3.21658000	0.53065900	0.60748400
H	-2.52469200	0.70798700	1.43335600
H	-3.61307100	1.50430600	0.29143600
H	-4.07123000	-0.03878000	0.99383500
H	-3.25473900	-0.42151300	-1.36883500

R25-(trans)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.92671400	0.14955200	0.39227800
C	-1.89216700	0.14419200	-0.44519400
C	-0.55620500	0.77713800	-0.17699900

P25-CC=CC•CCOO

H	-0.58162800	1.30008800	0.78674700
C	0.59407700	-0.24703000	-0.18284500
H	0.61321500	-0.78161700	-1.13995300
C	1.94134500	0.41711500	0.04114000
H	2.01038200	0.91076900	1.01553900
O	2.96064400	-0.62265900	0.00631900
O	4.15930700	-0.12635000	0.20891700
H	-0.34939600	1.54097100	-0.94105100
H	0.42397400	-0.99843100	0.59597000
H	2.18630800	1.14266400	-0.74114200
H	-1.99258100	-0.36129600	-1.40671800
H	-2.81993800	0.65527400	1.35258900
C	-4.25980000	-0.48498700	0.12990100
H	-4.28836200	-0.97161700	-0.84933900
H	-4.49784700	-1.23803100	0.89145800
H	-5.06694600	0.25740800	0.16432000

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.04895700	-0.00766800	-0.41830200
C	-1.82614800	-0.10683300	0.22183500
H	-1.76937900	0.26460500	1.24657200
C	-0.67071400	-0.64130100	-0.32114700
H	-0.70091200	-1.01692500	-1.34295700
C	0.63995900	-0.73039100	0.39476600
H	0.99704000	-1.76959600	0.42439600
H	0.53434400	-0.39878700	1.43331000
C	1.72537700	0.10811200	-0.29336100
H	1.46634500	1.17612100	-0.27186800
H	1.84843900	-0.19458600	-1.34133100
O	2.92917600	-0.12661600	0.42193700
O	3.97862700	0.58665900	-0.26878700
H	4.13576400	1.31663600	0.34729900
C	-4.28288700	0.56908400	0.19387100
H	-4.10451600	0.90908600	1.21844000
H	-4.65969900	1.42426300	-0.38433900
H	-5.10181800	-0.16328800	0.21990400
H	-3.12781900	-0.37388800	-1.44060100

TS25

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.03905000	-1.24495000	-0.05637700
H	0.84597000	-1.45961500	-1.11295700
H	1.02986600	-2.20342200	0.47969600

C	2.44657300	-0.62964900	0.06456400
H	3.19253000	-1.22680800	-0.46863500
H	2.74461400	-0.51258800	1.11347900
O	1.66856500	1.49159700	0.22128100
O	2.44001400	0.64074200	-0.57181100
H	0.60176600	0.81692700	0.30618600
C	-0.03271400	-0.30933700	0.48544800
H	-0.10444800	-0.30366300	1.57709800
C	-1.31717600	-0.23125700	-0.19481000
C	-2.48841200	0.08211800	0.39038400
H	-1.30574900	-0.40794700	-1.27098900
H	-2.50207200	0.26191000	1.46521200
C	-3.79893300	0.20690100	-0.32000400
H	-3.69929000	0.00573100	-1.39040700
H	-4.54370200	-0.48667500	0.09112300
H	-4.21845000	1.21448500	-0.20080100

R26-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393600	0.01912900	0.21624600
C	2.50767100	-0.37369400	-0.44139400
H	3.61461800	0.07695700	1.30107200
H	4.50795600	0.29247900	-0.30012900
H	2.53237300	-0.41673100	-1.53058100
C	1.20658100	-0.78156200	0.18939800
H	1.29137800	-0.72723600	1.28215600
C	0.00586100	0.07208200	-0.28137600
H	-0.03601000	0.02027100	-1.37829900
C	-1.28366200	-0.54535900	0.24668200
H	-1.38109900	-0.44387100	1.33248500
H	-1.38181400	-1.60131600	-0.02458500
O	-2.40657100	0.15928200	-0.35804800
O	-3.55264000	-0.24708400	0.13708900
H	1.00457700	-1.83346800	-0.05955400
C	0.13703600	1.54190200	0.13689500
H	-0.71143700	2.12975600	-0.22170500
H	0.17264800	1.63142600	1.22940800
H	1.05596300	1.97917100	-0.26129600

P26-C=CC•C(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.69379700	-0.74894500	0.12212400
C	-2.46807300	-0.38460100	-0.40070000
H	-3.89903400	-0.66604400	1.18449200

H	-4.48876300	-1.12747600	-0.50841500
H	-2.32732900	-0.49166000	-1.47652200
C	-1.39952300	0.11075700	0.32723600
H	-1.51494000	0.23088300	1.40453100
C	-0.07382400	0.50448600	-0.25325800
H	-0.11536900	0.38018100	-1.34276900
C	1.01680600	-0.44711100	0.27273600
H	0.75230400	-1.49240000	0.06032500
H	1.13941700	-0.33406000	1.35822900
O	2.22755600	-0.10284700	-0.38643200
O	3.27662400	-0.89864600	0.20668400
H	3.43218000	-1.54621600	-0.49613500
C	0.27152600	1.97242400	0.06554900
H	0.29394900	2.13674500	1.14893700
H	1.25287300	2.23444100	-0.33601100
H	-0.47742200	2.64549300	-0.36079800

TS26

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.40810600	0.85111200	0.58711600
H	-0.30829400	1.36491600	1.55486200
C	-1.76872400	0.11086800	0.64032800
H	-2.60531300	0.81615500	0.61711000
H	-1.84089400	-0.52658700	1.52946600
O	-1.00895900	-1.75017400	-0.40486300
O	-1.90423600	-0.68721400	-0.52686500
H	0.05439300	-1.12130100	-0.14700700
C	0.71352300	-0.18622400	0.48383100
H	0.88879600	-0.70892900	1.42904200
C	1.93656100	0.07032800	-0.26495400
C	3.13879100	-0.44814800	0.03853800
H	1.84960300	0.69070600	-1.15334000
H	4.01235000	-0.25411500	-0.57332100
H	3.28273000	-1.08054800	0.90976300
C	-0.40850300	1.90200800	-0.53029600
H	-1.24059300	2.60021200	-0.39503600
H	0.51620100	2.48508800	-0.53303500
H	-0.52467200	1.43384000	-1.51205300

R27-C=CCCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.77075500	-0.49856500	0.29660600
C	-2.75799800	0.05281400	-0.36369400
H	-3.72044300	-0.68680600	1.36564400

H	-4.69258600	-0.78050500	-0.20080500
H	-2.85101200	0.22245600	-1.43647200
C	-1.44897600	0.46940100	0.24559700
H	-1.47168300	0.29119800	1.32760700
C	-0.25360600	-0.27282400	-0.38025300
H	-0.21801900	-0.08026600	-1.45986500
C	1.08646700	0.11366900	0.23807500
H	1.09241200	-0.08905100	1.31455600
O	2.05530700	-0.83268700	-0.34395700
O	3.20355800	-0.80774300	0.28981400
H	-1.31507100	1.55069400	0.10659400
H	-0.39414500	-1.35215000	-0.25696600
C	1.55644700	1.53315600	-0.03898800
H	1.54303300	1.74518500	-1.11287800
H	0.91213500	2.25728800	0.46709300
H	2.57498600	1.65949400	0.33458400

P27-C=CC•CC(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.82877800	0.00785300	-0.48609200
C	-2.59858200	-0.51338800	-0.13713700
H	-4.05473600	1.05964900	-0.34324900
H	-4.60777300	-0.61291100	-0.91107000
H	-2.43612500	-1.57840500	-0.30478700
C	-1.54964400	0.20341200	0.41620800
C	-0.22531600	-0.38933100	0.77798300
H	0.04091900	-0.13281700	1.81315900
C	0.93285300	0.08842400	-0.12476300
H	0.72369500	-0.20522900	-1.16372700
O	2.05320700	-0.66850100	0.34595600
O	3.16253400	-0.43531700	-0.55044700
H	3.17948500	-1.27493100	-1.03171900
H	-1.69194700	1.26663200	0.59899800
C	1.19994800	1.58739000	-0.05190400
H	1.35799500	1.89926800	0.98578400
H	2.09322600	1.83444700	-0.62868500
H	0.35744000	2.15054200	-0.46378600
H	-0.27098800	-1.48185100	0.71924400

TS27

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.20445800	-0.98961700	0.13697900
H	0.24810300	-1.86684100	0.79620500
C	1.50567500	-0.17514100	0.32782500

H	1.60104800	0.13048700	1.37777500
O	0.41719100	1.81844900	0.12307600
O	1.38364500	1.00818600	-0.46563700
H	-0.54548900	1.01624300	0.17763200
C	-1.04346800	-0.16958300	0.42247900
H	-1.26977300	-0.05574300	1.48649800
C	-2.21898000	-0.34537100	-0.41922400
C	-3.48965500	-0.15504700	-0.02693900
H	-2.02681600	-0.62251300	-1.45548600
H	-4.32038200	-0.27407900	-0.71298600
H	-3.73459100	0.12331300	0.99383600
C	2.75233700	-0.90459600	-0.14667000
H	3.63939100	-0.28282900	-0.00227400
H	2.88324700	-1.83271900	0.41691900
H	2.67324300	-1.15431500	-1.20910500
H	0.18313100	-1.35795300	-0.89522000

R28-C=C(C)CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.01898100	-1.06360200	0.42371800
C	2.21673900	-0.10961100	-0.04718700
H	2.72819400	-2.10947100	0.41816700
H	3.99913700	-0.83580600	0.83059500
C	0.85364600	-0.43853600	-0.61545300
H	0.75320300	-1.52576100	-0.70813400
C	-0.31454100	0.10631700	0.22959000
H	-0.26261100	1.19805800	0.29935000
C	-1.65728900	-0.28120100	-0.36508500
H	-1.81106800	-1.36460200	-0.38715200
O	-2.69732500	0.29035000	0.47917000
O	-3.89536200	-0.00189300	0.02816300
H	0.77361600	-0.02659800	-1.63206000
H	-0.24317700	-0.28346200	1.25103200
H	-1.79958300	0.11692000	-1.37488000
C	2.62176100	1.34248000	-0.05417500
H	2.58883800	1.75444600	-1.07105400
H	1.94533100	1.95676700	0.55211200
H	3.63383500	1.47676800	0.33491100

P28-C=C(C)C•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.27743700	-0.84457700	-0.38615600
C	2.17755600	-0.07800000	-0.04769400
H	3.24580500	-1.92714400	-0.32566000

H	4.20429300	-0.39380600	-0.72035800
C	0.99606000	-0.68392200	0.38237700
C	-0.27258900	0.00644300	0.77161500
H	-0.58186700	-0.30532900	1.77927200
C	-1.42169900	-0.33976400	-0.18629600
H	-1.20856600	0.02327600	-1.20180500
O	-2.58140900	0.29226200	0.33440700
O	-3.69009600	-0.10065700	-0.50441300
H	-3.85750200	0.72561100	-0.98021200
H	0.98257800	-1.77144500	0.42833800
H	-0.14908000	1.09237600	0.79937000
H	-1.57715700	-1.42507800	-0.23552500
C	2.27716900	1.43287900	-0.14563000
H	1.51929600	1.84521700	-0.82029700
H	2.13365200	1.91011200	0.82983300
H	3.25698800	1.73501600	-0.52219300

TS28

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.64073400	0.98119700	-0.76292300
H	0.60972600	1.45490400	-1.75329900
C	2.08624800	0.51108200	-0.49411500
H	2.44441300	-0.15893400	-1.28470800
O	1.43628500	-1.37682100	0.57642400
O	2.11295500	-0.16760400	0.75293900
H	0.35985800	-0.96454900	0.08700100
C	-0.34307700	-0.17776900	-0.69421700
H	-0.36102500	-0.78091400	-1.60574600
C	-1.66397100	-0.03450600	-0.07166900
C	-2.71035900	-0.75493300	-0.52033100
H	-3.68560500	-0.69610600	-0.04942900
H	-2.61793100	-1.42127900	-1.37183700
H	0.39330900	1.74849200	-0.02521300
C	-1.80704800	0.88198300	1.11996300
H	-1.03390000	0.67585300	1.86866200
H	-1.70275200	1.93554300	0.83476500
H	-2.78434200	0.76074000	1.59244500
H	2.76916100	1.35932800	-0.38779600

R29-C=CC(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.25621700	-1.07567800	0.32724700
C	-2.35204300	-0.39232300	-0.36581700
H	-3.18023300	-1.19384000	1.40483800

H	-4.10963800	-1.54453300	-0.15092800
H	-2.46689200	-0.29680000	-1.44644600
C	-1.14112700	0.29319000	0.21281600
H	-1.14509500	0.12775900	1.29870700
C	0.14294500	-0.34548600	-0.36417100
H	0.10418100	-1.42885400	-0.20696000
H	0.18144300	-0.18421200	-1.44872800
C	1.42019500	0.18496200	0.26712200
H	1.42622200	0.06588900	1.35574900
H	1.62772700	1.22928800	0.02250600
O	2.52451100	-0.60557100	-0.26277900
O	3.68106800	-0.17141700	0.18143400
C	-1.21042900	1.81005400	-0.04817600
H	-0.38152300	2.34551600	0.42458000
H	-1.17810300	2.02361400	-1.12291700
H	-2.14266600	2.22376200	0.34622700

P29-C=CC•(C)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.40529400	-0.68944500	-0.47590400
C	-2.13803700	-0.83663300	0.04348900
H	-3.80098000	0.27428700	-0.77461900
H	-4.05654600	-1.54532000	-0.60486400
H	-1.82722200	-1.84828100	0.30291300
C	-1.19999700	0.16989400	0.27507900
C	-1.48890500	1.61562500	-0.02423300
H	-0.84321500	2.27821900	0.56083200
H	-1.32115900	1.85897600	-1.08322100
H	-2.52806800	1.87686900	0.19872400
C	0.16507200	-0.17391000	0.80491000
H	0.19358800	-1.21197500	1.15115500
H	0.41437200	0.46330500	1.66458900
C	1.26678600	0.02166900	-0.24765700
H	1.28569700	1.05484000	-0.61599900
H	1.10842500	-0.64811200	-1.10499400
O	2.49344600	-0.27973000	0.39981500
O	3.55044200	-0.00647400	-0.54673600
H	3.82625200	-0.90637700	-0.77324900

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.79257700	-0.38924800	0.80686400
H	-2.62974600	-0.15361500	1.47071200
H	-1.59345200	-1.46711000	0.83153100

O	-1.26476600	-0.51778800	-1.38916500
O	-2.21174900	-0.01634900	-0.49705400
H	-0.20609900	-0.07324000	-0.87143000
C	0.56073300	0.32530700	0.10698000
C	-0.53614600	0.43105400	1.17490500
H	-0.17151300	0.08820300	2.15136100
H	-0.83852600	1.47626200	1.28575700
C	1.14940300	1.64863300	-0.35065100
H	1.76659700	2.09980900	0.43830700
H	1.77871300	1.52882900	-1.23654200
H	0.35453700	2.35765000	-0.59854000
C	1.47341600	-0.81662100	0.26320300
C	2.76181000	-0.87647100	-0.09997000
H	1.02718000	-1.70460800	0.71053700
H	3.34376200	-1.77945700	0.04651900
H	3.28084600	-0.03555800	-0.54643600

R30-C=CC(CC)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.06018900	-1.56929100	-0.49036300
C	2.20784600	-0.96864800	0.33280200
H	3.85187600	-2.21402700	-0.12372300
H	3.00175700	-1.43967100	-1.56770600
H	2.30286500	-1.12648400	1.40802600
C	1.08360600	-0.05380500	-0.08430900
H	1.12397600	0.05051300	-1.17729600
C	-0.25911700	-0.72640500	0.28871100
H	-0.28895300	-1.72200800	-0.16766900
H	-0.29896800	-0.87937700	1.37440500
C	-1.50378000	0.02819700	-0.14952600
H	-1.50637600	0.24840400	-1.22196000
H	-1.67469100	0.95271400	0.40634900
O	-2.64287600	-0.84385600	0.11680100
O	-3.77865200	-0.24675700	-0.16017100
C	1.27397200	1.35403400	0.54591900
H	0.79736900	1.37791900	1.53474500
H	2.34392600	1.50603800	0.72582900
C	0.76801400	2.51835800	-0.31441500
H	1.27852200	2.53434500	-1.28347300
H	-0.30653300	2.46558000	-0.51114200
H	0.96307900	3.47632200	0.17766400

P30-C=CC•(CC)CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	3.20239600	-1.05368700	-0.53082800
C	1.87211800	-1.24804600	-0.22888900
H	3.78706500	-1.83851200	-0.99513000
H	3.71944800	-0.12733300	-0.30978800
H	1.45042100	-2.22070900	-0.48138700
C	0.99959400	-0.34085000	0.37524500
C	-0.41812200	-0.75114000	0.67192200
H	-0.54927400	-1.82325100	0.49330000
H	-0.65077700	-0.57058500	1.73080000
C	-1.46013300	0.00886300	-0.16152500
H	-1.30570200	-0.16832000	-1.23556700
H	-1.40963000	1.08902000	0.02146700
O	-2.72676700	-0.48554600	0.24715600
C	1.43819100	1.05011000	0.76453200
H	0.75394200	1.44821900	1.52308100
H	2.42581200	1.00206200	1.24049400
C	1.51164200	2.04452000	-0.41388500
H	2.20438000	1.69037300	-1.18207800
H	0.53407900	2.17940100	-0.88661800
H	1.85475700	3.02510200	-0.06856400
O	-3.72849900	0.28809400	-0.44957900
H	-4.04651700	-0.36447100	-1.09005900

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.78401400	-0.99314600	0.63118100
H	-2.61871800	-1.00669000	1.33850800
H	-1.58970900	-2.01012900	0.27050300
O	-1.26762000	-0.33962100	-1.47336500
O	-2.20667400	-0.18132200	-0.45309300
H	-0.20046500	-0.12441700	-0.83628600
C	0.56357900	-0.05815800	0.21962500
C	-0.52081300	-0.36505500	1.26333300
H	-0.14000800	-1.05463600	2.02673400
H	-0.82007600	0.55301300	1.77464900
C	1.11589800	1.36518800	0.22077900
H	1.61409200	1.55050900	1.18471100
H	1.89635200	1.44351300	-0.54246600
C	1.50454600	-1.16601400	-0.01016600
C	2.79268100	-1.09294200	-0.37242100
H	1.07462200	-2.15896500	0.12361600
H	3.37858300	-1.99234500	-0.52573100
H	3.31024400	-0.15196700	-0.51935800
C	0.07258500	2.45903100	-0.04289900

R31-C=CCCCCO•

H	0.54875100	3.44397700	-0.04661200
H	-0.41271600	2.30596100	-1.01084500
H	-0.71338400	2.47629400	0.71766000

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-4.19457000	-0.18035100	0.52430400
C	-3.18988700	-0.20658600	-0.34544100
H	-5.09120800	-0.77434900	0.38260600
H	-4.16278400	0.44347400	1.41355700
H	-3.26510600	-0.84764500	-1.22417100
C	-1.91385500	0.57599900	-0.22290700
H	-1.80921600	1.24447300	-1.08998900
H	-1.95685000	1.21942000	0.66422400
C	-0.66789200	-0.32472500	-0.14887600
H	-0.75306300	-0.98205300	0.72565000
H	-0.64427200	-0.98447300	-1.02656300
C	0.63687400	0.47684000	-0.07286600
H	0.62290400	1.13401700	0.80493600
H	0.72988700	1.12670200	-0.95142000
C	1.85442200	-0.42766600	0.00569200
H	1.96175900	-1.06495700	-0.87771000
H	1.85181400	-1.05906100	0.89966200
O	3.03520800	0.42256800	0.07597700
O	4.13549000	-0.28964600	0.15399600

P31-C=CCC•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	4.29611100	0.37946400	0.24489200
C	3.13732500	0.37214600	-0.40544700
H	5.06015100	1.12355200	0.04607900
H	4.52968800	-0.36400700	1.00228800
H	2.93743200	1.13790100	-1.15386500
C	2.02499200	-0.62000200	-0.18593300
H	1.84654900	-1.18603800	-1.11330400
H	2.35779800	-1.37032800	0.55378000
C	0.74253400	0.01940300	0.24819200
H	0.80331700	0.86834500	0.92534800
C	-0.57928800	-0.64678400	0.05882500
H	-0.59466600	-1.20839600	-0.88441900
H	-0.76721300	-1.39407400	0.85060700
C	-1.73843500	0.34980100	0.07630700
H	-1.75140900	0.91779100	1.01584900
H	-1.65583000	1.06406200	-0.75523700

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O	-2.92925800	-0.41341900	-0.04228000
O	-4.03530200	0.50961700	0.06065900
H	-4.34876800	0.51743800	-0.85517400

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.08849200	1.28945400	0.01883500
H	-1.04292700	1.58379100	-1.03523400
H	-1.13842800	2.21003600	0.61782300
C	-2.39703900	0.49717900	0.24279900
H	-3.25912300	1.02460900	-0.17693400
H	-2.56533000	0.30022100	1.30854400
O	-1.36123100	-1.52395300	0.19792300
O	-2.31571800	-0.72848200	-0.46447800
H	-0.45489700	-0.78667400	0.23944400
C	0.12748700	0.46449900	0.38091700
H	0.35258200	0.43003800	1.45032500
C	1.35284300	0.55173300	-0.50697900
H	1.78520300	1.56307300	-0.43719000
H	1.03724100	0.42841300	-1.55307800
C	2.40571500	-0.46700000	-0.16732400
C	3.64250200	-0.18592500	0.22863600
H	2.09288400	-1.50682500	-0.25558600
H	4.35957200	-0.96541600	0.46293600
H	3.99072400	0.83856400	0.33008300

R32-C=CCC(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.67914000	-1.10814100	-0.33959700
C	2.37433300	-1.08088500	-0.08460700
H	4.10938600	-1.79868600	-1.05735500
H	4.37214900	-0.44288900	0.16870300
H	1.71034400	-1.76066500	-0.61749700
C	1.69629000	-0.14376400	0.88766900
H	1.17423300	-0.73379500	1.65283600
H	2.47699300	0.42861500	1.41585400
C	0.71671600	0.79199000	0.22851300
C	-0.72210200	0.81336500	0.65013000
H	-0.82478700	0.54258200	1.70873600
H	-1.14707000	1.81768400	0.53155100
C	-1.58547800	-0.15764100	-0.17480900
H	-1.53694700	0.08766900	-1.24312700
H	-1.24320200	-1.19453800	-0.04352000
O	-2.91695500	-0.01473700	0.29602700

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O	-3.75263100	-0.85895700	-0.52808700
H	-3.96386800	-1.56704700	0.09723100
C	1.20862500	1.78710800	-0.77365500
H	0.45571400	2.00239200	-1.54156200
H	1.45112900	2.75523100	-0.30145500
H	2.11746200	1.44081400	-1.27576800

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.67914000	-1.10814100	-0.33959700
C	2.37433300	-1.08088500	-0.08460700
H	4.10938600	-1.79868600	-1.05735500
H	4.37214900	-0.44288900	0.16870300
H	1.71034400	-1.76066500	-0.61749700
C	1.69629000	-0.14376400	0.88766900
H	1.17423300	-0.73379500	1.65283600
H	2.47699300	0.42861500	1.41585400
C	0.71671600	0.79199000	0.22851300
C	-0.72210200	0.81336500	0.65013000
H	-0.82478700	0.54258200	1.70873600
H	-1.14707000	1.81768400	0.53155100
C	-1.58547800	-0.15764100	-0.17480900
H	-1.53694700	0.08766900	-1.24312700
H	-1.24320200	-1.19453800	-0.04352000
O	-2.91695500	-0.01473700	0.29602700
O	-3.75263100	-0.85895700	-0.52808700
H	-3.96386800	-1.56704700	0.09723100
C	1.20862500	1.78710800	-0.77365500
H	0.45571400	2.00239200	-1.54156200
H	1.45112900	2.75523100	-0.30145500
H	2.11746200	1.44081400	-1.27576800

TS32

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.16868600	1.00371600	0.74456200
H	1.09039600	0.76333800	1.80954700
H	1.27708400	2.09431300	0.65729800
C	2.45862500	0.34534800	0.20240200
H	3.31340600	0.55281300	0.85350200
H	2.68279800	0.68227600	-0.81691300
O	1.34964600	-1.37688400	-0.77466100
O	2.29893400	-1.06307300	0.21571400
H	0.46501200	-0.64534000	-0.46060500
C	-0.06920800	0.51902400	0.00129900

R33-C=CCOO•

C	-1.25436600	0.12395300	0.87747500
H	-1.72624900	1.03423100	1.28241400
H	-0.87261800	-0.43606100	1.74189300
C	-2.29122500	-0.70541000	0.17067600
C	-3.56986900	-0.37535000	0.01986200
H	-1.92949100	-1.65020900	-0.23441200
H	-4.27195600	-1.02491700	-0.49201400
H	-3.96852600	0.55749100	0.40961100
C	-0.40379000	1.27790300	-1.26684100
H	-1.20444300	0.78985200	-1.82839700
H	-0.74621300	2.29601400	-1.02669400
H	0.46903700	1.37075600	-1.92026500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.32345800	0.13895400	-0.26716500
C	1.21630500	-0.36510100	0.26701700
H	2.35079200	1.14240800	-0.68233200
H	3.24886800	-0.42546200	-0.30275700
H	1.20908100	-1.37364800	0.67400400
C	-0.06793300	0.38738600	0.37541700
H	-0.41691200	0.48496100	1.40810800
H	-0.00908200	1.37950500	-0.08143600
O	-1.10257800	-0.37018700	-0.33678500
O	-2.29913800	0.09828700	-0.07161500

P33-•C=CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.43242300	0.18102000	-0.34720000
C	1.36377900	-0.25364700	0.26834400
H	3.46631300	-0.10595500	-0.46875800
H	1.39483100	-1.18406500	0.84620800
C	0.03196100	0.44783200	0.26992400
H	-0.24026600	0.75678700	1.28824100
H	0.05151900	1.33625000	-0.37370100
O	-0.92106200	-0.50275700	-0.19736400
O	-2.22479500	0.08502300	0.00596300
H	-2.47452600	0.28762100	-0.90719100

TS33

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.35645100	-0.83274300	-0.08208800
H	0.04994700	-1.28999500	0.00517900
C	-1.21069600	0.46640100	0.00849900

H	-2.05091200	1.16268300	-0.03617900
C	0.17116800	1.08585800	0.18265800
H	0.25563500	2.03950200	-0.34819500
H	0.38198600	1.24849600	1.24947700
O	1.15390100	0.25378800	-0.40322000
O	1.08787700	-1.00014900	0.23604900
H	-2.19500700	-1.50689200	-0.18733000

R34-(trans)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.64596500	0.32705700	-0.23290000
C	0.57009500	-0.08521700	0.43528500
H	1.53907800	1.15657900	-0.93220600
H	0.64662400	-0.91407500	1.13650200
C	-0.77700300	0.53559700	0.29539500
H	-1.20987600	0.84764600	1.25046200
H	-0.77429000	1.38456700	-0.39454400
O	-1.69668500	-0.47269400	-0.25403400
O	-2.94534600	-0.08550100	-0.14544400
C	3.02176600	-0.24897300	-0.10302700
H	3.73747100	0.51273400	0.22973900
H	3.04809900	-1.07826500	0.60886800
H	3.38419900	-0.61440900	-1.07151600

P34-CC•=CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.74309100	0.12803000	0.24754500
C	0.65401200	0.11231300	-0.48113800
H	0.68557100	-0.25696400	-1.51311000
C	3.17327600	-0.18636200	0.17053600
H	3.43985300	-0.58937400	-0.81980000
H	3.78909500	0.70343900	0.34536000
H	3.45807400	-0.93182200	0.92187500
C	-0.69390000	0.58180500	-0.01035000
H	-0.64541400	0.94589100	1.02393000
H	-1.07571100	1.38902600	-0.64970400
O	-1.57130300	-0.53932000	-0.11309900
O	-2.90844700	-0.04544800	0.12774300
H	-3.07233600	-0.39676300	1.01473400

TS34

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.04446200	0.01432800	0.01103100
H	-0.06831100	-1.04831000	0.07781500

C	-0.25989600	1.06844100	0.04481300
H	-0.64959900	2.08785600	-0.00561600
C	1.25024100	0.91927700	0.15114300
H	1.77386000	1.69390400	-0.41872200
H	1.57179400	0.97071500	1.20169400
O	1.66094300	-0.30392300	-0.43493800
O	1.00396700	-1.34334400	0.25251900
C	-2.49501900	-0.25793500	-0.06466800
H	-2.84047200	-0.82141400	0.80959500
H	-3.06564300	0.68057800	-0.10774900
H	-2.74610000	-0.84986000	-0.95158100

R35-(trans)-CCC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.03700300	-0.01728000	-0.35180300
C	0.04242200	0.12203000	0.41604100
H	-0.97536600	-0.66445900	-1.22822000
H	0.00755000	0.76225900	1.29558100
C	1.33816800	-0.56559400	0.15443900
H	1.70510600	-1.13495400	1.01362100
H	1.29255700	-1.22079700	-0.72036600
O	2.35953300	0.45775900	-0.11739100
O	3.56557800	-0.05774200	-0.09306400
C	-2.37116700	0.62331800	-0.10789200
C	-3.49696300	-0.40791600	0.07943800
H	-2.61941400	1.26456800	-0.96491900
H	-2.31264600	1.27892100	0.76797500
H	-4.46118200	0.08947100	0.21965600
H	-3.58173900	-1.06307800	-0.79401700
H	-3.30850400	-1.03942600	0.95299100

P35-CC•C=CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.12866100	0.11337300	-0.19434600
C	-0.01842800	0.22215700	0.49398900
H	0.02571100	0.88045100	1.36988900
C	1.25663900	-0.50882800	0.17924900
H	1.57344600	-1.13096000	1.02712100
H	1.13549400	-1.15143000	-0.70228300
O	2.24897900	0.49039800	-0.05321900
C	-2.52025900	0.58604500	-0.20488700
C	-3.55119400	-0.54422800	-0.03432600
H	-2.71653200	1.11837200	-1.14512500
H	-2.65063500	1.33139800	0.59913700

TS35

H	-4.56778800	-0.14094200	-0.05142900
H	-3.46036200	-1.27935600	-0.83890900
H	-3.40380700	-1.06529600	0.91582900
O	3.51907700	-0.19495500	-0.13731100
H	3.69143700	-0.13689900	-1.08806200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.51595500	0.32014700	-0.22384200
H	0.23337400	-0.91420300	-0.20796700
C	0.42473700	1.18019700	0.09828200
H	0.23303300	2.25295600	0.17656100
C	1.84867700	0.71998900	0.37280100
H	2.58442600	1.44837200	0.01617900
H	2.00168100	0.55722700	1.44982200
O	2.12762200	-0.46432000	-0.35363500
O	1.19552900	-1.43968800	0.05283800
C	-1.96434900	0.35014900	-0.53317400
H	-2.30081300	1.39898300	-0.52499400
H	-2.12826500	-0.01854200	-1.55379500
C	-2.81362900	-0.47644200	0.44736800
H	-3.87169000	-0.42408600	0.17508400
H	-2.51137100	-1.52783500	0.43682300
H	-2.70246800	-0.10503900	1.47005100

R36-C=CC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.78976800	-0.87830700	-0.25783400
C	-1.81144100	-0.26221300	0.39677200
H	-2.74671500	-1.03847300	-1.33161100
H	-3.67567000	-1.24358600	0.25052800
H	-1.89685600	-0.11737400	1.47429100
C	-0.55327200	0.28307600	-0.22912200
H	-0.60004800	0.11282700	-1.31184700
C	0.64786500	-0.49848900	0.30635600
H	0.80636500	-0.33704200	1.37753600
H	0.55807800	-1.57090800	0.11287900
O	1.83960200	-0.02719700	-0.38748900
O	2.92589200	-0.59023000	0.08852600
C	-0.40386100	1.79224700	0.03476700
H	-0.38604900	1.99948200	1.11101100
H	0.52363700	2.17518300	-0.39797300
H	-1.24382900	2.34141600	-0.39875300

P36-C=C•C(C)COO

TS36

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.96232000	-0.66133300	0.26359000
C	-1.77456000	-0.67433700	-0.28505600
H	-3.34612600	0.20991300	0.80352500
H	-3.63758600	-1.51230600	0.20851600
C	-0.58314900	0.17725500	-0.46836100
H	-0.40777800	0.29849400	-1.54678300
C	-0.76387000	1.57964900	0.15440600
H	0.13284700	2.18137300	-0.01026100
H	-1.61876800	2.09296200	-0.29322700
H	-0.93657500	1.50189800	1.23273500
C	0.65283200	-0.54632700	0.09425300
H	0.73833200	-1.55301800	-0.33003600
H	0.58460200	-0.63172600	1.18836600
O	1.78097900	0.23397500	-0.27498100
O	2.95135200	-0.47382500	0.18305400
H	3.21881300	0.08176100	0.92958600

R37-C=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600

H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100
C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

P37-C=C•CCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.10608200	-0.30446000	-0.21976300
C	1.95343600	-0.05707500	0.34623700
H	3.35094100	0.07116200	-1.21898400
H	3.88426500	-0.88741600	0.26728000
C	0.68340500	0.63918800	0.09524100
H	0.52069200	1.42313100	0.84546300
H	0.71590400	1.14274400	-0.88568000
C	-0.51367700	-0.31860900	0.12880800
H	-0.59102600	-0.81126500	1.10500800
H	-0.41526700	-1.09242800	-0.64493700
O	-1.65968000	0.48407200	-0.10774600
O	-2.81010100	-0.37689700	0.02402200
H	-3.08273600	-0.45759300	-0.90149200

TS37

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.29901800	1.15121100	-0.17124000
H	0.22533800	1.48514200	-1.21318300
H	0.73799100	1.96978500	0.41644400
C	-1.13054700	0.86124100	0.34179600
H	-1.81232100	1.68083500	0.09732200
H	-1.13321200	0.68208500	1.42291700
O	-0.92269600	-1.39797400	0.12749000
O	-1.64129200	-0.27432800	-0.33728300
H	0.13681000	-1.08267600	-0.09166100
C	1.14468700	-0.06741500	-0.09245800
C	2.41926300	-0.34932700	0.05672000
H	2.79110800	-1.36878200	0.09535300
H	3.17166600	0.43776400	0.14224100

R38-C=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	3.04555100	0.12476000	0.13592000
C	1.96013500	-0.39298900	-0.43011200
H	3.08603900	0.34352300	1.19929100
H	3.93983200	0.34291100	-0.43787900
H	1.96473200	-0.59864500	-1.50046700
C	0.68725200	-0.73697800	0.29058600
H	0.47162100	-1.80720800	0.17379000
H	0.79227500	-0.54311700	1.36385100
C	-0.51633400	0.03922700	-0.25228400
H	-0.62376300	-0.11705900	-1.33097300
O	-1.69106900	-0.60382300	0.35785600
O	-2.80695800	-0.22447000	-0.21852700
C	-0.52312600	1.52213300	0.07881600
H	-0.45860600	1.67507900	1.16079600
H	0.33373800	2.01257500	-0.39047400
H	-1.44251000	1.98136800	-0.29011900

P38-C=C•CC(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.21116900	0.10439100	-0.03499500
C	2.02669600	-0.34688600	-0.35778500
H	3.49998800	0.27479700	1.00762600
H	3.97395700	0.32906900	-0.77695100
C	0.76075300	-0.78334000	0.24621300
H	0.57835600	-1.84089100	0.01944900
H	0.81873500	-0.70089100	1.34560600
C	-0.45415300	0.02134800	-0.25305300
H	-0.51288300	-0.06125100	-1.34578700
O	-1.56775200	-0.67610400	0.31190400
O	-2.76670400	-0.16939400	-0.31489100
H	-3.17479600	0.29858600	0.42710500
C	-0.42279300	1.48795200	0.15982600
H	-0.37712800	1.57846800	1.25078400
H	0.45545700	1.98247600	-0.26392800
H	-1.31607000	2.00283100	-0.20123300

TS38

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.24905800	-1.01037000	-0.17088700
H	-0.05285100	-1.29229500	-1.21327400
C	0.97258400	-0.20070300	0.33750300
H	0.86254400	-0.01190700	1.41265900
O	-0.11830100	1.80928000	0.13562700
O	0.97487200	1.05507000	-0.34031100

H	-0.97051000	1.11069100	-0.08279700
C	-1.50199400	-0.21882300	-0.08926800
C	-2.78550400	-0.45730000	0.05920100
H	-3.52556900	0.33633100	0.10025100
H	-3.17178700	-1.47566200	0.14170900
C	2.30309100	-0.86854900	0.03009800
H	3.13023100	-0.26270700	0.40767300
H	2.34854000	-1.85358400	0.50318400
H	2.43067200	-0.99638600	-1.04910100
H	-0.33855200	-1.93480900	0.41729000

R39-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000
C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100
H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900
H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

P39-C=C•C(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.06216700	-0.60030800	-0.23833800
C	-1.84954500	-0.36912200	-0.67279400
H	-3.50067400	-0.04046900	0.59369100
H	-3.70495100	-1.35667200	-0.68341600
C	-0.68135800	0.49823900	-0.43006300
H	-0.50168300	1.08548000	-1.34122300
C	0.59654500	-0.36203000	-0.24990400
H	0.69094200	-1.01041100	-1.12980200
O	1.66205000	0.59364100	-0.28636500

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O	2.90116000	-0.13268500	-0.43770900
H	3.30389800	0.01260000	0.42996200
C	0.62850800	-1.21399300	1.01478000
H	0.59731200	-0.59258200	1.91467100
H	-0.22755000	-1.89409800	1.03278200
H	1.54226400	-1.81232500	1.03694000
C	-0.92348300	1.49473000	0.72751200
H	-1.75392200	2.16119500	0.48050000
H	-1.17343500	0.97522700	1.65649800
H	-0.02888700	2.09931000	0.89484200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.29824900	0.64630900	-0.33774000
H	0.10619500	0.76399200	-1.41365100
C	-1.02095600	0.07495800	0.26825300
H	-0.91412700	0.00326100	1.35886700
O	-0.24841900	-2.09255300	0.30798200
O	-1.22217600	-1.23789400	-0.25260700
H	0.68648500	-1.56481100	-0.00324000
C	1.40469400	-0.33934600	-0.17754900
C	2.71417600	-0.30619900	-0.06922400
H	3.30991900	-1.20500600	0.06030800
H	3.27304000	0.63101100	-0.11360600
C	-2.26621700	0.86446700	-0.10873900
H	-3.15403400	0.36774200	0.28985900
H	-2.22620000	1.87572600	0.30216600
H	-2.36803500	0.93302300	-1.19620700
C	0.66470100	2.01786700	0.26392300
H	0.81051900	1.94076700	1.34563400
H	1.59205200	2.39485500	-0.17527200
H	-0.11893600	2.75468100	0.06859100

R40-(cis)-CC=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.44545000	0.40357200	-0.26473500
C	-1.26639800	0.94827300	0.03924300
H	-3.19585100	1.05813000	-0.70576800
H	-1.12578500	2.00609800	-0.17936600
C	-2.89161000	-1.01525800	-0.06752800
H	-2.11964700	-1.65306700	0.36828700
H	-3.77066200	-1.05714400	0.58738600
H	-3.19618100	-1.46086600	-1.02250900
C	-0.07029400	0.27028700	0.65047200

P40-CC=C•CCOO

H	-0.29225600	-0.75924000	0.94279400
H	0.23313100	0.80184600	1.56205800
C	1.11066900	0.27214600	-0.31462600
H	1.38676700	1.28182600	-0.63403300
H	0.92669200	-0.34335600	-1.19938000
O	2.25418500	-0.29279400	0.38898400
O	3.31235100	-0.35074900	-0.38603700

TS40

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.54040800	-0.49716000	-0.30203300
C	1.31531000	-0.81572200	0.03828900
C	0.10813000	-0.25926700	0.66861400
H	-0.15545100	-0.83029700	1.56788300
H	0.28796600	0.77731100	1.00005800
C	-1.09468200	-0.27314200	-0.28261600
H	-1.33054600	-1.29641900	-0.59694500
H	-0.88899600	0.32757500	-1.17942500
O	-2.17851100	0.27659800	0.45063900
O	-3.34983800	0.17164700	-0.38624100
H	-3.47587500	1.09799700	-0.63786200
H	3.16655000	-1.25159100	-0.78247800
C	3.20652400	0.84720500	-0.08611300
H	4.09781800	0.74110000	0.54363400
H	3.53710200	1.27411200	-1.04038800
H	2.53407700	1.56277600	0.39349300

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.11589700	1.06883600	-0.18118900
H	-0.15165500	1.41857900	-1.22024000
C	-1.56947000	0.94795600	0.33545300
H	-2.15243300	1.83925800	0.08552000
H	-1.58852400	0.78056400	1.41844700
O	-1.62956800	-1.32223300	0.14885000
O	-2.21232100	-0.12613800	-0.32939000
H	-0.54355600	-1.13115100	-0.07109200
C	0.57985500	-0.24250600	-0.10538200
C	1.81351100	-0.69039500	0.00203000
H	1.98229000	-1.76567900	0.05630000
C	3.05951700	0.16390600	0.04716800
H	2.82532300	1.23088900	0.02160500
H	3.63595900	-0.04199200	0.95687700
H	3.71341600	-0.06133400	-0.80370000

	H	0.40919000	1.83105100	0.41212100
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R41-(trans)-CC=CCCO•

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	2.18039800	0.25134600	0.16956800	
C	0.96255100	0.11084000	-0.34894500	
H	2.42759200	1.18040000	0.68494900	
H	0.70499300	-0.81239600	-0.86581600	
C	3.27398900	-0.77212300	0.10336900	
H	2.94976000	-1.67374300	-0.42398500	
H	4.15778100	-0.37517800	-0.41150500	
H	3.60471500	-1.06464700	1.10769900	
C	-0.12554600	1.14631900	-0.27553400	
H	0.23107500	2.03511100	0.25701400	
H	-0.41235000	1.47438200	-1.28398100	
C	-1.38506000	0.65537800	0.43175200	
H	-2.13953800	1.44216900	0.52684700	
H	-1.17373400	0.23086700	1.41680000	
O	-1.96498300	-0.40359600	-0.38523800	
O	-3.00855400	-0.94484300	0.19907800	

P41-CC=C•CCOO

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-2.44649900	0.18821300	0.36208000	
C	-1.30607700	0.22828500	-0.28219200	
C	0.04266000	0.80235500	-0.16483600	
H	0.27018700	1.44110800	-1.02759500	
H	0.09938200	1.44882700	0.72744200	
C	1.12371900	-0.28090200	-0.06771800	
H	1.10989200	-0.92517000	-0.95465300	
H	0.96677300	-0.90833700	0.82050300	
O	2.36163200	0.40796300	0.01756400	
O	3.40224300	-0.59233800	0.00108700	
H	3.69731500	-0.56115100	0.92263700	
C	-3.69140800	-0.53569600	-0.07936100	
H	-3.99653200	-1.28006900	0.66602200	
H	-4.53026300	0.16139900	-0.19329200	
H	-3.53567300	-1.04592900	-1.03240000	
H	-2.52645700	0.73079300	1.31429700	

TS41

Cartesian Coordinates (Å)				
At.	X	Y	Z	
C	-0.60921800	1.30346600	-0.16598600	
H	-0.81738900	1.61100600	-1.19812900	

C	-1.85471300	0.56064000	0.37012200
H	-2.77057800	1.12061400	0.15968400
H	-1.76976800	0.37322100	1.44664500
O	-0.93966400	-1.51036200	0.09717000
O	-1.99396600	-0.66848100	-0.32428400
H	-0.04471900	-0.86667000	-0.13248000
C	0.58552100	0.42199300	-0.12432300
C	1.88673100	0.56444000	0.01288400
H	-0.44641000	2.21245900	0.43066700
H	2.28528400	1.58137900	0.10594600
C	2.90636500	-0.53978100	0.04664400
H	3.63089200	-0.42835400	-0.76895000
H	3.47719300	-0.51559100	0.98251200
H	2.43643200	-1.52187400	-0.04503200

R42-C=CCCCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-4.19458300	-0.18033700	0.52429400
C	-3.18988700	-0.20659300	-0.34543600
H	-5.09122400	-0.77433000	0.38259000
H	-4.16280400	0.44349700	1.41354000
H	-3.26509800	-0.84766500	-1.22415700
C	-1.91385300	0.57599100	-0.22290000
H	-1.80920800	1.24445900	-1.08998600
H	-1.95685500	1.21942100	0.66422400
C	-0.66789100	-0.32473000	-0.14885400
H	-0.75304500	-0.98202400	0.72570000
H	-0.64428600	-0.98451200	-1.02651500
C	0.63687800	0.47683800	-0.07289800
H	0.62292000	1.13405300	0.80487500
H	0.72987700	1.12666000	-0.95148200
C	1.85442500	-0.42766600	0.00568900
H	1.96178200	-1.06496600	-0.87770300
H	1.85179900	-1.05905100	0.89966600
O	3.03520800	0.42257100	0.07599000
O	4.13549200	-0.28964200	0.15399500

P42-C=CC•CCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	4.34426000	-0.42740500	-0.22979600
C	3.11256400	0.17901600	-0.38385000
H	5.14521400	-0.27306100	-0.94214700
H	4.54835600	-1.07953200	0.61323200
H	2.97364700	0.82359100	-1.25229900

C	2.03455300	0.04126300	0.47414700
H	2.14553000	-0.60041100	1.34759500
C	0.70609000	0.70177100	0.28721600
H	0.49207800	1.35746700	1.14566400
H	0.73362100	1.34935100	-0.59769100
C	-0.45150200	-0.30985500	0.15533000
H	-0.47529900	-0.96572100	1.03296800
H	-0.28457200	-0.95187900	-0.71633200
C	-1.80137900	0.38686600	0.02246300
H	-1.82961100	1.02859800	-0.87126800
H	-2.00936200	1.01572000	0.89863500
O	-2.77914600	-0.63696800	-0.07783000
O	-4.06966700	0.01244900	-0.11833200
H	-4.31661400	-0.13790700	-1.04212200

TS42

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.90169600	0.57891900	-0.33226900
C	-0.62909700	1.40820700	-0.14250900
C	0.29223000	0.98477700	1.02444000
H	-2.49574800	0.52295000	0.58790300
H	-0.08041600	1.39905900	-1.08933200
H	-2.51542100	1.01491200	-1.12805700
H	-0.29138400	1.01216400	1.95167800
H	-0.08294100	-1.14790200	0.52461700
O	-1.23153700	-1.52230500	0.29631800
O	-1.63440200	-0.75147700	-0.78615500
H	1.08142400	1.74053900	1.13790400
C	0.92896600	-0.39716300	0.90316300
C	2.00813600	-0.65463400	-0.04079600
C	2.51054700	0.18866800	-0.96072200
H	2.43815900	-1.65358100	0.01945600
H	3.31714800	-0.11549500	-1.61821500
H	2.15654400	1.20707400	-1.07372700
H	-0.94235400	2.44567100	0.03052500
H	1.08799700	-0.88777300	1.86809900

R43-C=CC(C)CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.79460800	-1.17735900	-0.35666400
C	2.92815500	-0.46032200	0.35087800
H	4.62829900	-1.69204100	0.10926600
H	3.70627400	-1.27758900	-1.43517400
H	3.05649900	-0.38462200	1.43182100

C	0.43495500	-0.30535600	0.36138000
H	0.45070500	-1.39034500	0.19989400
H	0.41819900	-0.15811000	1.45042100
C	-0.84446000	0.27619300	-0.25477100
H	-0.81428400	0.17495000	-1.34653100
H	-0.93010700	1.34586100	-0.03720500
C	-2.08362700	-0.42723000	0.27212800
H	-2.19720500	-0.32150000	1.35568000
H	-2.10441600	-1.49110800	0.01630500
O	-3.24505400	0.19395300	-0.35028100
O	-4.36206500	-0.36855600	0.04961100
C	1.74476000	0.28687900	-0.20737900
H	1.73494500	0.14238800	-1.29630000
C	1.88215300	1.79318800	0.08155600
H	1.06894900	2.37029900	-0.36785000
H	1.87480500	1.98619300	1.16090200
H	2.82503700	2.17648900	-0.31863400

P43-C=CC•(C)CCCCO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.99312500	-0.75625300	-0.50769400
C	2.72604200	-0.86796400	0.02296200
H	4.61644000	-1.63139000	-0.64535200
H	4.41603500	0.19518500	-0.80824000
H	2.39077300	-1.87299600	0.27873500
C	0.44416900	-0.15623400	0.80474600
H	0.39952500	-1.20622900	1.11648800
H	0.25207900	0.44877800	1.70417000
C	-0.68818100	0.11784500	-0.20966400
H	-0.52729400	-0.48241900	-1.11201100
H	-0.67449700	1.16859100	-0.51830600
C	-2.05929400	-0.20328500	0.37486200
H	-2.25867400	0.40001000	1.27082000
H	-2.13080100	-1.26471900	0.65681400
O	-3.01234500	0.10192000	-0.63188200
C	1.81411500	0.15810300	0.26913800
C	2.12793400	1.59985300	-0.01970400
H	1.58172500	2.26540300	0.65791000
H	3.19447200	1.81663800	0.08518100
H	1.84125200	1.88607800	-1.04171800
O	-4.32032000	-0.12083600	-0.05861100
H	-4.58717600	-0.92399400	-0.52841400

TS43

Cartesian Coordinates (Å)

At.	X	Y	Z
C	-2.34708600	0.02798900	-0.22309300
C	-1.38477300	0.97820600	-0.93898000
C	-0.15472800	1.42095000	-0.12157600
H	-2.72149200	0.46199000	0.71175500
H	-1.07994500	0.52047000	-1.88685100
H	-3.19735700	-0.20752400	-0.87264700
H	-0.50550300	1.87545400	0.81281000
H	0.06524100	-0.55677200	0.76082900
O	-0.96085700	-1.12175200	1.19761600
O	-1.76332700	-1.24579700	0.06923700
H	0.36649000	2.21791800	-0.67147400
C	0.86140200	0.32530600	0.23841400
C	1.45829800	-0.39561400	-0.89147800
C	2.70527800	-0.88670300	-0.96541600
H	0.80094300	-0.56293000	-1.74171800
H	3.04269900	-1.42425000	-1.84464600
H	3.42967200	-0.76735500	-0.16754000
H	-1.95672900	1.87547100	-1.20797800
C	1.77896200	0.70760800	1.38759500
H	2.38624700	-0.13657400	1.72436600
H	2.46276800	1.51550600	1.09277800
H	1.19631900	1.06254000	2.24268100

R44-C=CCCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	4.83621000	0.18722300	0.55687500
C	3.83978500	0.21048200	-0.32246100
H	5.73161900	0.78540000	0.42509700
H	4.79811500	-0.43772800	1.44512900
H	3.92098600	0.85369700	-1.19915800
C	2.56504900	-0.57655000	-0.21442600
H	2.47515000	-1.24692700	-1.08201800
H	2.60106400	-1.21933200	0.67374000
C	1.31415100	0.31807100	-0.15741400
H	1.38391100	0.97780600	0.71670200
H	1.29777200	0.97686000	-1.03606700
C	0.00822500	-0.48115500	-0.09698100
H	0.02617700	-1.14191300	0.78039300
H	-0.05526700	-1.14087200	-0.97318600
C	-1.23610400	0.41327400	-0.03784700
H	-1.26982500	1.06770800	-0.91708700
H	-1.18599400	1.06793400	0.84043300
C	-2.51743900	-0.39985100	0.02408600

P44-C=CCC•CCCOO

H	-2.57136800	-1.03067900	0.91694400
H	-2.66029200	-1.02707900	-0.86148500
O	-3.63437800	0.53331800	0.08171900
O	-4.78453600	-0.09754800	0.13822700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-4.95888400	-0.38281500	-0.23307300
C	-3.81210600	-0.32358700	0.43570600
H	-5.73588800	-1.09526600	0.02315100
H	-5.16863200	0.28454000	-1.06476900
H	-3.63556900	-1.01348600	1.25990600
C	-2.68314700	0.62891300	0.14007900
H	-2.99296200	1.30593400	-0.67667500
H	-2.51541600	1.28313000	1.01011500
C	-1.40022400	-0.06369100	-0.20213900
C	-0.07620700	0.61118200	-0.06396600
H	-0.05321300	1.19430400	0.86903100
H	0.05762200	1.36098100	-0.86724900
C	1.11004100	-0.36376900	-0.10012400
H	1.09609500	-0.93192600	-1.03736500
H	1.01673600	-1.09221700	0.71306000
C	2.44867400	0.35555000	0.01859500
H	2.51920800	0.90775500	0.96809400
H	2.58704000	1.07254600	-0.80188200
O	3.45475700	-0.64412100	-0.04195800
O	4.72971800	0.03533200	-0.01482000
H	5.03716300	-0.19655300	0.87323500
H	-1.45686300	-0.98012800	-0.78490300

TS44

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.41786200	0.47362400	-0.43061700
C	-1.21633300	1.41239200	-0.29896600
C	-0.27829100	1.12979200	0.89320300
H	-3.04948700	0.49748100	0.46561600
H	-0.65319700	1.39353600	-1.23937200
H	-3.02378300	0.76132900	-1.29740500
H	-0.85454100	1.19546200	1.82418500
H	-0.63922500	-1.06949300	0.74230500
O	-1.69609500	-1.49837200	0.51972000
O	-2.05144400	-0.88292600	-0.69398300
H	0.47008300	1.93497200	0.94846000
C	0.42826900	-0.21516800	0.86090000

H	-1.60773600	2.43256200	-0.19759600
C	2.55594600	0.27349700	-0.38651200
C	3.79554300	-0.17205100	-0.20607600
H	2.39546400	1.33242100	-0.58453000
H	4.65482800	0.48824500	-0.25939500
H	4.00151900	-1.22004200	-0.00578300
C	1.31331700	-0.58180500	-0.32123500
H	0.74146500	-0.48268700	-1.25192100
H	1.60380100	-1.63449700	-0.23950000
H	0.85758200	-0.50059300	1.82485700

R45-C=CCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600
H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100
C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

P45-•CCCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.02145000	0.23831500	0.45714200
C	-2.01214500	0.09172100	-0.36193300
H	-3.99971100	0.69552500	0.45623300
H	-2.07103900	0.53950300	-1.36270500
C	-0.72752400	-0.64074500	-0.05746100
H	-0.78982000	-1.12064400	0.92257900
H	-0.56363900	-1.42902000	-0.80260300
C	0.47208300	0.30893200	-0.09405700
H	0.53411600	0.82884600	-1.05939000
H	0.39475300	1.06545600	0.69938100
O	1.62491200	-0.49686900	0.09476200
O	2.77167300	0.37323000	-0.02196700
H	3.05687200	0.42011200	0.90199600

TS45

Cartesian Coordinates (Å)

R46-C=CCC(C)OO•

At.	X	Y	Z
C	-0.02606100	-1.28368300	0.14972100
C	-1.39880500	-0.60700600	-0.12608400
C	-0.34082500	1.58013600	-0.33485100
C	-1.14691100	0.79613300	0.37614900
H	0.17588600	-1.35135200	1.22182900
H	-1.59900700	-0.62401300	-1.20150200
H	-0.17212200	1.51183400	-1.40898100
H	0.02521700	-2.28196300	-0.29987600
H	-2.19960600	-1.14698200	0.39274400
H	-1.18444800	0.91167900	1.46062500
H	0.82231900	1.39841300	0.22107400
O	1.64056000	0.38579700	0.37321100
O	1.06036100	-0.55218300	-0.47015000

P46-•C=CCC(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.04555100	0.12476000	0.13592000
C	1.96013500	-0.39298900	-0.43011200
H	3.08603900	0.34352300	1.19929100
H	3.93983200	0.34291100	-0.43787900
H	1.96473200	-0.59864500	-1.50046700
C	0.68725200	-0.73697800	0.29058600
H	0.47162100	-1.80720800	0.17379000
H	0.79227500	-0.54311700	1.36385100
C	-0.51633400	0.03922700	-0.25228400
H	-0.62376300	-0.11705900	-1.33097300
O	-1.69106900	-0.60382300	0.35785600
O	-2.80695800	-0.22447000	-0.21852700
C	-0.52312600	1.52213300	0.07881600
H	-0.45860600	1.67507900	1.16079600
H	0.33373800	2.01257500	-0.39047400
H	-1.44251000	1.98136800	-0.29011900

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.13910400	0.17584200	-0.17388300
C	2.08261100	-0.36158300	0.38011000
H	4.12512500	0.50123100	0.12297400
H	2.09804300	-0.56885500	1.45852800
C	0.80411700	-0.73962000	-0.32698300
H	0.89826000	-0.55362500	-1.40082200
H	0.61556800	-1.81158200	-0.19200500
C	-0.41383300	0.01807100	0.22684600

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H	-0.45572200	-0.11050500	1.31788000
O	-1.53093200	-0.67073500	-0.34301700
O	-2.72654200	-0.19752100	0.31801800
H	-3.14769200	0.29423700	-0.40084000
C	-0.41695300	1.50279700	-0.12020600
H	0.46386900	1.99473800	0.30126600
H	-0.39914300	1.64047000	-1.20679100
H	-1.30879100	1.98689500	0.28450200

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.85723700	-0.06109600	-0.31597600
C	-0.15327400	-1.41010500	0.03229900
C	1.97588800	-0.29819900	0.46807800
C	1.28530400	-1.11953400	-0.31864900
H	-0.75963500	0.13822300	-1.38729700
H	-0.27962300	-1.61019800	1.10124200
H	1.79478700	-0.13172500	1.52947500
H	-0.60653900	-2.22974200	-0.53742100
H	1.51703100	-1.15435900	-1.38452400
H	1.82265800	0.85951800	-0.10660200
O	0.80873100	1.64960000	-0.36381900
O	-0.19327200	1.04273200	0.37648500
C	-2.31354600	-0.01142600	0.12807100
H	-2.77789500	0.92978800	-0.17475800
H	-2.87129100	-0.83860100	-0.32056200
H	-2.38598200	-0.09939200	1.21617600

R47-C=CC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.78976800	-0.87830700	-0.25783400
C	-1.81144100	-0.26221300	0.39677200
H	-2.74671500	-1.03847300	-1.33161100
H	-3.67567000	-1.24358600	0.25052800
H	-1.89685600	-0.11737400	1.47429100
C	-0.55327200	0.28307600	-0.22912200
H	-0.60004800	0.11282700	-1.31184700
C	0.64786500	-0.49848900	0.30635600
H	0.80636500	-0.33704200	1.37753600
H	0.55807800	-1.57090800	0.11287900
O	1.83960200	-0.02719700	-0.38748900
O	2.92589200	-0.59023000	0.08852600
C	-0.40386100	1.79224700	0.03476700
H	-0.38604900	1.99948200	1.11101100

P47-•C=CC(C)COO

H	0.52363700	2.17518300	-0.39797300
H	-1.24382900	2.34141600	-0.39875300

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.90178700	-0.46930400	-0.41404800
C	-1.81248400	-0.74460900	0.25597800
H	-3.83558300	-0.94900300	-0.66595100
H	-1.71957100	-1.73380200	0.72414100
C	-0.62017100	0.16773700	0.45749400
H	-0.44475100	0.24630900	1.54017100
C	0.62473700	-0.51558800	-0.12879800
H	0.71682200	-1.54728300	0.23469700
O	1.74870800	0.24149700	0.29697800
O	2.92507900	-0.42903400	-0.20364600
H	3.19114300	0.17688300	-0.91036000
C	-0.82729100	1.57330200	-0.11401900
H	-1.01347900	1.52844600	-1.19240500
H	-1.68985400	2.05727500	0.35189700
H	0.05684600	2.19102700	0.05854900
H	0.57011100	-0.53877900	-1.22703800

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.11182600	-1.12301300	-0.01377100
C	1.05972800	0.06497600	0.34583100
C	-0.83440100	1.61974700	0.29176200
C	0.29669400	1.21604200	-0.27796900
H	0.09200200	-1.29461100	-1.09409200
H	1.05838700	0.16499200	1.43708100
H	-1.08616300	1.52534100	1.34736700
H	0.40956600	1.29651000	-1.36161600
H	-1.74712000	0.95609000	-0.35839200
O	-2.05355800	-0.30523100	-0.51788200
O	-1.24300300	-0.90021100	0.43987800
C	2.48019400	-0.16231900	-0.16910900
H	3.13154200	0.67050400	0.11086600
H	2.91197800	-1.07988500	0.24447700
H	2.49478300	-0.24716800	-1.26155500
H	0.42326200	-2.04083700	0.49942400

R48-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000

C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100
H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900
H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

P48-•C=CC(C)C(C)OO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.01437800	-0.50169400	-0.04993600
C	1.88406600	-0.43979900	-0.70615000
H	3.94226200	-1.05185300	-0.09577500
H	1.73745500	-1.11489300	-1.56045300
C	0.71749800	0.48307400	-0.42256400
H	0.53247200	1.05774400	-1.34110900
C	-0.56906600	-0.35521000	-0.22069200
H	-0.66710800	-1.04384600	-1.07164700
O	-1.62760100	0.60469300	-0.31357600
O	-2.87422000	-0.11784400	-0.42766700
H	-3.27690900	0.07968600	0.42954300
C	0.99156500	1.47429300	0.71368000
H	1.26767700	0.95891400	1.63797400
H	1.82261900	2.13269100	0.44668300
H	0.10960200	2.08946000	0.90676500
C	-0.62673100	-1.15059400	1.08016100
H	-1.54353100	-1.74356500	1.11476700
H	0.22610900	-1.83193100	1.14624700
H	-0.60634300	-0.48762600	1.94996100

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Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.29314600	0.74237300	-0.23549700

C	-0.83409800	-0.63370500	0.29571800
C	1.44856900	-1.51963700	0.50870600
C	0.28334600	-1.56193000	-0.12971900
H	-0.22198000	0.70540900	-1.32740000
H	-0.86533400	-0.56524100	1.38968900
H	1.60035900	-1.20550800	1.54064800
H	0.26480300	-1.83401100	-1.18764700
H	2.15223000	-0.71031400	-0.22837000
O	2.06589800	0.54920200	-0.57666900
O	1.05781600	0.98336100	0.26804200
C	-2.21461600	-0.99437600	-0.25584300
H	-2.51657300	-1.98501000	0.09671200
H	-2.98118400	-0.28145000	0.06068400
H	-2.20721600	-1.01928600	-1.35168500
C	-1.10532300	1.94752500	0.22541000
H	-2.13761600	1.87392600	-0.12554100
H	-1.11514500	2.01052500	1.31789900
H	-0.67044000	2.86895300	-0.16861900

R49-(trans)-CC=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.18039800	0.25134600	0.16956800
C	0.96255100	0.11084000	-0.34894500
H	2.42759200	1.18040000	0.68494900
H	0.70499300	-0.81239600	-0.86581600
C	3.27398900	-0.77212300	0.10336900
H	2.94976000	-1.67374300	-0.42398500
H	4.15778100	-0.37517800	-0.41150500
H	3.60471500	-1.06464700	1.10769900
C	-0.12554600	1.14631900	-0.27553400
H	0.23107500	2.03511100	0.25701400
H	-0.41235000	1.47438200	-1.28398100
C	-1.38506000	0.65537800	0.43175200
H	-2.13953800	1.44216900	0.52684700
H	-1.17373400	0.23086700	1.41680000
O	-1.96498300	-0.40359600	-0.38523800
O	-3.00855400	-0.94484300	0.19907800

P49-CC•=CCCOO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.37263600	0.01559300	-0.27674200
C	1.32039500	0.31545900	0.44398700
H	1.37762700	0.20550400	1.53603400
C	3.75737900	-0.44902400	-0.13670000

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H	4.01523800	-0.61739100	0.92174400
H	3.92187600	-1.39141100	-0.67208600
H	4.46932900	0.28119300	-0.53890400
C	-0.00779400	0.79419600	-0.09030900
H	-0.28586600	1.74271900	0.38594800
H	0.06175700	0.97463200	-1.16638200
C	-1.11676600	-0.22276200	0.18984500
H	-1.18281900	-0.44792100	1.26264400
H	-0.92691400	-1.16289100	-0.34713900
O	-2.32856800	0.36900700	-0.25379200
O	-3.39480900	-0.54571700	0.08267900
H	-3.61831500	-0.89152600	-0.79343500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.57772900	-0.24533500	-0.34153900
C	0.66285800	-1.49223300	-0.18383800
C	-1.22899300	-0.11329500	0.57247300
C	-0.29109000	-1.00931100	0.88514800
H	2.17567200	-0.07931500	0.55905000
H	0.15725700	-1.70216900	-1.13060400
H	2.24048300	-0.33820500	-1.21013100
H	1.26098900	-2.36782100	0.09540300
H	0.17991700	-0.91737800	1.86622500
H	-0.64006600	0.98105500	0.92925600
O	0.45853100	1.64890900	0.55571300
O	0.80784900	0.95392100	-0.60060800
C	-2.12115800	0.06843000	-0.60382000
H	-3.16343100	0.17342300	-0.27777800
H	-1.85992700	0.97239700	-1.16236000
H	-2.07801900	-0.79416900	-1.28045100

R50-C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800
C	0.02912800	0.36494300	-0.07789300
H	0.13282400	0.90845700	0.86749900

P50-C=C•CCCOO

H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

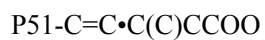
Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.76822000	-0.26430700	0.28922000
C	-2.62971200	-0.05588100	-0.31988800
H	-3.97676400	0.14977400	1.28164700
H	-4.56958100	-0.85254400	-0.15183200
C	-1.33839500	0.62218600	-0.13282700
H	-1.20830100	1.38740000	-0.91049100
H	-1.34943900	1.16415300	0.82992200
C	-0.13970700	-0.34568200	-0.16771700
H	-0.12070600	-0.87641300	-1.12474700
H	-0.25432700	-1.10223800	0.61542000
C	1.18096400	0.39170900	0.02400900
H	1.20893300	0.90973000	0.99474000
H	1.33430000	1.14053200	-0.76484800
O	2.20382500	-0.58953800	-0.03822500
O	3.46532200	0.10832600	0.05493500
H	3.75312900	-0.15884400	0.93972700

TS50

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.73052600	0.40699700	0.00747500
C	-0.60244300	1.39830100	-0.29286700
C	1.39167600	-0.11980100	0.10264500
C	0.72100800	1.15390200	0.46998600
H	-1.95970100	0.36758900	1.07971100
H	-0.40786900	1.39300800	-1.37116900
H	-2.63502800	0.70538200	-0.53476600
H	-0.96650800	2.40115200	-0.03707600
H	1.41267700	1.98890300	0.28332800
H	0.51347600	1.15160600	1.54881200
H	0.37739500	-1.12087000	0.25312100
O	-0.62049300	-1.56403600	0.46233100
O	-1.47007300	-0.91537100	-0.46047300
C	2.58258000	-0.47489300	-0.32340600
H	3.36615900	0.26829000	-0.49051100
H	2.85015800	-1.50684000	-0.52931000



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.25621700	-1.07567800	0.32724700
C	-2.35204300	-0.39232300	-0.36581700
H	-3.18023300	-1.19384000	1.40483800
H	-4.10963800	-1.54453300	-0.15092800
H	-2.46689200	-0.29680000	-1.44644600
C	-1.14112700	0.29319000	0.21281600
H	-1.14509500	0.12775900	1.29870700
C	0.14294500	-0.34548600	-0.36417100
H	0.10418100	-1.42885400	-0.20696000
H	0.18144300	-0.18421200	-1.44872800
C	1.42019500	0.18496200	0.26712200
H	1.42622200	0.06588900	1.35574900
H	1.62772700	1.22928800	0.02250600
O	2.52451100	-0.60557100	-0.26277900
O	3.68106800	-0.17141700	0.18143400
C	-1.21042900	1.81005400	-0.04817600
H	-0.38152300	2.34551600	0.42458000
H	-1.17810300	2.02361400	-1.12291700
H	-2.14266600	2.22376200	0.34622700



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.44918200	-1.08216900	0.18210600
C	-2.42930000	-0.39068700	-0.25591500
H	-3.58445200	-1.30202100	1.24661600
H	-4.21705500	-1.47634900	-0.47966400
C	-1.21865600	0.30548900	0.22026000
H	-1.18316800	0.18499500	1.31950200
C	0.04571300	-0.36323800	-0.36941500
H	0.05629600	-0.23269800	-1.45693300
H	-0.00044500	-1.44056000	-0.17932600
C	1.34655600	0.17655900	0.21874700
H	1.33761400	0.11662700	1.31836800
H	1.52510300	1.22014900	-0.06503200
O	2.38249200	-0.63907200	-0.30886800
O	3.63483100	-0.07035600	0.13372400
H	3.91662000	-0.73702900	0.77645100
C	-1.29845500	1.81418000	-0.09046300
H	-0.45768400	2.35651700	0.35062700
H	-1.28887900	1.98588200	-1.17145200
H	-2.22259000	2.23910300	0.31007200

TS51

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.67278200	-1.01256300	-0.00784100
C	0.21642700	-1.32283400	-0.36844700
C	-0.81135200	0.93088900	0.07344700
C	-0.87065800	-0.52367700	0.39768500
H	1.85617400	-1.13316300	1.06719100
H	0.07980200	-1.17578600	-1.44640000
H	2.33575200	-1.69220500	-0.55561400
H	0.05326700	-2.39000300	-0.16870500
H	-0.65072900	-0.62537400	1.47096700
H	0.55329000	1.30705500	0.29758100
O	1.63464700	1.22615200	0.53399100
O	2.10255000	0.28516000	-0.40974100
C	-1.64238100	1.85223000	-0.36030500
H	-2.68817700	1.62543200	-0.57618700
H	-1.33530400	2.88068900	-0.52587200
C	-2.27086100	-1.10840900	0.13697200
H	-3.03648500	-0.57084300	0.70333600
H	-2.52728700	-1.04919200	-0.92577200
H	-2.30162200	-2.16092500	0.43641100

R52-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393600	0.01912900	0.21624600
C	2.50767100	-0.37369400	-0.44139400
H	3.61461800	0.07695700	1.30107200
H	4.50795600	0.29247900	-0.30012900
H	2.53237300	-0.41673100	-1.53058100
C	1.20658100	-0.78156200	0.18939800
H	1.29137800	-0.72723600	1.28215600
C	0.00586100	0.07208200	-0.28137600
H	-0.03601000	0.02027100	-1.37829900
C	-1.28366200	-0.54535900	0.24668200
H	-1.38109900	-0.44387100	1.33248500
H	-1.38181400	-1.60131600	-0.02458500
O	-2.40657100	0.15928200	-0.35804800
O	-3.55264000	-0.24708400	0.13708900
H	1.00457700	-1.83346800	-0.05955400
C	0.13703600	1.54190200	0.13689500
H	-0.71143700	2.12975600	-0.22170500
H	0.17264800	1.63142600	1.22940800
H	1.05596300	1.97917100	-0.26129600

P52-C=C•CC(C)COO

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.77214200	-0.03281900	0.02425800
C	2.57769700	-0.41095300	-0.35205100
H	4.03594500	0.07915100	1.08143100
H	4.56767500	0.18653800	-0.68420900
C	1.27039000	-0.80578300	0.19167200
H	1.31612400	-0.78980700	1.29636200
C	0.10133600	0.09107500	-0.28320300
H	0.08645600	0.06808300	-1.37971200
C	-1.21774300	-0.51395100	0.20315000
H	-1.28479000	-0.47345800	1.30170800
H	-1.30934600	-1.56302100	-0.10799400
O	-2.26606300	0.24687800	-0.37807100
O	-3.50899800	-0.36165300	0.03481500
H	-3.83943900	0.30720500	0.65171100
H	1.06209400	-1.84670100	-0.09121600
C	0.26806900	1.54301000	0.17866100
H	0.27195800	1.60321200	1.27421900
H	1.21292600	1.95843700	-0.18119900
H	-0.55046200	2.16508800	-0.18997100

TS52

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.21811900	0.99340600	-0.01448200
C	1.01495800	-0.50080300	-0.31298200
C	-1.50134400	-0.59599500	0.10754800
C	-0.16633200	-1.13950800	0.46295500
H	1.38253300	1.16676200	1.05702700
H	0.79993500	-0.58907600	-1.38537300
H	2.09360200	1.35595400	-0.56605000
H	0.00635700	-1.00004100	1.53963900
H	-1.37775300	0.82152400	0.27899500
O	-0.88964100	1.79803200	0.47845200
O	0.15902500	1.83249000	-0.46655000
C	-2.63846800	-1.09163600	-0.32530800
H	-2.75247500	-2.16268300	-0.50986900
H	-3.51204700	-0.47689900	-0.51981100
C	2.31246700	-1.25957400	-0.00283200
H	2.56784500	-1.18791700	1.06109600
H	2.21404100	-2.32132800	-0.24927400
H	3.15502800	-0.85951200	-0.57574900
H	-0.16854300	-2.22630800	0.28475600



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.77075500	-0.49856500	0.29660600
C	-2.75799800	0.05281400	-0.36369400
H	-3.72044300	-0.68680600	1.36564400
H	-4.69258600	-0.78050500	-0.20080500
H	-2.85101200	0.22245600	-1.43647200
C	-1.44897600	0.46940100	0.24559700
H	-1.47168300	0.29119800	1.32760700
C	-0.25360600	-0.27282400	-0.38025300
H	-0.21801900	-0.08026600	-1.45986500
C	1.08646700	0.11366900	0.23807500
H	1.09241200	-0.08905100	1.31455600
O	2.05530700	-0.83268700	-0.34395700
O	3.20355800	-0.80774300	0.28981400
H	-1.31507100	1.55069400	0.10659400
H	-0.39414500	-1.35215000	-0.25696600
C	1.55644700	1.53315600	-0.03898800
H	1.54303300	1.74518500	-1.11287800
H	0.91213500	2.25728800	0.46709300
H	2.57498600	1.65949400	0.33458400



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.95818800	-0.48951600	0.13818400
C	-2.82943200	0.03404400	-0.26460200
H	-4.14267100	-0.72458300	1.19200100
H	-4.77478200	-0.71660100	-0.54327500
C	-1.52610300	0.48469100	0.24599700
H	-1.50614600	0.36750400	1.34476800
C	-0.34462800	-0.28579800	-0.37589800
H	-0.33283100	-0.12908600	-1.45997800
C	1.01376400	0.11889500	0.20680600
H	1.00697700	-0.04151500	1.29636300
O	1.92207400	-0.82037400	-0.37907000
O	3.21332700	-0.64892400	0.24745400
H	3.24871800	-1.44605400	0.79518700
H	-1.41198000	1.55856500	0.05164100
C	1.42874000	1.55489800	-0.09887000
H	0.77716200	2.27061700	0.41159400
H	2.45166300	1.72518000	0.24214400
H	1.38319700	1.74554700	-1.17598400
H	-0.48743600	-1.35845700	-0.21123400

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.36063200	-0.09772000	0.24046400
C	0.39925400	-1.24772400	-0.09775900
C	-1.82827300	-0.02990000	0.03064400
C	-1.01123900	-1.16358000	0.53218100
H	1.42349900	0.03241100	1.32888800
H	0.30845000	-1.31382900	-1.18837600
H	-0.90844800	-1.07628500	1.62238300
H	-0.98970400	1.12087700	0.21867000
O	-0.08891700	1.70318700	0.49574000
O	0.92256400	1.15178400	-0.31840500
C	-3.01147600	0.11522100	-0.52137100
H	-3.65335500	-0.74820300	-0.71331400
H	-3.41100200	1.08214600	-0.81180300
H	-1.55097300	-2.10343100	0.34149200
H	0.86331100	-2.18139300	0.24237500
C	2.75027400	-0.32639700	-0.34668000
H	3.41047200	0.50692100	-0.09509400
H	3.18375700	-1.24950800	0.04811100
H	2.69978700	-0.40886700	-1.43688800

6.3 The optimized geometries of all the reactions at B3LYP/6-31G(2df,p) level for concerted elimination reactions of alkenyl peroxy radicals (TS_n is the transition state of the reaction R_n)

HO₂

Cartesian Coordinates (Å)			
At.	X	Y	Z
O	0.05542600	0.71633300	0.00000000
O	0.05542600	-0.60791900	0.00000000
H	-0.88681000	-0.86730700	0.00000000

R1-C=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.91835900	0.09048500	0.42665700
C	1.87818400	0.19779700	-0.39324800
H	2.90798300	-0.58638900	1.27642800
H	3.82454200	0.66777700	0.27832600
H	1.93022800	0.88835900	-1.23452100
C	0.59054900	-0.56586800	-0.25540300
H	0.38996300	-1.13772200	-1.17105400
H	0.65903400	-1.28457500	0.56761100

P1-C=CC=C

C	-0.58751200	0.37234800	-0.01511800
H	-0.52283700	0.88269600	0.94964500
H	-0.69489100	1.11937400	-0.80778300
O	-1.79765000	-0.43751800	-0.00987500
O	-2.86378700	0.29775700	0.20537600

TS1

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.30137300	-0.00004700	-0.00001200
H	-1.86984200	-0.69651200	-0.60949700
H	-1.86899300	0.69693500	0.60978900
C	-0.00001300	0.00000800	-0.00003900
C	1.30139400	-0.00002300	-0.00000800
H	1.86948000	0.60969200	-0.69660800
H	1.86930700	-0.60974300	0.69667000

R2-C=CC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.95131300	0.10346600	0.00004500
O	1.76535600	0.20097900	-0.00007500
O	1.33212100	-0.98809700	-0.00006700
H	0.11312500	-0.74727400	0.00000500
C	-2.12156100	-0.50664000	0.00007300
H	-3.05472000	0.05129000	0.00011300
H	-2.20612400	-1.58825500	0.00005900
C	-0.22016900	1.24947700	0.00003300
H	0.06304300	1.75169600	-0.91958400
H	0.06311900	1.75166600	0.91964300

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.78976800	-0.87830700	-0.25783400
C	-1.81144100	-0.26221300	0.39677200
H	-2.74671500	-1.03847300	-1.33161100
H	-3.67567000	-1.24358600	0.25052800
H	-1.89685600	-0.11737400	1.47429100
C	-0.55327200	0.28307600	-0.22912200
H	-0.60004800	0.11282700	-1.31184700
C	0.64786500	-0.49848900	0.30635600
H	0.80636500	-0.33704200	1.37753600
H	0.55807800	-1.57090800	0.11287900
O	1.83960200	-0.02719700	-0.38748900
O	2.92589200	-0.59023000	0.08852600
C	-0.40386100	1.79224700	0.03476700

H	-0.38604900	1.99948200	1.11101100
H	0.52363700	2.17518300	-0.39797300
H	-1.24382900	2.34141600	-0.39875300

P2-C=CC(C)=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.98108300	0.00430400	0.00031900
C	0.83192700	-0.67703900	0.00004300
H	2.93805000	-0.50539700	0.00041800
H	2.01331500	1.08849400	0.00046100
H	0.86731300	-1.76522600	-0.00007000
C	-0.51522700	-0.10151400	-0.00009800
C	-1.58548500	-0.90779100	-0.00015400
H	-2.59733500	-0.51698600	-0.00026900
H	-1.48037400	-1.98813400	-0.00008600
C	-0.65823600	1.39960600	-0.00012600
H	-0.17847700	1.84285300	0.88026200
H	-0.17728700	1.84294800	-0.87981200
H	-1.70958000	1.69604800	-0.00081000

TS2

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.30697300	0.30460800	0.23373600
H	-0.54351200	-0.17936400	-0.67022000
C	-0.69452500	0.32661500	1.21602100
H	-0.80198000	-0.48420000	1.92737400
H	-1.22864500	1.23798500	1.45614900
O	-2.31164300	-0.37171300	0.06457700
O	-1.73462700	-0.55221700	-1.04757000
C	1.31285200	-0.79130600	0.30388800
C	2.53781400	-0.77596600	-0.21917800
H	3.19944500	-1.62895700	-0.11951500
H	2.93079600	0.07818300	-0.75973800
H	0.97849500	-1.68229200	0.83425800
C	0.74617700	1.62700400	-0.39213800
H	1.56878000	2.07599100	0.17552500
H	1.09340400	1.48825400	-1.42031700
H	-0.08236800	2.34010900	-0.41354400

R3-C=CC(C)C(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.82935700	-0.96561300	-0.48057000
C	-1.93274300	-0.28814300	0.22876000
H	-2.72823700	-1.09626100	-1.55452100

P3-C=CC(C)=CC

H	-3.70274800	-1.41412400	-0.01917300
H	-2.07992800	-0.17412100	1.30257100
C	-0.69877400	0.36962200	-0.33580900
H	-0.73972400	0.28647500	-1.42880200
C	0.56331400	-0.40588900	0.09273300
H	0.48525900	-1.44166300	-0.25051700
O	1.66139000	0.18602700	-0.69375200
O	2.74051800	-0.55904300	-0.66313500
C	-0.64173800	1.86355200	0.03235200
H	-0.69085400	2.01379400	1.11550900
H	-1.49079700	2.38995900	-0.41209600
H	0.27943900	2.32306800	-0.33499700
C	0.93303500	-0.37114200	1.56774600
H	1.87488700	-0.90476000	1.71196500
H	1.05384000	0.65299700	1.92991800
H	0.16117700	-0.86555300	2.16397300

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.08085200	-1.06166200	-0.00002800
C	-0.75320100	-0.89919600	0.00003800
H	-2.52384400	-2.05139400	0.00003600
H	-2.77263100	-0.22673900	-0.00012300
H	-0.13589800	-1.79295600	0.00016600
C	-0.04352800	0.38051000	0.00000800
C	1.29983000	0.47103100	0.00002800
H	1.72578600	1.47369700	0.00010500
C	-0.87987300	1.63857900	-0.00000600
H	-1.53258300	1.68347600	-0.87996800
H	-1.53251100	1.68353800	0.88001100
H	-0.24988300	2.53111500	-0.00007500
C	2.32106700	-0.62648200	-0.00003100
H	2.97506500	-0.54395000	-0.87772700
H	2.97494300	-0.54430700	0.87781100
H	1.89090400	-1.62915400	-0.00029200

TS3

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.44986600	-0.12781300	0.31619800
H	0.25196800	-0.88952700	-0.51730800
C	0.70552400	0.55357400	0.75396900
H	1.16813100	0.19280400	1.66803600
O	2.14472700	-0.58073800	-0.37266500
O	1.36459000	-1.34500400	-1.01992800

C	-1.39808300	0.54950200	-0.60956100
C	-2.69957800	0.28800300	-0.73251400
H	-0.96772000	1.31619400	-1.24877600
H	-3.31185300	0.82757900	-1.44634700
H	-3.20553900	-0.46223400	-0.13522200
C	-1.04496000	-1.17003400	1.26461100
H	-1.77207400	-0.71631600	1.94761300
H	-1.56036400	-1.96344900	0.71518300
H	-0.26027700	-1.63831100	1.86490400
C	1.17207100	1.89978600	0.29537500
H	0.63963900	2.68670400	0.84788600
H	2.24073100	2.02531600	0.48478300
H	0.99219100	2.06906100	-0.76848600

R4-C=CC(C)C(C₂)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.03961300	0.35145400	0.25345100
C	1.90028200	0.62737900	-0.37471200
H	3.24387400	-0.61483800	0.70120100
H	3.82694300	1.09319300	0.33594100
H	1.77971500	1.61780900	-0.80861600
C	0.73129300	-0.30820200	-0.58331700
H	0.52407200	-0.31656500	-1.66428400
C	-0.56583400	0.26783600	0.05236900
O	-1.61426700	-0.64831900	-0.49937600
O	-2.81630100	-0.38023400	-0.05658900
C	1.01613800	-1.75484600	-0.15998000
H	1.85110500	-2.15735200	-0.74013500
H	1.28135300	-1.82913300	0.89834900
H	0.14262600	-2.38578600	-0.33524100
C	-0.90512700	1.67128100	-0.44696800
H	-0.25946100	2.41617200	0.02386600
H	-0.79246200	1.74623100	-1.53293500
H	-1.94085000	1.89968400	-0.18673900
C	-0.60895300	0.18632300	1.57489500
H	-1.54371500	0.61055600	1.94555600
H	-0.54220600	-0.84724900	1.92080900
H	0.22908700	0.74835900	1.99552400

P4-C=CC(C)=CC₂

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.68491000	-0.48357500	-0.00409600
C	1.37284300	-0.74847000	-0.01100700
H	3.41306700	-1.28696400	-0.02141000

H	3.08558500	0.52318100	0.01794400
H	1.08529700	-1.79372800	-0.03964200
C	0.28658400	0.23724500	0.00160400
C	-1.01786600	-0.13070000	0.00043900
C	0.74195800	1.67995300	0.01247100
H	1.37429600	1.87471400	0.88668000
H	1.35224900	1.90157100	-0.87106400
H	-0.07776200	2.39507400	0.03796600
C	-1.50724300	-1.56046100	0.01590800
H	-2.24018000	-1.69537100	0.82182000
H	-2.03632500	-1.79390800	-0.91779700
H	-0.72963500	-2.30943400	0.15362000
C	-2.17801200	0.83519300	-0.01674800
H	-2.75438100	0.75913600	0.91537100
H	-1.89785000	1.87871700	-0.15048500
H	-2.87340600	0.57190100	-0.82443300

TS4

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.56811800	-0.03156300	0.25752200
H	-0.04295500	-1.17814600	-0.16937900
C	0.65020100	0.67825900	0.07713200
O	1.84302600	-1.07428400	-0.52719200
O	0.92627400	-1.95716000	-0.53847100
C	-1.66904000	0.17394600	-0.72849500
C	-2.97823900	0.10823200	-0.48340200
H	-1.36067000	0.38589600	-1.74793400
H	-3.69877900	0.26204600	-1.27901900
H	-3.38682500	-0.09229700	0.50035400
C	-1.02417700	-0.39672100	1.67161700
H	-1.46197200	0.46178100	2.19451400
H	-1.78482800	-1.18075900	1.63102300
H	-0.20460000	-0.77963800	2.28193600
C	0.94242800	1.44356600	-1.18731300
H	0.44089800	2.42112100	-1.15942700
H	2.01519700	1.62248800	-1.29001600
H	0.60129800	0.92631600	-2.08505200
C	1.54665200	1.02365700	1.23356900
H	1.21644300	1.97383700	1.67922500
H	1.53533800	0.27382300	2.02423900
H	2.57882000	1.15882800	0.90105300

R5-C₂C=CCCO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

P5-C₂C=CC=C

C	2.00466100	-0.02455900	-0.00021400
C	0.87528400	-0.61401700	0.40746800
H	0.87442400	-1.70178200	0.47604100
C	-0.43214500	0.03090700	0.77892300
H	-0.75345500	-0.32314700	1.76732800
C	-1.52153400	-0.32499900	-0.22802400
O	-2.77523900	0.23269800	0.26203700
O	-3.76579200	-0.01751800	-0.56260800
C	3.22349400	-0.84752300	-0.33469800
H	4.07559000	-0.56273900	0.29595700
H	3.04384600	-1.91724300	-0.20171900
H	3.53846600	-0.67938100	-1.37267300
C	2.19681200	1.46121600	-0.16130000
H	1.30581500	2.04480800	0.07453200
H	3.01201000	1.81594500	0.48215600
H	2.49246600	1.70014900	-1.19078800
H	-0.35028400	1.11859200	0.84545400
H	-1.65950000	-1.40590100	-0.32875700
H	-1.33055700	0.10309800	-1.21589400

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.90930500	-0.05112500	-0.00000100
C	-0.36336700	-0.48792900	-0.00001700
H	-0.52297100	-1.56591900	-0.00003600
C	-1.57910200	0.30584500	-0.00004300
C	-2.81226800	-0.21381200	0.00003400
C	2.05683700	-1.02613000	-0.00000600
H	1.71241300	-2.06325600	-0.00001500
H	2.69975200	-0.87874800	-0.87814600
H	2.69970400	-0.87873300	0.87817800
C	1.32127200	1.39692900	0.00002500
H	0.47954600	2.09029400	0.00038200
H	1.94191400	1.62009800	0.87771300
H	1.94136800	1.62031100	-0.87799600
H	-1.47473200	1.38797800	-0.00016300
H	-3.69667600	0.41291900	-0.00000500
H	-2.97638400	-1.28762000	0.00013300

TS5

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.60084600	0.29430400	0.66466900
H	-0.41261300	1.31983700	0.98110900
H	-1.26124700	0.52216900	-0.47568800

C	-1.70651100	-0.33127000	1.25095300
H	-1.78102900	-1.41181300	1.30343900
H	-2.40634100	0.21970600	1.86621400
O	-3.03010500	-0.24593100	-0.39647600
O	-2.31450800	0.38877900	-1.22602400
C	0.57710900	-0.50184800	0.24043800
C	1.81725600	-0.06893600	-0.02150000
H	0.37838800	-1.56699200	0.12298600
C	2.26100700	1.36755400	0.07427300
H	3.09272900	1.47032200	0.78341200
H	2.63824600	1.72011900	-0.89451800
H	1.46773300	2.04806200	0.38774700
C	2.89645400	-1.03186200	-0.44525200
H	3.30355600	-0.76144000	-1.42865300
H	3.74283200	-1.01107400	0.25413900
H	2.52783300	-2.05933300	-0.50167800

R6-C₂C=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.19310700	-0.11248600	-0.06830000
C	-1.03450200	-0.77632000	-0.15178600
H	-0.99025300	-1.76250000	0.31107200
C	0.24759000	-0.34781500	-0.81007400
H	0.54150700	-1.09384700	-1.56029100
C	1.39740300	-0.23019300	0.19621400
O	2.61036100	-0.07602800	-0.62344500
O	3.70183200	-0.23958600	0.08619100
C	1.28828100	0.94066500	1.15838300
H	2.17208300	0.98121100	1.79848000
H	1.20449900	1.88427000	0.60971800
H	0.39962900	0.82361100	1.78395800
C	-3.38016000	-0.72512100	0.63238200
H	-4.23326100	-0.82370600	-0.05137800
H	-3.15113300	-1.71498900	1.03501300
H	-3.72078900	-0.08903700	1.45967300
C	-2.45228000	1.25573700	-0.64412900
H	-1.58103300	1.69627600	-1.13068900
H	-3.26494100	1.21583900	-1.38072500
H	-2.78404800	1.94644400	0.14153000
H	0.14027900	0.60365300	-1.33828700
H	1.53056200	-1.16911500	0.74382500

P6-C₂C=CC=CC

Cartesian Coordinates (Å)			
At.	X	Y	Z

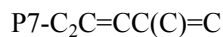
TS6

C	-1.42400700	-0.10389800	-0.00000300
C	-0.08745000	-0.26931900	0.00000400
H	0.27378400	-1.29516400	-0.00001700
C	0.92993500	0.76602300	0.00006000
C	2.26153200	0.58816200	0.00001900
C	3.02227800	-0.70414000	-0.00004100
H	3.67737100	-0.77019400	-0.87830800
H	3.67766000	-0.77008300	0.87801700
H	2.37591600	-1.58391700	0.00012100
C	-2.34525000	-1.29531500	0.00002500
H	-1.79385500	-2.23902600	0.00001500
H	-3.00530700	-1.28530900	0.87803000
H	-3.00539200	-1.28533900	-0.87791800
C	-2.13034100	1.22575100	-0.00004900
H	-2.78379600	1.31469900	0.87785300
H	-1.45320600	2.08049200	-0.00017700
H	-2.78389000	1.31453100	-0.87789600
H	0.57733900	1.79392400	0.00014000
H	2.88318900	1.48179500	0.00004700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.36433300	-0.16189700	0.64850400
H	0.90333500	-1.07358700	-0.16017600
C	1.57988700	0.52523900	0.81787900
H	2.20163300	0.22656800	1.65583400
O	2.77967200	-0.73740900	-0.45917400
O	1.90244500	-1.57997800	-0.82353800
C	-0.77258200	0.39833300	-0.12159700
C	-2.06260800	0.03952700	-0.05516800
H	-0.51572500	1.17983100	-0.83294000
C	1.96011700	1.81649600	0.16461400
H	1.55312200	2.65941600	0.74096300
H	3.04597500	1.93203000	0.12902400
H	1.57337300	1.89943500	-0.85354600
C	-2.61427600	-1.03050300	0.85050500
H	-1.85867300	-1.50153400	1.48116200
H	-3.39235200	-0.61980400	1.50707900
H	-3.09587400	-1.82239900	0.26206800
C	-3.09409000	0.71462900	-0.92262400
H	-3.60408300	-0.01192300	-1.56931200
H	-3.87700900	1.18588100	-0.31349600
H	-2.65091700	1.48366100	-1.56055500
H	0.09556900	-0.80941600	1.48291500



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.09555400	-0.16848200	-0.05657600
C	0.95961600	0.42604300	-0.43745500
H	0.96174000	0.94192900	-1.39875200
C	-0.36144700	0.49384500	0.28700700
H	-0.26645500	0.06134600	1.28822900
C	-1.38126600	-0.35581500	-0.47432600
H	-1.59641800	0.04484700	-1.47008700
H	-1.05868100	-1.39635900	-0.56774000
O	-2.63149100	-0.35296400	0.27675000
O	-3.58235000	-0.98612500	-0.37034700
C	-0.84168900	1.94979500	0.42820000
H	-0.12731900	2.53312600	1.01545600
H	-0.93427900	2.42497600	-0.55525700
H	-1.81689600	1.99683200	0.91944300
C	3.32258000	-0.11365600	-0.93233700
H	3.65943900	-1.12325700	-1.20097400
H	3.14153000	0.44268600	-1.85530500
H	4.16046800	0.36079900	-0.40524100
C	2.28945700	-0.92687500	1.23127300
H	1.40097000	-0.95020800	1.86397100
H	2.58119000	-1.96458700	1.02490100
H	3.10860900	-0.48854200	1.81541900



Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.19831600	-0.09110800	-0.00014700
C	-0.00618500	-0.69220800	-0.00029900
H	0.02596700	-1.78133000	0.00015200
C	-1.38669500	-0.19416100	-0.00020800
C	-2.38355900	-1.09432400	0.00013000
C	2.44599300	-0.94221800	0.00012600
H	3.06941500	-0.72577800	-0.87783200
H	3.06900700	-0.72588100	0.87837500
H	2.21712800	-2.01048000	-0.00001300
C	1.50125600	1.38477600	0.00002700
H	0.62444000	2.02534800	-0.00018000
H	2.10972500	1.64404600	0.87682600
H	2.11032200	1.64422400	-0.87629300
H	-3.42497700	-0.79136100	0.00035200
H	-2.18771800	-2.16162100	0.00014200
C	-1.72734500	1.27776900	0.00005100

TS7

H	-1.32630300	1.78801600	0.88243100
H	-1.32623700	1.78840500	-0.88208200
H	-2.81146000	1.41525800	0.00004500

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.62839100	0.76999100	-0.08056600
H	1.00969000	-0.42680400	0.37500700
C	1.71588100	0.82017600	-0.95470800
H	1.62013400	0.53084600	-1.99491700
H	2.63791100	1.32090300	-0.68437400
O	2.60281400	-1.09868400	-0.46303500
O	1.78038000	-1.46447400	0.42876700
C	-0.72864100	0.52176700	-0.68029500
C	-1.77235800	-0.10937800	-0.12775900
C	-1.76376400	-0.76024000	1.23140100
H	-2.43459200	-0.23340700	1.92289300
H	-2.13952200	-1.78846800	1.16158000
H	-0.77328800	-0.79951800	1.68635100
C	-3.08275600	-0.21994900	-0.86492600
H	-3.04510200	0.26841200	-1.84192000
H	-3.36168600	-1.27079700	-1.01634700
H	-3.89856900	0.23528600	-0.28805000
H	-0.86715000	0.91937300	-1.68485500
C	0.68481000	1.65728600	1.17177300
H	0.29089000	2.65567200	0.95207800
H	0.09117000	1.24892100	1.99283400
H	1.71518300	1.76692400	1.52435000

R8-(cis)-CC=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.60976500	0.37217800	-0.17521500
C	-1.45984300	0.85573800	0.29866400
H	-1.34354700	1.93720000	0.33017600
C	-0.27820700	0.07054400	0.80162200
H	0.04853100	0.47310100	1.76964600
C	0.91501100	0.11845300	-0.15915400
O	1.92604600	-0.75802600	0.45802200
O	2.89447700	-1.04842100	-0.37796300
C	1.52115000	1.49432100	-0.38338400
H	0.81658500	2.13519800	-0.91998000
H	1.77139700	1.97099800	0.56995300
H	2.43010900	1.39983500	-0.98140100
C	-3.02200700	-1.06271100	-0.32422500

P8-CC=CC=CC

H	-2.25533300	-1.76693400	0.00545600
H	-3.93547500	-1.26555300	0.24823600
H	-3.25667900	-1.28987500	-1.37152800
H	-3.35914300	1.09508400	-0.49474700
H	-0.53817800	-0.97817500	0.96810800
H	0.65952200	-0.35044100	-1.11424100

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.98364400	0.51773800	0.00001000
C	-0.68574900	0.85848600	-0.00002400
H	-0.44357200	1.92047400	-0.00002900
C	0.46236700	-0.03132200	-0.00002800
C	1.73435200	0.38985000	0.00002100
C	-2.57004600	-0.86239700	0.00001500
H	-1.81280600	-1.64913100	-0.00028600
H	-3.21048100	-1.01385800	0.87839800
H	-3.21093200	-1.01364800	-0.87807500
H	1.92723900	1.46282800	0.00008200
H	-2.71308200	1.32564000	0.00001000
H	0.27329500	-1.10302200	-0.00008700
C	2.94011000	-0.49735800	0.00000500
H	3.57204800	-0.31175600	-0.87824600
H	3.57187100	-0.31206300	0.87844900
H	2.66207400	-1.55544100	-0.00020900

TS8

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.09625000	-0.31704400	-0.06672200
H	-0.37762800	-0.73314400	-1.03491000
H	0.40269200	0.86669900	-0.44264100
C	1.12833300	-0.76531400	0.44988000
H	1.30234800	-0.67218500	1.51876000
O	2.23417700	1.05065700	0.11907900
O	1.35508200	1.74067100	-0.48354300
C	-1.20478400	0.05850500	0.84443000
C	-2.50784600	0.13516200	0.55880400
H	-0.89113900	0.31060000	1.85664400
H	-3.17727300	0.43544100	1.36256900
C	-3.17772700	-0.14647300	-0.75418000
H	-3.94185600	-0.92633700	-0.64499400
H	-3.69719500	0.74551200	-1.12678700
H	-2.47953300	-0.46963200	-1.52974300
C	2.06444100	-1.65944200	-0.29666200

H	1.93474800	-1.56200800	-1.37830100
H	3.10828500	-1.45078900	-0.04720200
H	1.86547700	-2.70713200	-0.03098400

R9-(trans)-CC=CCC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.44844800	-0.51438200	-0.11228200
C	-1.42752800	0.14674000	0.42990600
H	-1.55413900	1.20107600	0.67403500
C	-0.08545300	-0.45686500	0.73881700
H	0.18666900	-0.26699100	1.78608500
C	1.03600100	0.09375700	-0.14843300
O	2.22894200	-0.68136100	0.23490100
O	3.20830700	-0.52534600	-0.62384500
C	1.33343000	1.57536800	0.01584200
H	0.49573400	2.17375800	-0.35216600
H	1.50627900	1.82491200	1.06769800
H	2.22399400	1.83492000	-0.56067700
C	-3.79188600	0.07135600	-0.42727600
H	-4.58963100	-0.45426100	0.11204900
H	-3.84265700	1.13105700	-0.16086000
H	-4.02456800	-0.02338900	-1.49521500
H	-2.32099200	-1.57115900	-0.34884400
H	-0.12461900	-1.54340700	0.60898700
H	0.84924700	-0.14870200	-1.19899300

P9-CC=CC=CC

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.80063300	-0.43160500	0.00012300
C	-0.66813300	0.28316500	0.00002900
H	-0.73151000	1.37172600	-0.00015800
C	0.66813400	-0.28314900	0.00007000
C	1.80064200	0.43161300	-0.00008800
C	-3.18439600	0.14011600	-0.00003100
H	-3.16790000	1.23398200	-0.00023300
H	-3.75348800	-0.19124100	-0.87838000
H	-3.75375400	-0.19086000	0.87827800
H	1.72952200	1.51934700	-0.00025000
H	-1.72950900	-1.51934000	0.00021500
H	0.73150700	-1.37171100	0.00026200
C	3.18439300	-0.14012300	-0.00004400
H	3.75350500	0.19052100	-0.87864200
H	3.75381200	0.19144400	0.87802200
H	3.16777200	-1.23398100	0.00053300

TS9

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.08578100	-0.38115500	0.36838700
H	-0.05951500	-0.77668700	1.38663900
H	-0.57007700	0.84468600	0.58915500
C	-1.18409000	-0.76602400	-0.41333100
H	-1.09557800	-0.70205400	-1.49463300
O	-2.19785700	1.13644300	-0.39736700
O	-1.43608500	1.78641500	0.38305000
C	1.23862900	-0.11999900	-0.24444800
C	2.40854300	-0.18849400	0.39216900
H	1.22473300	0.16352200	-1.29737400
H	2.41684400	-0.46830100	1.44582600
C	3.74510800	0.08940200	-0.22734200
H	3.65008000	0.35752200	-1.28381100
H	4.25917300	0.91252400	0.28534800
H	4.40846500	-0.78202300	-0.15693100
C	-2.33491100	-1.56301100	0.11004800
H	-2.45426100	-1.43350400	1.18946200
H	-3.27228400	-1.29130800	-0.38275400
H	-2.16103400	-2.63156100	-0.07927700

R10-C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.56239600	0.06847500	0.48518900
C	2.53893600	0.22193300	-0.34827400
H	3.53726800	-0.65915000	1.29188100
H	4.46822400	0.65825700	0.39429600
H	2.60531200	0.96444000	-1.14349400
C	1.25056500	-0.54873700	-0.28913500
H	1.11491100	-1.10640100	-1.22727900
H	1.30223500	-1.29383200	0.51385800
C	0.02912800	0.36494300	-0.07789300
H	0.13282400	0.90845700	0.86749900
H	-0.01653000	1.11791400	-0.87354000
C	-1.26812100	-0.42491300	-0.06709500
H	-1.31242500	-1.14913800	0.75232300
H	-1.44874100	-0.94764900	-1.01180900
O	-2.36024500	0.51893900	0.12519700
O	-3.52231800	-0.09182600	0.15224200

P10-C=CCC=C

Cartesian Coordinates (Å)			
At.	X	Y	Z

TS10

C	-2.37146900	-0.17589900	0.14750400
C	-1.17487600	-0.17787900	-0.43076800
H	-3.17930800	-0.80838300	-0.20514900
H	-2.59338100	0.46471200	0.99690600
H	-0.98738700	-0.83745600	-1.27707700
C	0.00004400	0.66360000	0.00085300
H	0.31269000	1.31761900	-0.82404500
H	-0.31244000	1.31538600	0.82755900
C	1.17479800	-0.17917200	0.43018800
C	2.37150400	-0.17550200	-0.14783300
H	0.98697300	-0.84145600	1.27431500
H	3.17918000	-0.80931100	0.20280400
H	2.59366900	0.46800300	-0.99497600

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.00363600	0.95711000	0.31428800
C	0.32416400	0.92568600	-0.44850900
C	1.52503200	1.22227700	0.17880000
O	2.29635500	-0.82051900	0.28895200
O	1.34905700	-1.41051000	-0.31024300
H	-1.35697500	1.99775000	0.36209100
H	-0.83938100	0.63409300	1.34870300
H	0.25142700	1.18009700	-1.50821600
H	0.62090500	-0.39227400	-0.54505100
H	2.39959700	1.53108400	-0.38048300
H	1.59582500	1.31937700	1.25651500
C	-2.70392400	-0.89906500	0.26839700
H	-2.48792600	-1.18670400	1.29371300
C	-2.06911500	0.10752300	-0.32263000
H	-2.31635000	0.35992300	-1.35404300
H	-3.46553600	-1.47630200	-0.24497900

R11-C=CC(C)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.25621700	-1.07567800	0.32724700
C	-2.35204300	-0.39232300	-0.36581700
H	-3.18023300	-1.19384000	1.40483800
H	-4.10963800	-1.54453300	-0.15092800
H	-2.46689200	-0.29680000	-1.44644600
C	-1.14112700	0.29319000	0.21281600
H	-1.14509500	0.12775900	1.29870700
C	0.14294500	-0.34548600	-0.36417100
H	0.10418100	-1.42885400	-0.20696000

P11-C=CC(C)C=C

H	0.18144300	-0.18421200	-1.44872800
C	1.42019500	0.18496200	0.26712200
H	1.42622200	0.06588900	1.35574900
H	1.62772700	1.22928800	0.02250600
O	2.52451100	-0.60557100	-0.26277900
O	3.68106800	-0.17141700	0.18143400
C	-1.21042900	1.81005400	-0.04817600
H	-0.38152300	2.34551600	0.42458000
H	-1.17810300	2.02361400	-1.12291700
H	-2.14266600	2.22376200	0.34622700

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.18605700	-0.95555500	0.19456100
C	1.24018200	-0.25619700	-0.42277500
H	1.33939300	-0.04617300	-1.48846900
C	0.00001100	0.30703200	0.22935100
H	0.00004100	0.01540500	1.28658600
C	-1.24013400	-0.25628800	-0.42279000
C	-2.18593100	-0.95573100	0.19457200
H	-1.33943400	-0.04610900	-1.48844500
H	-3.05956800	-1.32594600	-0.33150000
H	-2.12428100	-1.18844800	1.25414900
H	2.12457100	-1.18815800	1.25416400
H	3.05962600	-1.32580400	-0.33158900
C	-0.00014500	1.84935000	0.14269000
H	0.00003700	2.18178600	-0.90163800
H	-0.88969900	2.26377600	0.62634600
H	0.88907200	2.26400600	0.62675000

TS11

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.93250200	-0.82817100	-0.15756100
C	-0.41954100	-0.59469500	-0.86237000
C	-1.61655000	-1.14704000	-0.43187800
O	-2.49244000	0.68861900	0.38855800
O	-1.55793900	1.48965200	0.08667200
H	1.28713300	-1.82079600	-0.47936100
H	-0.33135700	-0.43754300	-1.93970200
H	-0.77733000	0.65262800	-0.47819100
H	-2.45787100	-1.25309300	-1.10573500
H	-1.72354600	-1.63507100	0.52883300
C	2.67467600	1.02350100	0.01993300
C	1.93741900	0.17143700	-0.68470400

H	2.03854900	0.17057900	-1.77053500
H	3.36608500	1.70352400	-0.46621900
H	2.62526900	1.08401600	1.10172400
C	0.82206000	-0.84607200	1.36981000
H	0.43050900	0.10151700	1.75282600
H	0.16053200	-1.64660500	1.71121800
H	1.80166100	-1.01908600	1.82392800

R12-C=CC(C₂)CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.16519100	-1.10891000	0.08263500
C	2.13525100	-0.59628900	-0.58200500
H	2.04622800	-0.81165100	-1.64765000
C	1.02077200	0.28038600	-0.04239900
C	-0.30187800	-0.50453000	-0.28102200
H	-0.24991800	-1.45552700	0.26093700
H	-0.38044300	-0.75590000	-1.34563400
C	-1.57761100	0.21564700	0.13022100
H	-1.74651800	1.14604700	-0.41772800
H	-1.63400400	0.41711300	1.20278700
O	-2.68516700	-0.67731100	-0.19488700
O	-3.84009200	-0.14534000	0.13092900
H	3.32244400	-0.94238200	1.14269300
H	3.90357100	-1.72570900	-0.41868700
C	1.02644300	1.59645000	-0.85436400
H	0.86300500	1.40601400	-1.92062100
H	0.25000600	2.28798900	-0.51222700
H	1.99073600	2.10266100	-0.74981300
C	1.20849000	0.59534600	1.45016400
H	0.43451400	1.27856200	1.81182000
H	1.16795900	-0.31246800	2.06049900
H	2.17455200	1.07787100	1.62590500

P12-C=CC(C₂)C=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.33956900	-0.78760300	0.10371700
C	1.09135700	-0.66193600	0.54299400
H	0.76768700	-1.27252700	1.38577700
C	-0.00000300	0.24753500	0.00000300
C	-1.09144400	-0.66174400	-0.54312500
C	-2.33960000	-0.78755000	-0.10372800
H	-0.76789300	-1.27206500	-1.38615400
H	-3.03241800	-1.47697700	-0.57491600
H	-2.72771300	-0.21684000	0.73293500

H	2.72779200	-0.21661300	-0.73270300
H	3.03231800	-1.47720200	0.57475800
C	0.50334200	1.13735800	-1.15253300
H	0.84923200	0.53861200	-2.00093000
H	-0.30368800	1.78461500	-1.50824200
H	1.33215800	1.77304700	-0.82483800
C	-0.50324300	1.13727000	1.15265000
H	-1.33194500	1.77315000	0.82502300
H	-0.84926500	0.53846000	2.00094600
H	0.30386700	1.78436000	1.50848100

TS12

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.89921800	-0.40377300	0.02020800
C	-0.44416900	-0.61014400	-0.71781800
C	-1.50906100	-1.33081400	-0.19672800
O	-2.80798400	0.37685700	0.25122800
O	-2.05940900	1.29930600	-0.19005400
H	-0.33992600	-0.64231400	-1.80523000
H	-1.08517900	0.57008900	-0.58139200
H	-2.27126500	-1.74885900	-0.84290700
H	-1.55360100	-1.64250400	0.83927300
C	2.00738500	1.90236700	-0.07170700
C	1.59466400	0.77398500	-0.63861900
H	1.76058000	0.64069400	-1.70877100
H	2.49763000	2.67503200	-0.65453100
H	1.87631500	2.11121500	0.98427500
C	0.69016600	-0.18370200	1.52506500
H	0.02376600	0.66104500	1.72181800
H	0.26117400	-1.07135800	1.99856000
H	1.64660400	0.01279000	2.01813300
C	1.78125700	-1.65731600	-0.20117900
H	1.95064900	-1.83835400	-1.26793300
H	2.75820400	-1.53417000	0.27763500
H	1.29743300	-2.54622100	0.21634300

R13-C=CCC(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.59393500	0.01913200	0.21624900
C	2.50767100	-0.37369200	-0.44139300
H	2.53237500	-0.41672800	-1.53058000
C	1.20658200	-0.78156400	0.18939600
C	0.00586100	0.07208000	-0.28137900
H	-0.03600900	0.02027000	-1.37830100

C	-1.28366200	-0.54536200	0.24667800
H	-1.38110000	-0.44387400	1.33248100
H	-1.38181200	-1.60131900	-0.02458900
O	-2.40657100	0.15927800	-0.35805200
O	-3.55263900	-0.24707700	0.13709700
H	3.61461500	0.07695900	1.30107500
H	4.50795300	0.29248500	-0.30012300
H	1.29137700	-0.72724000	1.28215500
H	1.00457900	-1.83347000	-0.05955800
C	0.13703500	1.54190000	0.13689400
H	-0.71143800	2.12975300	-0.22170400
H	0.17264900	1.63142200	1.22940700
H	1.05596200	1.97917000	-0.26129800

P13-C=CCC(C)=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.53739900	0.21908600	-0.09923600
C	1.41375100	-0.44037000	-0.36293600
H	1.27026400	-0.88389700	-1.34775400
C	0.26886700	-0.63672500	0.59974700
C	-1.03235500	-0.04179300	0.09165700
C	-2.06595700	-0.81160000	-0.24575600
H	-2.99507400	-0.38956800	-0.61601900
H	-2.02453900	-1.89322200	-0.16185000
H	2.71586500	0.67710600	0.86999600
H	3.32719600	0.32283800	-0.83587800
C	-1.07556500	1.46019200	-0.01033200
H	-0.93228000	1.92229800	0.97529000
H	-0.26570500	1.83504000	-0.64663500
H	-2.02783700	1.81046900	-0.41581900
H	0.53252100	-0.18394800	1.56495100
H	0.12275600	-1.70985600	0.77485800

TS13

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.03143000	0.52296600	0.83274900
C	0.33851700	0.77578700	0.17361700
C	1.47955500	0.59792500	0.95082500
O	2.15309800	-1.28490800	0.06801700
O	1.22269600	-1.43576900	-0.77684200
H	0.56179300	-0.36104400	-0.48906900
H	2.42226000	1.06509600	0.69056500
H	1.43709800	0.13201700	1.92845000
C	-2.70522200	-1.13213500	-0.04847400

C	-2.10164600	0.05026500	-0.11419700
H	-2.38879100	0.74704500	-0.90024600
H	-3.47311700	-1.42386500	-0.75708000
H	-2.45531700	-1.85829400	0.72037600
H	-1.36146800	1.46184400	1.30310300
H	-0.91163100	-0.20936900	1.63849900
C	0.36270300	1.83226100	-0.93091900
H	-0.27935400	1.55816000	-1.77301300
H	0.01169400	2.80058300	-0.55306100
H	1.37562000	1.97083000	-1.31953000

R14-C=CC(C)C(C)COO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	3.19043500	-1.13205500	0.65383400
C	2.40484500	-0.37249100	-0.10255900
H	2.66265500	-0.22477800	-1.15084600
C	1.16353400	0.33692300	0.37611800
C	-0.12119200	-0.30452800	-0.23037900
H	-0.07944400	-1.37069400	0.02745400
C	-1.36694900	0.25338400	0.45303200
H	-1.63876200	1.25514200	0.10979900
H	-1.27541100	0.25934500	1.54417600
O	-2.48236500	-0.62688500	0.12211200
O	-3.62633000	-0.13234000	0.53414900
H	2.98109600	-1.30030900	1.70694800
H	4.07566700	-1.61604100	0.25489600
H	1.10111900	0.18507300	1.46214900
C	-0.23683500	-0.19041300	-1.75761800
H	-1.15160000	-0.67852100	-2.10389800
H	-0.27608700	0.85462800	-2.08235100
H	0.60714200	-0.67027600	-2.25975600
C	1.28233000	1.85199900	0.11947400
H	2.16223500	2.25074900	0.63209400
H	1.39603100	2.07279800	-0.94652900
H	0.40792100	2.39976300	0.48436000

P14-C=CC(C)C(C)=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-2.42297800	-0.98316800	0.06050000
C	-1.41470700	-0.21491500	0.45879800
H	-1.35520600	0.08028800	1.50620700
C	-0.32437900	0.32198900	-0.43916100
C	1.04020700	-0.27106300	-0.10258100
C	1.73637800	-0.93728900	-1.02286300

H	2.71425000	-1.35602000	-0.80540700
H	1.35641900	-1.09134600	-2.02802200
H	-2.52655300	-1.29777200	-0.97446700
H	-3.18567300	-1.33042500	0.74966600
C	1.57391000	-0.07168900	1.29444300
H	1.64881200	0.99078100	1.55444000
H	0.91873500	-0.53283800	2.04283900
H	2.56741800	-0.51382000	1.40112500
H	-0.56094100	0.02319100	-1.46677200
C	-0.30157100	1.86621100	-0.38989800
H	-1.25960800	2.27071100	-0.72970600
H	-0.12998900	2.23475500	0.62660100
H	0.49118300	2.26203400	-1.03192600

TS14

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.97966300	0.40925800	0.69564600
C	0.46326300	0.77138500	0.23996600
C	1.56317700	0.36579800	0.99314400
O	2.26246300	-1.22726300	-0.32615200
O	1.36949800	-1.13502200	-1.21909700
H	0.70600900	-0.15054000	-0.68613400
H	2.51583100	0.87409000	0.90004000
H	1.49235000	-0.34495900	1.80470200
C	-2.57070600	-0.71634000	-0.94564900
C	-1.91227000	0.34817200	-0.49722200
H	-2.03951500	1.28979100	-1.02788900
H	-3.21191300	-0.65219200	-1.81844200
H	-2.50335100	-1.69072600	-0.47416600
H	-1.32158200	1.25987900	1.30763700
C	0.59009900	2.08757200	-0.53290700
H	0.06798000	2.05821800	-1.49291800
H	0.17005100	2.92119900	0.04350400
H	1.63933100	2.31835400	-0.73711300
C	-1.04690300	-0.84659100	1.57123000
H	-2.08664000	-1.08578600	1.80960300
H	-0.60605900	-1.71470300	1.07052700
H	-0.52015800	-0.69987300	2.51739800

R15-C₂C=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.62519300	-0.01278700	-0.03080900
C	1.50076500	-0.57707100	0.42264100
H	1.49625100	-1.66181900	0.53389500

C	0.20202700	0.08142900	0.79573000
H	0.27678700	1.17193700	0.74182200
H	-0.03450400	-0.15757000	1.84311100
C	-0.96572500	-0.39526100	-0.08998800
H	-1.04320400	-1.48807400	-0.04874700
H	-0.76885300	-0.13179100	-1.13492800
C	-2.28766900	0.21326200	0.34416300
H	-2.29749800	1.30438500	0.25860900
H	-2.56047100	-0.06336000	1.36770100
O	-3.32598300	-0.30172900	-0.53808800
O	-4.50248500	0.19798100	-0.23756300
C	3.83106100	-0.85700700	-0.36083300
H	4.12256700	-0.73377200	-1.41207400
H	4.70047300	-0.55422900	0.23727100
H	3.64752000	-1.91922800	-0.18078100
C	2.82549000	1.46416200	-0.25410500
H	1.94222300	2.06331600	-0.02809900
H	3.65216600	1.83903900	0.36308700
H	3.10742600	1.66077700	-1.29645200

P15-C₂C=CCC=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.42892500	-0.08555300	0.03678700
C	0.17934700	-0.44722000	0.34773200
H	-0.02551100	-1.51247300	0.45048700
C	-1.03132400	0.42760000	0.56128600
H	-0.75827500	1.48740600	0.50615400
H	-1.43181100	0.25972600	1.57020500
C	-2.11655300	0.13798400	-0.44644000
C	-3.33073500	-0.31841200	-0.15671900
H	-1.84216100	0.31090600	-1.48644100
H	-4.06845900	-0.51554900	-0.92746600
H	-3.63817700	-0.50990200	0.86797700
C	2.50744800	-1.12475100	-0.14561600
H	2.94318400	-1.06865000	-1.15192700
H	3.33526900	-0.96318300	0.55742900
H	2.12667700	-2.13815100	0.00426800
C	1.89962900	1.33317700	-0.15616000
H	1.10924000	2.07488400	-0.03167300
H	2.70130100	1.57414900	0.55402000
H	2.32830500	1.46388600	-1.15825500

TS15

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-0.09820200	-1.32276800	0.52019000
C	-1.35416100	-1.06934500	-0.32240100
C	-2.59756100	-0.89016800	0.26514200
O	-2.72736200	1.28020600	-0.02376800
O	-1.64145700	1.44770100	-0.65440900
H	-0.07088400	-2.38647400	0.79748800
H	-0.18139800	-0.76538200	1.45781500
H	-1.34320100	-1.52706500	-1.31398100
H	-1.25097900	0.22913200	-0.66828800
H	-3.51682100	-1.03178900	-0.29004900
H	-2.70892300	-0.75970800	1.33594700
C	2.04427700	-0.00104200	0.04465000
C	1.17221900	-0.98193700	-0.21206500
H	1.37916100	-1.62195000	-1.07037600
C	3.26660300	0.18942900	-0.81863700
H	4.18599100	0.10955000	-0.22377900
H	3.31748000	-0.54819300	-1.62360500
H	3.27778900	1.18997400	-1.27019300
C	1.92295100	0.99084600	1.17275800
H	1.02976600	0.84923900	1.78256800
H	2.79720000	0.93420800	1.83410300
H	1.89861600	2.01511300	0.77994000

R16-(cis)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-3.09137900	0.32750700	-0.27855200
C	-1.94400000	0.92045300	0.05452200
H	-3.86708400	0.95410600	-0.71660000
H	-1.85285300	1.98899200	-0.13863400
C	-3.46976900	-1.11653200	-0.12240700
H	-2.66902600	-1.72751900	0.29995200
H	-4.34796800	-1.22044100	0.52702500
H	-3.74824800	-1.55083900	-1.09053300
C	-0.72028400	0.29312300	0.66277400
H	-0.89189400	-0.76339600	0.89218300
H	-0.50281600	0.78497200	1.62211300
C	0.51415900	0.42771800	-0.24924000
H	0.68880600	1.48348700	-0.48765500
H	0.32947500	-0.08454900	-1.19974700
C	1.76029800	-0.14703200	0.40124700
H	1.67474100	-1.21993700	0.60027200
H	2.02152800	0.36556700	1.33255600
O	2.86988600	0.03720400	-0.52398200
O	3.98901300	-0.44243700	-0.03239200

P16-CC=CCC=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.78742100	0.60303100	-0.21113900
C	-0.50202900	0.82769200	0.06605300
H	-2.36584000	1.43860300	-0.60348000
H	-0.10620800	1.82360300	-0.12652900
C	-2.56473500	-0.67044200	-0.04574800
H	-3.41125800	-0.52375800	0.63680100
H	-2.99238100	-0.99176500	-1.00376100
H	-1.96184600	-1.49383800	0.34333400
C	0.51677400	-0.14621000	0.60635600
H	0.04514800	-1.11130400	0.82444700
H	0.91625000	0.23097900	1.55724000
C	1.66066000	-0.35202400	-0.35566800
C	2.93239900	-0.05433400	-0.10980400
H	1.38339400	-0.76310200	-1.32561000
H	3.71228400	-0.21901200	-0.84584500
H	3.24656500	0.36332000	0.84310000

TS16

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.43871300	-1.20895600	0.38623300
C	-0.95215900	-1.07792600	-0.24370500
C	-2.08917700	-0.93133500	0.53650500
O	-2.41764600	1.19984600	0.15160600
O	-1.46614600	1.38958500	-0.66300700
H	0.57753600	-2.24885300	0.71690500
H	0.48213300	-0.59170100	1.28864000
H	-1.07655800	-1.59848100	-1.19578500
H	-0.99690400	0.20289500	-0.67330600
H	-3.07632100	-1.16292200	0.15562500
H	-2.02836700	-0.73735400	1.60174600
C	2.46434900	0.10298400	-0.44910700
C	1.54470000	-0.85516800	-0.57153200
H	1.57191500	-1.46760300	-1.47275000
H	3.18679200	0.20681200	-1.25764000
C	2.64479800	1.07757200	0.67781400
H	1.89696000	0.96661100	1.46580900
H	3.63512800	0.96319100	1.13621300
H	2.59068000	2.10893200	0.30849600

R17-(trans)-CC=CCCCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z

C	-2.92685100	0.14952200	0.39228900
C	-1.89229800	0.14417100	-0.44520300
H	-1.99273100	-0.36131100	-1.40673400
C	-0.55617200	0.77701400	-0.17690500
H	-0.58153600	1.29970700	0.78701200
H	-0.34952100	1.54110700	-0.94074500
C	0.59421200	-0.24703100	-0.18304900
H	0.61325800	-0.78161000	-1.14017100
H	0.42431500	-0.99850200	0.59575000
C	1.94145700	0.41719700	0.04081700
H	2.01053900	0.91101200	1.01513600
H	2.18646000	1.14258700	-0.74160100
O	2.96076800	-0.62261500	0.00619700
O	4.15936400	-0.12638300	0.20933600
C	-4.25999700	-0.48492900	0.12998300
H	-4.49801000	-1.23795100	0.89158900
H	-5.06707100	0.25755800	0.16457200
H	-4.28877400	-0.97153400	-0.84926100
H	-2.82008900	0.65525500	1.35259100

P17-CC=CCC=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.70207700	0.30673100	0.20917900
C	-0.53915300	0.01206700	-0.36771800
H	-0.48339200	-0.83400100	-1.05298900
C	0.75645900	0.74926800	-0.13935400
H	0.56955500	1.60110700	0.52830700
H	1.12727300	1.16161000	-1.08738600
C	1.82103100	-0.13829800	0.45576400
C	2.98640000	-0.42590700	-0.11486300
H	1.57428600	-0.57356900	1.42343800
H	3.71231400	-1.07752200	0.36004200
H	3.26396300	-0.01538200	-1.08210700
C	-2.99025500	-0.42952900	-0.00976900
H	-3.38262100	-0.83377800	0.93193400
H	-3.76633500	0.23538200	-0.40941200
H	-2.86372500	-1.26135800	-0.70889800
H	-1.74574500	1.15151600	0.89763000

TS17

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.20125600	-1.29980300	-0.33125700
C	1.04336400	-0.92704900	0.48107800
C	2.31153400	-0.96220000	-0.07928600

O	2.58763800	1.20056000	-0.27941600
O	1.49833200	1.57632000	0.24682200
H	-0.29317900	-2.39583400	-0.34848700
H	-0.06407400	-0.98162100	-1.37127000
H	0.97605000	-1.14175000	1.54993200
H	1.01912200	0.42350200	0.51383000
H	3.20375400	-1.02959200	0.53110000
H	2.45947600	-1.08867900	-1.14613400
C	-2.26902000	0.13650800	-0.42659600
C	-1.46682500	-0.70431900	0.22225500
H	-1.72143900	-0.99514800	1.24262700
C	-3.52848600	0.73515100	0.12466800
H	-3.47710700	1.83099800	0.12945900
H	-4.39795100	0.46729200	-0.48865700
H	-3.71934800	0.39959500	1.14822800
H	-2.00893200	0.42647500	-1.44504400

R18-C=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.32345800	0.13895400	-0.26716500
C	1.21630500	-0.36510100	0.26701700
H	2.35079200	1.14240800	-0.68233200
H	3.24886800	-0.42546200	-0.30275700
H	1.20908100	-1.37364800	0.67400400
C	-0.06793300	0.38738600	0.37541700
H	-0.41691200	0.48496100	1.40810800
H	-0.00908200	1.37950500	-0.08143600
O	-1.10257800	-0.37018700	-0.33678500
O	-2.29913800	0.09828700	-0.07161500

P18-C=C=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.30137300	-0.00004700	-0.00001200
H	-1.86984200	-0.69651200	-0.60949700
H	-1.86899300	0.69693500	0.60978900
C	-0.00001300	0.00000800	-0.00003900
C	1.30139400	-0.00002300	-0.00000800
H	1.86948000	0.60969200	-0.69660800
H	1.86930700	-0.60974300	0.69667000

TS18

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.95131300	0.10346600	0.00004500
O	1.76535600	0.20097900	-0.00007500

O	1.33212100	-0.98809700	-0.00006700
H	0.11312500	-0.74727400	0.00000500
C	-2.12156100	-0.50664000	0.00007300
H	-3.05472000	0.05129000	0.00011300
H	-2.20612400	-1.58825500	0.00005900
C	-0.22016900	1.24947700	0.00003300
H	0.06304300	1.75169600	-0.91958400
H	0.06311900	1.75166600	0.91964300

R19-C=CC(C)OO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	2.37995800	-0.22114300	-0.16869600
C	1.20019100	-0.71744100	0.18629800
H	2.53311700	0.83529000	-0.36125500
H	3.25045500	-0.85979300	-0.27131900
H	1.09341300	-1.78418100	0.37129500
C	-0.05919300	0.07118500	0.39265200
H	-0.38771100	-0.00897800	1.43563200
O	-1.09639000	-0.65443900	-0.37746500
O	-2.30374000	-0.32057000	0.00979400
C	-0.04520100	1.52605400	-0.04315400
H	0.64555300	2.10264100	0.57831400
H	0.25887100	1.61961600	-1.08922500
H	-1.04718800	1.94354800	0.07532200

P19-C=C=CC

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.93566600	-0.21333900	-0.00002600
C	-0.69219500	0.17375000	0.00000500
H	-2.48103000	-0.38233700	0.92483600
H	-2.48101700	-0.38223100	-0.92491500
C	0.55270800	0.55936100	0.00003600
H	0.76299000	1.62876900	0.00009800
C	1.74472400	-0.36499000	-0.00000900
H	2.37340500	-0.19034500	-0.88117400
H	2.37339300	-0.19044400	0.88118500
H	1.43483500	-1.41209700	-0.00007000

TS19

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.38350500	0.42367900	0.46679600
H	-0.60399400	0.44338300	1.53545300
H	0.43814800	-0.64241500	0.41140800
C	0.61356400	1.29243000	0.01367200

H	0.65652800	1.60711100	-1.02316100
H	1.22446500	1.86081700	0.70341100
O	2.15867300	-0.11127400	-0.26576700
O	1.57944400	-1.16677200	0.12700200
C	-1.51622600	0.03688800	-0.40653500
C	-2.69492800	-0.41355700	0.01895300
H	-1.33316400	0.12804700	-1.47684700
H	-3.48219100	-0.68723300	-0.67392900
H	-2.91815500	-0.52198200	1.07646900

R20-(cis)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-1.81928900	0.52831900	-0.14283600
C	-0.56610900	0.90860400	0.11292400
H	-2.52210200	1.30716100	-0.43526300
H	-0.30831800	1.95977100	0.00795100
C	0.56001300	0.03352500	0.54898100
H	1.01676500	0.37313300	1.48379400
H	0.29033500	-1.01949800	0.64871100
O	1.61586400	0.11465100	-0.47203600
O	2.72064500	-0.45673700	-0.05570200
C	-2.40944200	-0.84779300	-0.07087700
H	-3.20901100	-0.88536200	0.67918800
H	-2.87090700	-1.11345600	-1.02937900
H	-1.67987300	-1.62098400	0.17775200

P20-CC=C=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.55271800	0.55942900	0.00004500
H	-0.76298200	1.62883700	-0.00002200
C	-1.74472000	-0.36502200	0.00001100
H	-2.37366000	-0.19006800	0.88090400
H	-2.37313300	-0.19083300	-0.88145400
H	-1.43486000	-1.41216000	0.00047800
C	0.69218600	0.17377100	-0.00010000
C	1.93566700	-0.21337900	0.00001700
H	2.48123800	-0.38230000	-0.92473400
H	2.48090000	-0.38227000	0.92498800

TS20

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.31712600	0.65207900	-0.00002300
O	2.22927000	-0.33044900	0.00004300
O	1.36002900	-1.25143600	-0.00002300

H	0.33725300	-0.54952700	-0.00008500
C	-1.63535000	0.55065000	0.00002300
H	-2.22546100	1.46799500	0.00003700
C	0.80272900	1.42181400	-0.00001600
H	1.26473700	1.77101000	-0.91876600
H	1.26468500	1.77106400	0.91874100
C	-2.42217800	-0.72865700	0.00000800
H	-1.77287500	-1.60800600	-0.00051900
H	-3.07524600	-0.78666500	0.87937900
H	-3.07593200	-0.78610000	-0.87889800

R21-(trans)-CC=CCOO•

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	1.64596500	0.32705700	-0.23290000
C	0.57009500	-0.08521700	0.43528500
H	1.53907800	1.15657900	-0.93220600
H	0.64662400	-0.91407500	1.13650200
C	-0.77700300	0.53559700	0.29539500
H	-1.20987600	0.84764600	1.25046200
H	-0.77429000	1.38456700	-0.39454400
O	-1.69668500	-0.47269400	-0.25403400
O	-2.94534600	-0.08550100	-0.14544400
C	3.02176600	-0.24897300	-0.10302700
H	3.73747100	0.51273400	0.22973900
H	3.04809900	-1.07826500	0.60886800
H	3.38419900	-0.61440900	-1.07151600

P21-CC=C=C

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	0.47470300	0.41651100	0.00003500
C	-0.65914100	-0.37857800	0.00000000
C	-1.96211500	0.08060700	-0.00000900
H	-0.50525600	-1.45813500	0.00001500
H	-2.80399100	-0.60060300	-0.00000100
H	-2.18354100	1.14307100	-0.00002200
H	0.34522800	1.49773700	0.00003000
C	1.87539500	-0.10023400	-0.00000300
H	1.90264000	-1.19405300	0.00067500
H	2.43563500	0.25054700	-0.87794300
H	2.43623600	0.25160900	0.87710800

TS21

Cartesian Coordinates (Å)			
At.	X	Y	Z
C	-0.33435000	0.04751700	0.00003200

O	2.38205900	0.24893900	-0.00024600
O	1.98942300	-0.95460600	-0.00018600
H	0.76328800	-0.75667500	-0.00006600
C	-1.47932200	-0.61225500	0.00016100
H	-1.46442800	-1.70085500	0.00017800
C	0.34592800	1.22502000	-0.00005700
H	0.61341600	1.73868700	-0.91878000
H	0.61360100	1.73871900	0.91859500
C	-2.84520900	0.02224900	0.00029000
H	-3.42084300	-0.29114900	-0.87938700
H	-3.42066100	-0.29111600	0.88009700
H	-2.77851200	1.11254200	0.00026200
