Supporting Information I

Investigating the kinetics of the intramolecular H-migration reaction class of methyl-

ester peroxy radicals in low-temperature oxidation mechanisms of biodiesel

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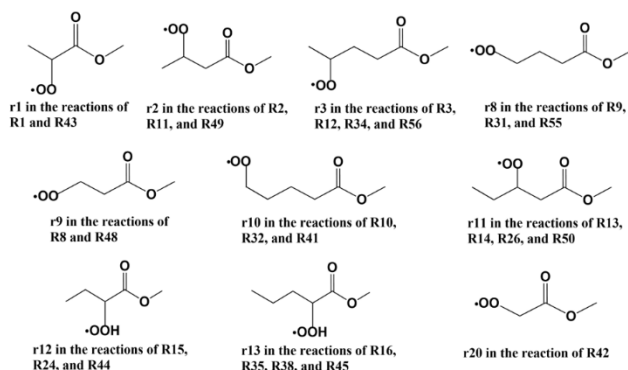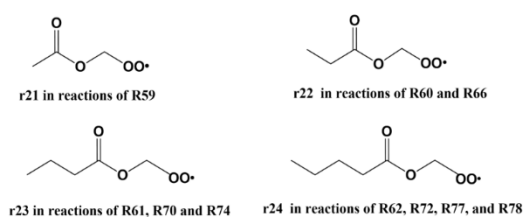
Branched-methyl ester peroxy radicals
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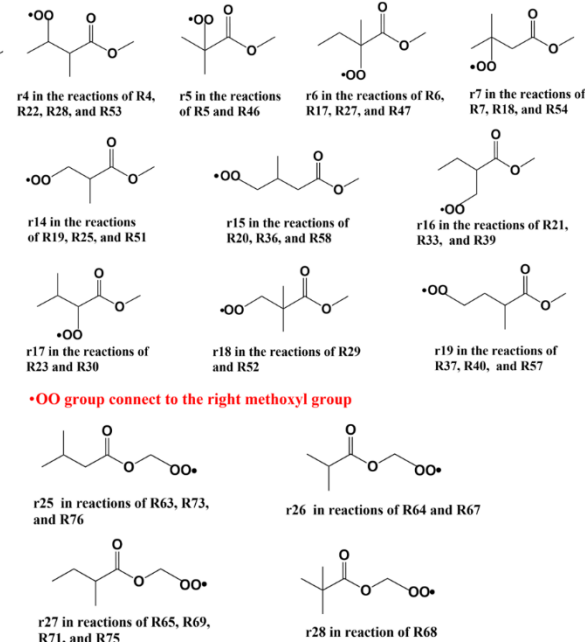
Figure S1. The structures of the studied methyl-ester peroxy radicals.

Table S1. A list of the reactions of intramolecular H-migration class in this work.

No.	Reaction equation
R1	$CH_3CH(OO·)C(=O)OCH_3 \rightarrow C·H_2CH(OOH)C(=O)OCH_3$
R2	$CH_3CH(OO·)CH_2C(=O)OCH_3 \rightarrow C·H_2CH(OOH)CH_2C(=O)OCH_3$
R3	$CH_3CH(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow C·H_2CH(OOH)CH_2CH_2C(=O)OCH_3$
R4	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow C·H_2CH(OOH)CH(CH_3)C(=O)OCH_3$
R5	$(CH_3)_2C(OO·)C(=O)OCH_3 \rightarrow C·H_2(CH_3)C(OOH)C(=O)OCH_3$
R6	$CH_3CH_2C(OO·)(CH_3)C(=O)OCH_3 \rightarrow CH_3CH_2C(OOH)(C·H_2)C(=O)OCH_3$
R7	$(CH_3)_2C(OO·)CH_2C(=O)OCH_3 \rightarrow C·H_2(CH_3)C(OOH)CH_2C(=O)OCH_3$
R8	$CH_2(OO·)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C·HC(=O)OCH_3$
R9	$CH_2(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C·HCH_2C(=O)OCH_3$
R10	$CH_2(OO·)CH_2CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C·HCH_2CH_2C(=O)OCH_3$
R11	$CH_3CH(OO·)CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)C·HC(=O)OCH_3$
R12	$CH_3CH(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)C·HCH_2C(=O)OCH_3$
R13	$CH_3CH_2CH(OO·)CH_2C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)C·HC(=O)OCH_3$
R14	$CH_3CH_2CH(OO·)CH_2C(=O)OCH_3 \rightarrow CH_3C·HCH(OOH)CH_2C(=O)OCH_3$
R15	$CH_3CH_2CH(OO·)C(=O)OCH_3 \rightarrow CH_3C·HCH(OOH)C(=O)OCH_3$
R16	$CH_3CH_2CH_2CH(OO·)C(=O)OCH_3 \rightarrow CH_3CH_2C·HCH(OOH)C(=O)OCH_3$
R17	$CH_3CH_2C(OO·)(CH_3)C(=O)OCH_3 \rightarrow CH_3C·HC(OOH)(CH_3)C(=O)OCH_3$
R18	$(CH_3)_2C(OO·)CH_2C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)C·H(=O)OCH_3$
R19	$CH_3CH(CH_2OO·)C(=O)OCH_3 \rightarrow CH_3C·(CH_2OOH)C(=O)OCH_3$
R20	$CH_3CH(CH_2OO·)CH_2C(=O)OCH_3 \rightarrow CH_3C·(CH_2OOH)CH_2C(=O)OCH_3$
R21	$CH_3CH_2CH(CH_2OO·)C(=O)OCH_3 \rightarrow CH_3CH_2C·(CH_2OOH)C(=O)OCH_3$
R22	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)C·(CH_3)C(=O)OCH_3$
R23	$(CH_3)_2CHCH(OO·)C(=O)OCH_3 \rightarrow (CH_3)_2C·CH(OOH)C(=O)OCH_3$
R24	$CH_3CH_2CH(OO·)C(=O)OCH_3 \rightarrow C·H_2CH_2CH(OOH)C(=O)OCH_3$
R25	$CH_3CH(CH_2OO·)C(=O)OCH_3 \rightarrow C·H_2CH(CH_2OOH)C(=O)OCH_3$
R26	$CH_3CH_2CH(OO·)CH_2C(=O)OCH_3 \rightarrow C·H_2CH_2CH(OOH)CH_2C(=O)OCH_3$
R27	$CH_3CH_2C(OO·)(CH_3)C(=O)OCH_3 \rightarrow C·H_2CH_2C(OOH)(CH_3)C(=O)OCH_3$
R28	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH(C·H_2)C(=O)OCH_3$
R29	$(CH_3)_2C(CH_2OO·)C(=O)OCH_3 \rightarrow C·H_2(CH_3)C(CH_2OOH)C(=O)OCH_3$
R30	$(CH_3)_2CHCH(OO·)C(=O)OCH_3 \rightarrow C·H_2(CH_3)CHCH(OOH)C(=O)OCH_3$

R31	$CH_2(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C\cdot HC(=O)OCH_3$
R32	$CH_2(OO\cdot)CH_2CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C\cdot HCH_2C(=O)OCH_3$
R33	$CH_3CH_2CH(CH_2OO\cdot)C(=O)OCH_3 \rightarrow CH_3C\cdot HCH(CH_2OOH)C(=O)OCH_3$
R34	$CH_2(OO\cdot)CH(CH_3)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)C\cdot HC(=O)OCH_3$
R35	$CH_3CH(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH_2C\cdot HC(=O)OCH_3$
R36	$CH_3CH_2CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3C\cdot HCH_2CH(OOH)C(=O)OCH_3$
R37	$CH_2(OO\cdot)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C\cdot(CH_3)C(=O)OCH_3$
R38	$CH_3CH_2CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow C\cdot H_2CH_2CH_2CH(OOH)C(=O)OCH_3$
R39	$CH_3CH_2CH(CH_2OO\cdot)C(=O)OCH_3 \rightarrow C\cdot H_2CH_2CH(CH_2OOH)C(=O)OCH_3$
R40	$CH_2(OO\cdot)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH(C\cdot H_2)C(=O)OCH_3$
R41	$CH_2(OO\cdot)CH_2CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH_2CH\cdot C(=O)OCH_3$
R42	$CH_2(OO\cdot)C(=O)OCH_3 \rightarrow CH_2(OOH)C(=O)OC\cdot H_2$
R43	$CH_3CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3CH(OOH)C(=O)OC\cdot H_2$
R44	$CH_3CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)C(=O)OC\cdot H_2$
R45	$CH_3CH_2CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3CH_2CH_2CH(OOH)C(=O)OC\cdot H_2$
R46	$(CH_3)_2C(OO\cdot)C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)C(=O)OC\cdot H_2$
R47	$CH_3CH_2(CH_3)C(OO\cdot)C(=O)OCH_3 \rightarrow CH_3CH_2(CH_3)C(OOH)C(=O)OC\cdot H_2$
R48	$CH_2(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C(=O)OC\cdot H_2$
R49	$CH_3CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH_2C(=O)OC\cdot H_2$
R50	$CH_3CH_2CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)CH_2C(=O)OC\cdot H_2$
R51	$CH_2(OO\cdot)CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)C(=O)OC\cdot H_2$
R52	$(CH_3)_2C(CH_2OO\cdot)C(=O)OCH_3 \rightarrow (CH_3)_2C(CH_2OOH)C(=O)OC\cdot H_2$
R53	$CH_3CH(OO\cdot)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH(CH_3)C(=O)OC\cdot H_2$
R54	$(CH_3)_2C(OO\cdot)CH_2C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)CH_2C(=O)OC\cdot H_2$
R55	$CH_2(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH_2C(=O)OC\cdot H_2$
R56	$CH_3CH(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH_2CH_2C(=O)OC\cdot H_2$
R57	$CH_2(OO\cdot)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH(CH_3)C(=O)OC\cdot H_2$
R58	$CH_2(OO\cdot)CH(CH_3)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)CH_2C(=O)OC\cdot H_2$
R59	$CH_3C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2C(=O)OCH_2(OOH)$
R60	$CH_3CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3C\cdot HC(=O)OCH_2(OOH)$
R61	$CH_3CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3CH_2C\cdot HC(=O)OCH_2(OOH)$
R62	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3CH_2CH_2C\cdot HC(=O)OCH_2(OOH)$
R63	$(CH_3)_2CHCH_2C(=O)OCH_2(OO\cdot) \rightarrow (CH_3)_2CHC\cdot HC(=O)OCH_2(OOH)$
R64	$(CH_3)_2CHC(=O)OCH_2(OO\cdot) \rightarrow (CH_3)_2C\cdot C(=O)OCH_2(OOH)$
R65	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot) \rightarrow CH_3CH_2C\cdot(CH_3)C(=O)OCH_2(OOH)$
R66	$CH_3CH_2C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2CH_2C(=O)OCH_2(OOH)$
R67	$(CH_3)_2CHC(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2(CH_3)CHC(=O)OCH_2(OOH)$
R68	$(CH_3)_3CC(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2(CH_3)_2CC(=O)OCH_2(OOH)$
R69	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot) \rightarrow CH_3CH_2CH(C\cdot H_2)C(=O)OCH_2(OOH)$
R70	$CH_3CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3C\cdot HCH_2C(=O)OCH_2(OOH)$
R71	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot) \rightarrow CH_3C\cdot HCH(CH_3)C(=O)OCH_2(OOH)$
R72	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3CH_2C\cdot HCH_2C(=O)OCH_2(OOH)$
R73	$(CH_3)_2CHCH_2C(=O)OCH_2(OO\cdot) \rightarrow (CH_3)_2C\cdot CH_2C(=O)OCH_2(OOH)$
R74	$CH_3CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2CH_2CH_2C(=O)OCH_2(OOH)$
R75	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2CH_2CH(CH_3)C(=O)OCH_2(OOH)$
R76	$(CH_3)_2CHCH_2C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2(CH_3)CHCH_2C(=O)OCH_2(OOH)$
R77	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow CH_3C\cdot H_2CH_2CH_2C(=O)OCH_2(OOH)$
R78	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot) \rightarrow C\cdot H_2CH_2CH_2CH_2C(=O)OCH_2(OOH)$

2. T1 diagnostic values for some representative species in this work

Table S2. T_1 diagnostic values for some reactants, transition states, and products.

Species	T_1^a
r20	0.022
r21	0.021
TS42	0.020

TS59	0.021
p41	0.016
p58	0.016

[a] T_1 diagnostic value were calculated at the CCSD(T)/cc-pVTZ level.

3. Figure S2-S4. Potential energy profiles for internal rotations
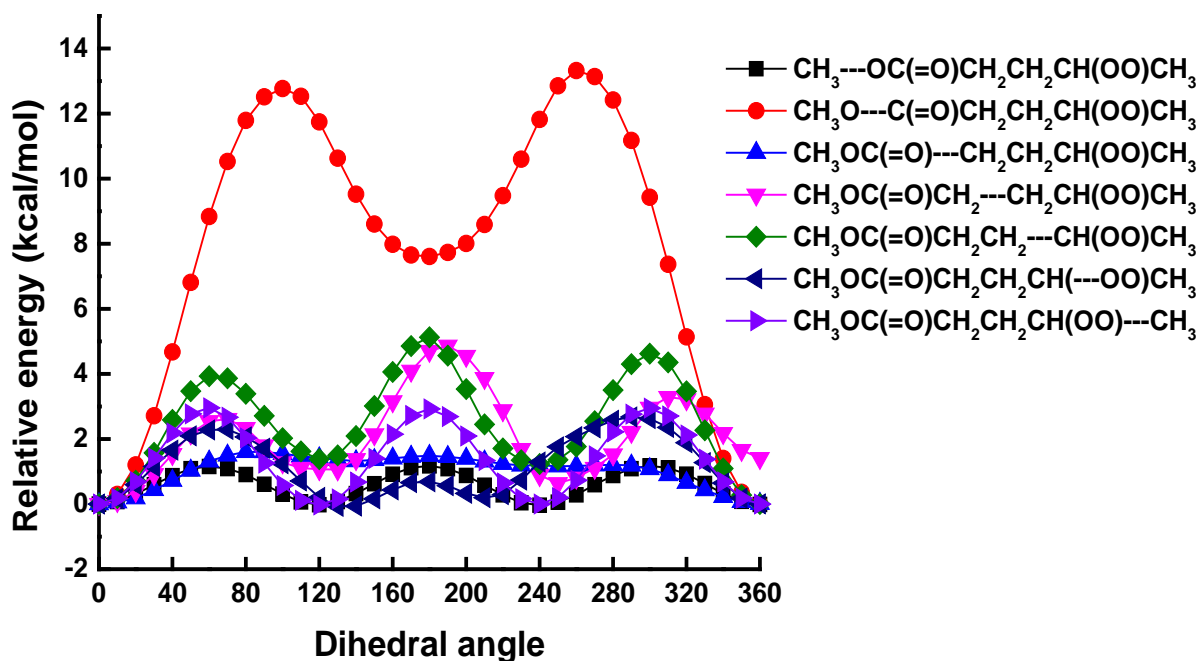
Figure S2. Potential energy profiles of the reactant for internal rotations in reaction R3 at M06-2X/6-311++G(d,p) level.
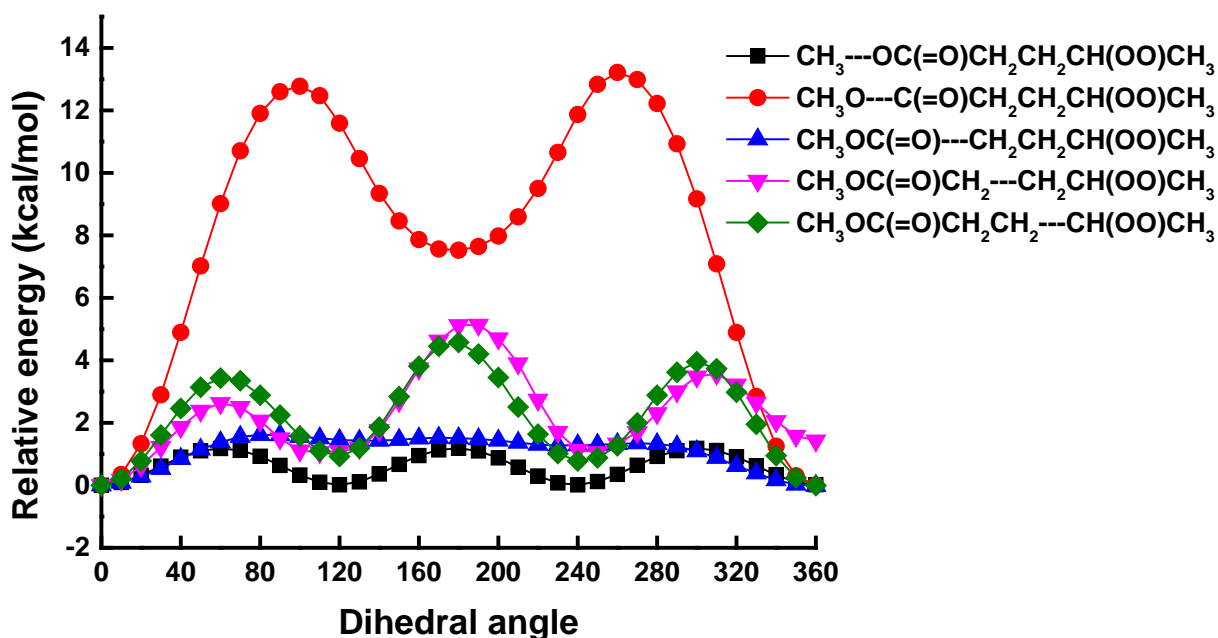
Figure S3. Potential energy profiles of the transition state for internal rotations in reaction R3 at M06-2X/6-311++G(d,p) level.
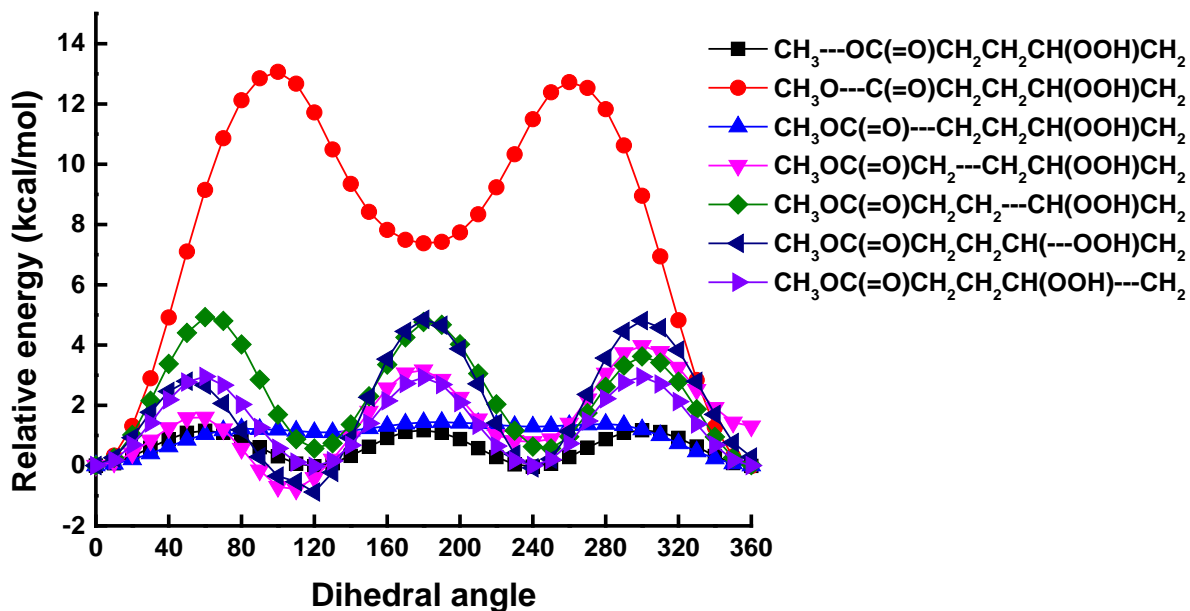
Figure S4. Potential energy profiles of the product for internal rotations in reaction R3 at M06-2X/6-311++G(d,p) level.

4. The calculated values of the barrier width L for all studied reactions

Table S3. Calculated barrier width L (Å) for all the reactions in this work.

Reactions	Barrier width L	Reactions	Barrier width L	Reactions	Barrier width L
R1	1.07	R28	0.89	R55	0.89
R2	1.04	R29	0.89	R56	0.91
R3	1.02	R30	0.87	R57	0.83
R4	1.03	R31	0.92	R58	0.93
R5	1.11	R32	0.87	R59	1.17
R6	1.13	R33	0.95	R60	1.09
R7	1.03	R34	1.01	R61	1.09
R8	0.91	R35	0.98	R62	1.09
R9	1.03	R36	0.93	R63	1.05
R10	1.03	R37	0.93	R64	1.13
R11	0.91	R38	0.95	R65	1.13
R12	1.00	R39	0.76	R66	0.86
R13	0.94	R40	0.83	R67	0.83
R14	1.05	R41	0.90	R68	0.77
R15	1.03	R42	1.13	R69	0.81
R16	1.08	R43	1.09	R70	0.85
R17	1.07	R44	1.15	R71	0.81
R18	0.90	R45	1.13	R72	0.99
R19	0.98	R46	1.15	R73	0.96
R20	1.03	R47	1.16	R74	0.61

R21	0.98	R48	1.06	R75	0.52
R22	0.99	R49	1.07	R76	0.6
R23	1.13	R50	1.07	R77	0.57
R24	0.99	R51	1.03	R78	0.78
R25	1.02	R52	1.01		
R26	0.98	R53	1.03		
R27	1.06	R54	1.10		

5. Lennard-Jones parameters used in this work

Table S4. Lennard-Jones parameters σ (Å) and ε (K) used in this work [1].

	Ar	$C_4H_7O_4$[a]	$C_5H_9O_4$[b]	$C_6H_{11}O_4$[c]	$C_6H_{11}O_4$[d]
σ	3.47	6.08	6.37	6.67	6.57
ε	114	455.19	474.91	493.13	491.50

[a] Represents $CH_3CH(OO\cdot)C(=O)OCH_3$ radical.

[b] Represents $CH_3CH(OO\cdot)CH_2C(=O)OCH_3$ radical.

[c] Represents $CH_3CH(OO\cdot)CH_2CH_2C(=O)OCH_3$ radical.

[d] Represents $(CH_3)_3CC(=O)OCH_2(OO\cdot)$ radical.

[1] Wang H, Frenklach M. Transport properties of polycyclic aromatic hydrocarbons for flame modeling. Combust Flame 1994;96:163-170.

6. Energy barriers for intramolecular H-migration reactions of methyl-ester peroxy radicals

Table S5. Energy barriers for all the H-migration reactions in this work (kcal/mol).

Reaction subclass	No.	Reaction equation	Energy barriers
1, 4-H(p)-(L, L)	R1	$CH_3CH(OO\cdot)C(=O)OCH_3 \rightarrow C\cdot H_2CH(OOH)C(=O)OCH_3$	36.75
	R2	$CH_3CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow C\cdot H_2CH(OOH)CH_2C(=O)OCH_3$	36.59
	R3	$CH_3CH(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow C\cdot H_2CH(OOH)CH_2CH_2C(=O)OCH_3$	35.69
	R4	$CH_3CH(OO\cdot)CH(CH_3)C(=O)OCH_3 \rightarrow C\cdot H_2CH(OOH)CH(CH_3)C(=O)OCH_3$	35.12
	R5	$(CH_3)_2C(OO\cdot)C(=O)OCH_3 \rightarrow C\cdot H_2(CH_3)C(OOH)C(=O)OCH_3$	37.39
	R6	$CH_3CH_2C(OO\cdot)(CH_3)C(=O)OCH_3 \rightarrow CH_3CH_2C(OOH)(C\cdot H_2)C(=O)OCH_3$	37.64
	R7	$(CH_3)_2C(OO\cdot)CH_2C(=O)OCH_3 \rightarrow C\cdot H_2(CH_3)C(OOH)CH_2C(=O)OCH_3$	36.63
			36.54[a], 2.52[b]
1, 4-H(s)-(L, L)	R8	$CH_2(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C\cdot HC(=O)OCH_3$	33.98
	R9	$CH_2(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C\cdot HCH_2C(=O)OCH_3$	32.99
	R10	$CH_2(OO\cdot)CH_2CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)C\cdot HCH_2CH_2C(=O)OCH_3$	32.42
	R11	$CH_3CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)C\cdot HC(=O)OCH_3$	34.65
	R12	$CH_3CH(OO\cdot)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)C\cdot HCH_2C(=O)OCH_3$	32.70
	R13	$CH_3CH_2CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)C\cdot HC(=O)OCH_3$	34.56
	R14	$CH_3CH_2CH(OO\cdot)CH_2C(=O)OCH_3 \rightarrow CH_3C\cdot HCH(OOH)CH_2C(=O)OCH_3$	32.74
	R15	$CH_3CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3C\cdot HCH(OOH)C(=O)OCH_3$	31.72
	R16	$CH_3CH_2CH_2CH(OO\cdot)C(=O)OCH_3 \rightarrow CH_3CH_2C\cdot HCH(OOH)C(=O)OCH_3$	31.22
	R17	$CH_3CH_2C(OO\cdot)(CH_3)C(=O)OCH_3 \rightarrow CH_3C\cdot HC(OOH)(CH_3)C(=O)OCH_3$	30.77
	R18	$(CH_3)_2C(OO\cdot)CH_2C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)C\cdot H(=O)OCH_3$	33.85
			32.87[a], 3.88[b]

1, 4-H(t)-(L, L)	R19	$CH_3CH(CH_2OO·)C(=O)OCH_3 \rightarrow CH_3C·(CH_2OOH)C(=O)OCH_3$	31.18
	R20	$CH_3CH(CH_2OO·)CH_2C(=O)OCH_3 \rightarrow CH_3C·(CH_2OOH)CH_2C(=O)OCH_3$	31.30
	R21	$CH_3CH_2CH(CH_2OO·)C(=O)OCH_3 \rightarrow CH_3CH_2C·(CH_2OOH)C(=O)OCH_3$	31.39
	R22	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)C·(CH_3)C(=O)OCH_3$	30.79
	R23	$(CH_3)_2CHCH(OO·)C(=O)OCH_3 \rightarrow (CH_3)_2C·CH(OOH)C(=O)OCH_3$	31.45
			$31.22^a, 0.66^b$
1, 5-H(p)-(L, L)	R24	$CH_3CH_2CH(OO·)C(=O)OCH_3 \rightarrow C·H_2CH_2CH(OOH)C(=O)OCH_3$	24.45
	R25	$CH_3CH(CH_2OO·)C(=O)OCH_3 \rightarrow C·H_2CH(CH_2OOH)C(=O)OCH_3$	24.93
	R26	$CH_3CH_2CH(OO·)CH_2C(=O)OCH_3 \rightarrow C·H_2CH_2CH(OOH)CH_2C(=O)OCH_3$	24.42
	R27	$CH_3CH_2C(OO·)(CH_3)C(=O)OCH_3 \rightarrow C·H_2CH_2C(OOH)(CH_3)C(=O)OCH_3$	25.09
	R28	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH(C·H_2)C(=O)OCH_3$	22.70
	R29	$(CH_3)_2C(CH_2OO·)C(=O)OCH_3 \rightarrow C·H_2(CH_3)C(CH_2OOH)C(=O)OCH_3$	23.89
	R30	$(CH_3)_2CHCH(OO·)C(=O)OCH_3 \rightarrow C·H_2(CH_3)CHCH(OOH)C(=O)OCH_3$	24.77
			$24.32^a, 2.39^b$
1, 5-H(s)-(L, L)	R31	$CH_2(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C·HC(=O)OCH_3$	19.29
	R32	$CH_2(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C·HCH_2C(=O)OCH_3$	21.76
	R33	$CH_3CH_2CH(CH_2OO·)C(=O)OCH_3 \rightarrow CH_3C·HCH(CH_2OOH)C(=O)OCH_3$	21.53
	R34	$CH_3CH(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OO·)CH_2C·HC(=O)OCH_3$	21.27
	R35	$CH_3CH_2CH_2CH(OO·)C(=O)OCH_3 \rightarrow CH_3C·HCH_2CH(OOH)C(=O)OCH_3$	20.74
	R36	$CH_2(OO·)CH(CH_3)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)C·HC(=O)OCH_3$	19.04
			$20.61^a, 1.70^b$
1, 5-H(t)-(L, L)	R37	$CH_2(OO·)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C·(CH_3)C(=O)OCH_3$	17.23
			17.23^a
1, 6-H(p)-(L, L)	R38	$CH_3CH_2CH_2CH(OO·)C(=O)OCH_3 \rightarrow C·H_2CH_2CH_2CH(OOH)C(=O)OCH_3$	23.74
	R39	$CH_3CH_2CH(CH_2OO·)C(=O)OCH_3 \rightarrow C·H_2CH_2CH(CH_2OOH)C(=O)OCH_3$	24.21
	R40	$CH_2(OO·)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH(C·H_2)C(=O)OCH_3$	23.57
			$23.84^a, 0.64^b$
1, 6-H(s)-(L, L)	R41	$CH_2(OO·)CH_2CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH_2CH·C(=O)OCH_3$	20.51
			$20.51^a, 0.00^b$
1, 6-H(p)-(L, R)	R42	$CH_2(OO·)C(=O)OCH_3 \rightarrow CH_2(OOH)C(=O)OC·H_2$	30.25
	R43	$CH_3CH(OO·)C(=O)OCH_3 \rightarrow CH_3CH(OOH)C(=O)OC·H_2$	30.80
	R44	$CH_3CH_2CH(OO·)C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)C(=O)OC·H_2$	30.93
	R45	$CH_3CH_2CH_2CH(OO·)C(=O)OCH_3 \rightarrow CH_3CH_2CH_2CH(OOH)C(=O)OC·H_2$	30.69
	R46	$(CH_3)_2C(OO·)C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)C(=O)OC·H_2$	32.07
	R47	$CH_3CH_2(CH_3)C(OO·)C(=O)OCH_3 \rightarrow CH_3CH_2(CH_3)C(OOH)C(=O)OC·H_2$	32.03
			$31.13^a, 1.82^b$
1, 7-H(p)-(L, R)	R48	$CH_2(OO·)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2C(=O)OC·H_2$	31.48
	R49	$CH_3CH(OO·)CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH_2C(=O)OC·H_2$	31.04
	R50	$CH_3CH_2CH(OO·)CH_2C(=O)OCH_3 \rightarrow CH_3CH_2CH(OOH)CH_2C(=O)OC·H_2$	30.55
	R51	$CH_2(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)C(=O)OC·H_2$	30.65
	R52	$(CH_3)_2C(CH_2OO·)C(=O)OCH_3 \rightarrow (CH_3)_2C(CH_2OOH)C(=O)OC·H_2$	29.59
	R53	$CH_3CH(OO·)CH(CH_3)C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH(CH_3)C(=O)OC·H_2$	29.84
	R54	$(CH_3)_2C(OO·)CH_2C(=O)OCH_3 \rightarrow (CH_3)_2C(OOH)CH_2C(=O)OC·H_2$	32.56
			$30.82^a, 2.97^b$
1, 8-H(p)-(L, R)	R55	$CH_2(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH_2C(=O)OC·H_2$	24.79
	R56	$CH_3CH(OO·)CH_2CH_2C(=O)OCH_3 \rightarrow CH_3CH(OOH)CH_2CH_2C(=O)OC·H_2$	24.55
	R57	$CH_2(OO·)CH_2CH(CH_3)C(=O)OCH_3 \rightarrow CH_2(OOH)CH_2CH(CH_3)C(=O)OC·H_2$	23.44
	R58	$CH_2(OO·)CH(CH_3)CH_2C(=O)OCH_3 \rightarrow CH_2(OOH)CH(CH_3)CH_2C(=O)OC·H_2$	26.69
			$24.87^a, 3.25^b$
1, 6-H(p)-(R, L)	R59	$CH_3C(=O)OCH_2(OO·) \rightarrow C·H_2C(=O)OCH_2(OOH)$	31.14
			$31.14^a, 0.00^b$
1, 6-H(s)-(R, L)	R60	$CH_3CH_2C(=O)OCH_2(OO·) \rightarrow CH_3C·HC(=O)OCH_2(OOH)$	27.00
	R61	$CH_3CH_2CH_2C(=O)OCH_2(OO·) \rightarrow CH_3CH_2C·HC(=O)OCH_2(OOH)$	26.39
	R62	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO·) \rightarrow CH_3CH_2CH_2C·HC(=O)OCH_2(OOH)$	26.25
	R63	$(CH_3)_2CHCH_2C(=O)OCH_2(OO·) \rightarrow (CH_3)_2CHC·HC(=O)OCH_2(OOH)$	26.12
			$26.44^a, 0.88^b$
1, 6-H(t)-(R, L)	R64	$(CH_3)_2CHC(=O)OCH_2(OO·) \rightarrow (CH_3)_2C·C(=O)OCH_2(OOH)$	23.27
	R65	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO·) \rightarrow CH_3CH_2C·(CH_3)C(=O)OCH_2(OOH)$	23.04
			$23.16^a, 0.23^b$
1, 7-H(p)-(R, L)	R66	$CH_3CH_2C(=O)OCH_2(OO·) \rightarrow C·H_2CH_2C(=O)OCH_2(OOH)$	26.34
	R67	$(CH_3)_2CHC(=O)OCH_2(OO·) \rightarrow C·H_2(CH_3)CHC(=O)OCH_2(OOH)$	25.04

	R68	$(CH_3)_3CC(=O)OCH_2(OO\cdot)\rightarrow C\cdot H_2(CH_3)_2CC(=O)OCH_2(OOH)$	24.16
	R69	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot)\rightarrow CH_3CH_2CH(C\cdot H_2)C(=O)OCH_2(OOH)$	24.29
			24.96[a], 2.18[b]
1, 7-H(s)-(R, L)	R70	$CH_3CH_2CH_2C(=O)OCH_2(OO\cdot)\rightarrow CH_3C\cdot HCH_2C(=O)OCH_2(OOH)$	22.46
	R71	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot)\rightarrow CH_3C\cdot HCH(CH_3)C(=O)OCH_2(OOH)$	21.62
	R72	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot)\rightarrow CH_3CH_2C\cdot HCH_2C(=O)OCH_2(OOH)$	22.51
			22.20[a], 0.89[b]
1, 7-H(t)-(R, L)	R73	$(CH_3)_2CHCH_2C(=O)OCH_2(OO\cdot)\rightarrow (CH_3)_2C\cdot CH_2C(=O)OCH_2(OOH)$	19.36
			19.36[a], 0.00[b]
1, 8-H(p)-(R, L)	R74	$CH_3CH_2CH_2C(=O)OCH_2(OO\cdot)\rightarrow C\cdot H_2CH_2CH_2C(=O)OCH_2(OOH)$	20.83
	R75	$CH_3CH_2CH(CH_3)C(=O)OCH_2(OO\cdot)\rightarrow C\cdot H_2CH_2CH(CH_3)C(=O)OCH_2(OOH)$	18.99
	R76	$(CH_3)_2CHCH_2C(=O)OCH_2(OO\cdot)\rightarrow C\cdot H_2(CH_3)CHCH_2C(=O)OCH_2(OOH)$	20.83
			20.22[a], 1.84[b]
1, 8-H(s)-(R, L)	R77	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot)\rightarrow CH_3C\cdot H_2CH_2CH_2C(=O)OCH_2(OOH)$	17.3
			17.3[a], 0.00[b]
1, 9-H(p)-(R, L)	R78	$CH_3CH_2CH_2CH_2C(=O)OCH_2(OO\cdot)\rightarrow C\cdot H_2CH_2CH_2CH_2C(=O)OCH_2(OOH)$	23.04
			23.04[a], 0.00[b]

[a] The average energy barrier of reactions in each class.

[b] The maximum deviation of energy barriers in each class.

7. High-pressure-limit rate constants of studied reactions

Table S6. Calculated high-pressure-limit rate constants, rate rules, ratios of rate constants of reactions to the average values of the reactions and uncertainty factor values of the rate rule in subclasses of (L, L).

Reaction	Modified Arrhenius parameters			T=800K	
	$\text{Log } A \text{ (s}^{-1})$	n	E (cal/mol)	$k(s^{-1})$	$k/k_{ave}{}^e$
R1	-20.49	9.73	17959.1	9.44E+02	0.63
R2	-15.76	8.34	20640	8.77E+02	0.63
R3	-13.77	7.63	20844.4	6.24E+02	0.46
R4	-14.64	8.03	19729.4	2.57E+03	2.38
R5	-15.50	8.18	21266	3.76E+02	0.35
R6	-17.27	8.79	20707.2	6.11E+02	0.56
R7	-12.07	7.44	21817.7	2.16E+03	2.00
1, 4-H(p)-(L, L)	**-16.21**	**8.46**	**19809.34**	**1.08E+03**	**6.83#**
R8	-27.30	11.61	10441.8	3.58E+03	0.49
R9	-13.09	7.5	18297.1	4.88E+03	0.67
R10	-13.83	7.46	18027.8	6.87E+03	0.95
R11	-28.31	12.04	10516.5	5.78E+03	0.80
R12	-28.60	11.89	10507.4	3.16E+03	0.43
R13	-12.52	7.21	18653.1	2.14E+03	0.29
R14	-9.28	6.45	19190.2	2.10E+03	0.29
R15	-12.11	7.23	17362	1.63E+04	2.25

R16	-11.64	7.22	16682.8	1.33E+04	1.83
R17	-26.31	11.35	10465.1	1.58E+04	2.17
R18	-27.30	11.61	10441.8	5.98E+03	0.82
1, 4-H(s)-(L, L)	**-20.64**	**9.70**	**13638.46**	**7.26E+03**	**7.78[#]**
R19	-25.41	11.12	9668.72	1.69E+04	0.41
R20	-10.60	6.82	16730.6	4.34E+04	1.04
R21	-24.09	10.67	10161.1	1.32E+04	0.32
R22	-24.12	10.96	9401.16	1.13E+05	2.76
R23	-13.77	7.79	16681	1.91E+04	0.46
1, 4-H(t)-(L, L)	**-25.36**	**11.18**	**9557.70**	**4.11E+04**	**8.58[#]**
R24	0.94	3.29	17930.7	3.79E+05	0.81
R25	1.03	3.36	18586.4	4.90E+05	1.05
R26	2.14	2.82	18786.6	1.52E+05	0.33
R27	0.45	3.38	18235.1	1.95E+05	0.42
R28	4.97	2.41	18130	1.34E+06	2.88
R29	3.40	2.53	18809	3.99E+05	0.85
R30	4.51	2.24	20235.6	3.07E+05	0.66
1, 5-H(p)-(L, L)	**1.44**	**3.13**	**17855.64**	**4.67E+05**	**8.83[#]**
R31	-0.98	3.68	12144.3	2.40E+06	**0.59**
R32	2.54	2.79	16362.6	1.59E+06	0.39
R33	2.80	2.72	15556.9	2.84E+05	0.70
R34	-4.49	4.76	10226.2	3.45E+06	0.84
R35	1.09	3.37	14624.2	7.61E+06	1.86
R36	-0.77	3.77	12254.8	6.65E+06	1.63
1, 5-H(s)-(L, L)	**-3.39**	**4.54**	**11669.09**	**4.09E+06**	**4.79[#]**
R37	-2.75	4.29	9232.1	1.59E+07	1.00
1, 5-H(t)-(L, L)	**-2.75**	**4.29**	**9232.1**	**1.77E+07**	**1.00[#]**
R38	-0.77	3.57	16189.3	1.45E+05	0.87
R39	4.84	1.91	19781	9.74E+04	0.58
R40	3.04	2.55	18403.9	2.57E+05	1.54
1, 6-H(p)-(L, L)	**1.09**	**3.06**	**17433.73**	**1.67E+05**	**2.64[#]**
R41	-5.05	4.55	11710.2	9.33E+04	1
1, 6-H(s)-(L, L)	**-5.05**	**4.55**	**11710.2**	**1.03E+05**	**1[#]**

e k_{ave} is the average rate constants at 800 K for each reaction class.

The uncertainty factor values of the high-pressure-limit rule at 800 K for each class in this work (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class).

Table S7. Calculated high-pressure-limit rate constants, rate rules, ratios of rate constants of reactions to the average values of the reactions and uncertainty factor values of the rate rule in subclasses of (L, R).

Reaction	Modified Arrhenius parameters			T=800K	
	Log A (s^{-1})	n	E (cal/mol)	k(s^{-1})	$k/k_{ave}{}^e$
R42	-11.90	7	17304.2	5.08E+03	1.20
R43	-9.80	6.42	19061.3	4.30E+03	1.02
R44	-12.26	7.11	17866.6	3.22E+03	0.76
R45	-12.63	7.28	17291.5	6.07E+03	1.44
R46	-11.83	7.11	18816.6	4.70E+03	1.11
R47	-12.11	7.08	18804.2	1.99E+03	0.47
1, 6-H(p)-(L, R)	**-12.63**	**7.26**	**17647.34**	**4.23E+03**	**3.05#**
R48	-11.42	6.68	18724.8	7.33E+02	0.57
R49	-11.92	6.97	17971.4	2.47E+03	1.93
R50	-11.23	6.47	18114.3	3.92E+02	0.31
R51	-11.67	6.78	18041.8	1.25E+03	0.98
R52	-10.17	6.27	17776.3	1.54E+03	1.20
R53	-9.38	6.19	17895.5	2.04E+03	1.59
R54	-13.15	7.23	18724.9	5.22E+02	0.41
1, 7-H(p)-(L, R)	**-12.33**	**6.96**	**17542.68**	**1.28E+03**	**6.30#**
R55	-3.23	3.97	16663.7	5.35E+03	0.59
R56	-4.52	4.35	15812.8	6.35E+03	0.69
R57	-1.94	3.64	16264.3	1.55E+04	1.70
R58	-4.66	4.5	16221.1	9.33E+03	1.02
1, 8-H(p)-(L, R)	**-3.65**	**4.14**	**16076.59**	**9.14E+03**	**2.90#**

e k_{ave} is the average rate constants at 800 K for each reaction class.

The uncertainty factor values of the high-pressure-limit rule at 800 K for each class in this work (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class).

Table S8. Calculated high-pressure-limit rate constants, rate rules, ratios of rate constants of reactions to the average values of the reactions and uncertainty factor values of the rate rule in subclasses of (R, L).

	Modified Arrhenius parameters	T=800K

Reaction	Log A (s^{-1})	n	E (cal/mol)	k(s^{-1})	k/k_{ave} [e]
R59	-5.56	5.11	21347.7	2.71E+03	1
1, 6-H(p)-(R, L)	**-5.56**	**5.11**	**21347.7**	**2.71E+03**	1
R60	-7.96	5.75	16197.9	6.52E+04	0.48
R61	-8.05	5.99	15496.9	1.25E+05	0.92
R62	-6.98	5.76	15796.7	2.58E+05	1.90
R63	-7.31	5.68	15395.8	9.39E+04	0.69
1, 6-H(s)-(R, L)	**-7.49**	**5.82**	**15654.47**	**1.36E+05**	**3.96**[#]
R64	-7.70	5.87	12845.4	6.88E+05	0.57
R65	-6.63	5.65	12957.3	1.73E+06	1.43
1, 6-H(t)-(R, L)	**-6.99**	**5.72**	**12920.73**	**1.21E+06**	**2.5**[#]
R66	-0.45	3.3	19570	1.66E+04	0.30
R67	0.72	3.18	19041.5	5.73E+04	1.03
R68	2.30	2.65	19042.3	6.15E+04	1.11
R69	1.42	2.95	18492.7	8.68E+04	1.56
1, 7-H(p)-(R, L)	**0.91**	**3.08**	**18655.06**	**5.56E+04**	**5.22**[#]
R70	1.08	3.07	16511.6	3.34E+05	1.13
R71	2.07	2.7	16071.3	3.33E+05	1.13
R72	-4.14	4.52	13577.8	2.20E+05	0.74
1, 7-H(s)-(R, L)	**-0.79**	**3.57**	**15157.98**	**2.96E+05**	**1.52**[#]
R73	-0.84	3.59	12313.3	1.80E+06	1.00
1, 7-H(t)-(R, L)	**-0.84**	**3.59**	**12313.3**	**1.80E+06**	**1.00**[#]
R74	4.01	2.03	16607.5	2.40E+05	0.56
R75	6.12	1.45	16254.8	7.67E+05	1.78
R76	5.55	1.6	17377.9	2.88E+05	0.67
1, 8-H(p)-(R, L)	**4.91**	**1.78**	**16253.18**	**4.32E+05**	**3.19**[#]
R77	5.90	1.5	14264.9	2.34E+06	1.00
1, 8-H(s)-(R, L)	**5.90**	**1.5**	**14264.9**	**2.34E+06**	**1.00**[#]
R78	2.41	2.43	17819.2	3.91E+04	1.00
1, 9-H(p)-(R, L)	**2.41**	**2.43**	**17819.2**	**3.91E+04**	**1.00**[#]

[e] k_{ave} is the average rate constants at 800 K for each reaction class.

[#] The uncertainty factor values of the high-pressure-limit rule at 800 K for each class in this work (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class).

8. Pressure-dependent rate constants of studied reactions

Table S9. Calculated pressure-dependent rate constants, rate rules, ratios of rate constants of reactions to the average values of the reactions and uncertainty factor values of the rate rule in subclasses of (L, L) at different pressures.

| Reaction | Pressure (atm) | Modified Arrhenius parameters | | | T=800K | |
		Log A (s⁻¹)	n	E (cal/mol)	k (s⁻¹)	k/k_{ave}^e
R1	0.01	-1.00	3.51	23788.9	8.35E+02	0.46
	0.1	-5.94	5.10	22366	9.04E+02	0.50
	1.0	-13.68	7.57	20078.9	9.54E+02	0.74
	10	-18.50	9.10	18600.8	9.62E+02	0.63
	100	-20.18	9.63	18072.6	9.63E+02	0.58
R2	0.01	6.60	1.11	9363.28	8.27E+02	0.50
	0.1	1.91	2.61	7982.33	8.65E+02	0.52
	1.0	-5.48	4.97	5767.52	8.90E+02	0.69
	10	-9.74	6.31	4450.62	8.93E+02	0.63
	100	-11.06	6.73	4034.68	8.93E+02	0.57
R3	0.01	-0.59	3.47	24907.5	6.49E+02	0.43
	0.1	-4.13	4.59	23844.1	6.60E+02	0.43
	1.0	-10.14	6.50	22011.5	6.67E+02	0.52
	10	-13.03	7.41	21109.5	6.67E+02	0.48
	100	-13.69	7.62	20899.9	6.68E+02	0.44
R4	0.01	4.56	1.93	25545.6	2.43E+03	2.27
	0.1	-0.30	3.49	24115.6	2.54E+03	2.24
	1.0	-8.11	5.98	21780.6	2.62E+03	2.04
	10	-12.83	7.47	20324.9	2.63E+03	2.39
	100	-14.37	7.96	19840.7	2.63E+03	2.18
R5	0.01	-1.40	3.72	25573.1	3.99E+02	0.37
	0.1	-5.27	4.96	24420.8	4.09E+02	0.36
	1.0	-11.53	6.95	22519.7	4.15E+02	0.32
	10	-14.63	7.93	21554.2	4.16E+02	0.38
	100	-15.39	8.16	21316.7	4.16E+02	0.35
R6	0.01	-1.49	3.81	25543.6	6.09E+02	0.57
	0.1	-5.59	5.11	24319.7	6.23E+02	0.55

	1.0	-12.53	7.32	22216	6.33E+02	0.49
	10	-16.32	8.52	21037	6.34E+02	0.58
	100	-17.37	8.85	20705.1	6.35E+02	0.53
R7	0.01	8.83	0.70	28048.3	2.57E+03	2.40
	0.1	3.67	2.35	26539.9	2.72E+03	2.40
	1.0	-4.58	4.99	24087.1	2.83E+03	2.20
	10	-9.90	6.67	22454	2.11E+03	1.92
	100	-11.84	7.29	21844.3	2.85E+03	2.36
1, 4-H(p)-(L, L)	**0.01**	**1.85**	**2.74**	**25286.01**	**1.07E+03**	**6.46[#]**
	0.1	**-2.61**	**4.17**	**23983.03**	**1.13E+03**	**6.65[#]**
	1.0	**-9.81**	**6.46**	**21850.28**	**1.29E+03**	**6.81[#]**
	10	**-13.29**	**7.56**	**20714.24**	**1.10E+03**	**6.32[#]**
	100	**-15.73**	**8.33**	**20019.77**	**1.21E+03**	**6.84[#]**
R8	0.01	-6.63	5.01	16586.1	2.42E+03	0.44
	0.1	-12.17	6.79	15003.2	2.84E+03	0.46
	1.0	-20.14	9.35	12672.2	3.39E+03	0.47
	10	-25.17	10.94	11138.2	3.59E+03	0.48
	100	-26.96	11.51	10581.1	3.62E+03	0.48
R9	0.01	6.79	1.16	24239.1	3.36E+03	0.61
	0.1	1.51	2.85	22715.1	3.85E+03	0.62
	1.0	-6.38	5.38	20391.7	4.53E+03	0.64
	10	-11.22	6.91	18910.7	4.77E+03	0.64
	100	-12.83	7.42	18407.6	4.80E+03	0.64
R10	0.01	5.72	1.50	23689.8	6.05E+03	1.10
	0.1	0.85	3.05	22264.5	6.37E+03	1.03
	1.0	-6.81	5.50	19986.9	6.63E+03	0.93
	10	-11.34	6.94	18593.4	6.66E+03	0.89
	100	-12.75	7.38	18151.9	6.66E+03	0.88
R11	0.01	-3.91	4.26	1776	3.99E+03	0.73
	0.1	-9.92	6.19	16043.7	4.74E+03	0.77
	1.0	-18.69	9.01	13494.4	5.84E+03	0.82
	10	-24.90	10.98	11612.5	6.31E+03	0.84
	100	-27.58	11.83	10775.3	6.40E+03	0.85

R12	0.01	3.23	2.23	23011.1	2.64E+03	0.48
	0.1	-0.96	3.57	21771.9	2.86E+03	0.46
	1.0	-8.02	5.82	19657	3.20E+03	0.45
	10	-11.92	7.05	18452.7	3.30E+03	0.44
	100	-12.99	7.39	18116.6	3.31E+03	0.44
R13	0.01	-13.87	7.25	14948.2	2.04E+03	0.37
	0.1	-17.76	8.49	13787.3	2.09E+03	0.34
	1.0	-24.26	10.56	11819.8	2.12E+03	0.30
	10	-27.55	11.60	10797.9	2.13E+03	0.28
	100	-28.35	11.85	10544.9	2.13E+03	0.28
R14	0.01	1.30	2.82	22872.8	1.69E+03	0.31
	0.1	-2.46	4.02	21753.6	1.81E+03	0.29
	1.0	-8.72	5.01	19860.4	1.97E+03	0.28
	10	-11.75	6.96	18919.6	2.00E+03	0.27
	100	-12.43	7.18	18702.7	2.01E+03	0.27
R15	0.01	14.96	-1.30	26302.3	9.83E+03	1.79
	0.1	8.80	0.69	24566.4	1.20E+04	1.95
	1.0	0.13	3.48	22084.4	1.53E+04	2.15
	10	-6.05	5.44	20222.2	1.68E+04	2.24
	100	-8.68	6.27	19407.8	1.70E+04	2.26
R16	0.01	9.57	0.32	23788	9.61E+04	1.75
	0.1	3.98	2.11	22178.1	1.11E+04	1.80
	1.0	-4.31	4.77	19761.9	1.35E+04	1.89
	10	-9.74	6.49	18111.3	1.44E+04	1.92
	100	-11.71	7.11	17495	1.45E+04	1.93
R17	0.01	7.28	0.98	22595.1	1.41E+04	2.57
	0.1	2.09	2.64	21091.9	1.51E+04	2.45
	1.0	-5.83	5.17	18768.5	1.60E+04	2.25
	10	-10.71	6.73	17276.4	1.62E+04	2.16
	100	-12.31	7.23	16777.7	1.62E+04	2.15
R18	0.01	-6.14	4.93	16526.1	4.55E+03	0.83
	0.1	-11.26	6.57	15030.5	5.11E+03	0.83
	1.0	-19.29	9.13	12658.2	5.97E+03	0.84

	10	-24.30	10.72	11122.2	6.26E+03	0.84
	100	-26.00	11.26	10588.4	6.31E+03	0.84
1, 4-H(s)-(L, L)	**0.01**	**0.14**	**3.08**	**19838.30**	**5.48E+03**	**8.31#**
	0.1	**-5.09**	**4.76**	**18328.45**	**6.18E+03**	**8.36#**
	1.0	**-13.13**	**7.33**	**15967.11**	**7.14E+03**	**8.16#**
	10	**-18.32**	**8.98**	**14379.71**	**7.49E+03**	**8.36#**
	100	**-20.24**	**9.58**	**13778.77**	**7.55E+03**	**8.49#**
R19	0.01	-1.90	3.59	16571.7	9.90E+03	0.38
	0.1	-7.95	5.54	14858.8	1.19E+04	0.38
	1.0	-16.46	8.28	12409.4	1.50E+04	0.38
	10	-22.39	10.16	10617.7	1.62E+04	0.38
	100	-24.82	10.93	982.97	1.65E+04	0.39
R20	0.01	13.54	-0.92	23774.5	2.35E+04	0.90
	0.1	7.33	1.08	22018.1	2.86E+04	0.90
	1.0	-1.30	3.86	19558.2	3.67E+04	0.92
	10	-7.47	5.83	17703.8	4.03E+04	0.95
	100	-10.03	6.63	16909.9	4.10E+04	0.96
R21	0.01	-3.29	4.05	16339.2	9.86E+03	0.38
	0.1	-8.71	5.79	14770.7	1.13E+04	0.36
	1.0	-16.82	8.38	12401	1.35E+04	0.34
	10	-21.97	10.02	10829.8	1.44E+04	0.34
	100	-23.75	10.58	10274.2	1.45E+04	0.34
R22	0.01	4.74	1.61	17746.9	7.54E+04	2.90
	0.1	-2.44	3.94	15768.8	9.41E+04	2.96
	1.0	-11.69	6.94	13221.8	1.17E+05	2.95
	10	-19.56	9.46	10906.3	1.23E+05	2.90
	100	-24.12	10.90	9507.9	1.24E+05	2.89
R23	0.01	9.56	0.32	23559	1.12E+04	0.43
	0.1	3.63	2.23	21863.1	1.33E+04	0.42
	1.0	-4.98	4.99	19376.5	1.65E+04	0.41
	10	-10.92	6.88	17577	1.78E+04	0.42
	100	-13.29	7.63	16839.6	1.81E+04	0.42
1, 4-H(t)-(L, L)	**0.01**	**-1.36**	**3.46**	**16339.46**	**2.60E+04**	**7.65#**

	0.1	**-7.06**	**5.31**	**14798.64**	**3.18E+04**	**8.32[#]**
	1.0	**-15.25**	**7.97**	**12549.22**	**3.98E+04**	**8.65[#]**
	10	**-21.37**	**9.92**	**10774.54**	**4.23E+04**	**8.56[#]**
	100	**-24.38**	**10.88**	**9864.83**	**4.28E+04**	**8.54[#]**
R24	0.01	25.51	-4.66	24805.7	1.59E+05	**0.75**
	0.1	18.87	-2.49	23039.6	2.19E+05	**0.75**
	1.0	10.99	0.08	20936.9	3.80E+05	**0.81**
	10	4.65	2.11	19089.5	3.66E+05	**0.75**
	100	1.70	3.05	18185.7	3.78E+05	**0.76**
R25	0.01	28.18	-5.45	26084	1.76E+05	0.83
	0.1	21.26	-3.17	24283.2	2.57E+05	0.88
	1.0	13.23	-0.54	22196.1	4.82E+05	1.03
	10	6.16	1.73	20161.6	4.72E+05	0.97
	100	2.27	2.97	18978.9	4.96E+05	1.00
R26	0.01	21.97	-3.55	24556	9.23E+04	0.44
	0.1	16.35	-1.73	22974	1.11E+05	0.38
	1.0	8.82	0.70	20844.4	1.59E+05	0.34
	10	4.01	2.23	19400.9	1.51E+05	0.31
	100	2.44	2.72	18915.5	1.53E+05	0.31
R27	0.01	22.40	-3.68	24525.7	1.07E+05	0.51
	0.1	16.36	-1.72	22845.2	1.33E+05	0.45
	1.0	8.51	0.82	20655	2.08E+05	0.44
	10	2.99	2.58	19012.6	1.92E+05	0.40
	100	0.89	3.24	18363.6	1.96E+05	0.39
R28	0.01	30.27	-6.11	25163.9	6.06E+05	2.87
	0.1	23.31	-3.81	23378.6	8.88E+05	3.03

	1.0	15.81	-1.34	21504.2	1.35E+06	2.88
	10	8.89	0.89	19541.8	1.52E+06	3.13
	100	4.97	2.14	18358.7	1.54E+06	3.10
R29	0.01	26.78	-5.01	25443	1.92E+05	0.91
	0.1	20.35	-2.92	23692.1	2.52E+05	0.86
	1.0	12.50	-0.37	21567	4.05E+05	0.86
	10	6.51	1.55	19806.4	3.98E+05	0.82
	100	3.94	2.36	19019.2	4.08E+05	0.82
R30	0.01	28.12	-5.37	26944.9	1.48E+05	0.70
	0.1	21.68	-3.28	25179	1.92E+05	0.66
	1.0	13.68	-0.68	22991.9	3.02E+05	0.64
	10	7.65	1.25	21212.9	2.98E+05	0.61
	100	5.08	2.06	20424	3.05E+05	0.61
1, 5-H(p)-(L, L)	**0.01**	**24.83**	**-4.45**	**24223.22**	**2.11E+05**	**6.56[#]**
	0.1	**18.80**	**-2.48**	**22665.91**	**2.93E+05**	**7.99[#]**
	1.0	**12.11**	**-0.26**	**21021.82**	**4.70E+05**	**8.54[#]**
	10	**5.38**	**1.89**	**19036.79**	**4.85E+05**	**10.03[#]**
	100	**2.40**	**2.84**	**18148.64**	**4.97E+05**	**10.07[#]**
R31	0.01	21.01	-3.51	17972.6	8.22E+05	**0.25**
	0.1	14.73	-1.42	16428.1	1.27E+06	0.37
	1.0	8.29	0.72	14870.6	2.06E+06	0.52
	10	2.51	2.58	13241.8	2.43E+06	0.59
	100	-0.29	3.47	12399.3	2.53E+06	0.61
R32	0.01	19.39	-2.87	21448.1	6.87E+05	0.21

	0.1	14.12	-1.16	19972.7	9.90E+05	0.28
	1.0	7.23	1.06	18032.8	1.47E+06	0.38
	10	3.12	2.37	16801.8	1.63E+06	0.40
	100	1.94	2.74	16440.1	1.65E+06	0.40
R33	0.01	27.27	-5.25	23078.6	8.34E+05	0.25
	0.1	20.50	-3.02	21337.4	1.32E+06	0.38
	1.0	13.23	-0.62	19509.5	2.19E+06	0.57
	10	6.77	1.46	17670.2	2.75E+06	0.67
	100	3.44	2.52	16661.4	2.91E+06	0.70
R34	0.01	1.85	2.77	12240	3.38E+06	1.03
	0.1	1.69	2.81	12193.4	3.38E+06	0.97
	1.0	0.81	3.09	11917.9	3.40E+06	0.88
	10	-1.44	3.80	11214	3.44E+06	0.84
	100	-3.67	4.50	10513.6	3.46E+06	0.83
R35	0.01	10.45	0.42	17555.2	7.58E+06	2.31
	0.1	10.35	0.45	17525.8	7.59E+06	2.18
	1.0	9.65	0.68	17310.2	7.64E+06	1.98
	10	7.19	1.45	16552.8	7.79E+06	1.91
	100	3.61	2.59	15437.4	7.96E+06	1.91
R36	0.01	6.58	1.45	14555	6.36E+06	1.94
	0.1	6.47	1.48	14521.1	6.36E+06	1.82
	1.0	5.73	1.72	14292.8	6.40E+06	1.66
	10	3.47	2.43	13591.6	6.48E+06	1.59
	100	0.70	3.30	12721.3	6.55E+06	1.57

1, 5-H(s)-(L, L)	**0.01**	**5.53**	**1.68**	**14282.86**	**3.28E+06**	**11.04**[#]
	0.1	**5.57**	**1.68**	**14340.96**	**3.49E+06**	**7.67**[#]
	1.0	**4.52**	**2.03**	**14104.12**	**3.85E+06**	**5.18**[#]
	10	**1.30**	**3.06**	**13150.25**	**4.09E+06**	**4.78**[#]
	100	**-1.83**	**4.05**	**12185.81**	**4.18E+06**	**4.82**[#]
R37	0.01	19.15	-3.02	14373.7	2.93E+06	1.00
	0.1	13.73	-1.15	13305.8	5.71E+06	1.00
	1.0	9.00	0.50	12480.5	1.11E+07	1.00
	10	3.05	2.46	10947.4	1.55E+07	1.00
	100	-1.14	3.80	9731.32	1.72E+07	1.00
1, 5-H(t)-(L, L)	**0.01**	**19.15**	**-3.02**	**14373.7**	**2.93E+06**	**1.00**[#]
	0.1	**13.73**	**-1.15**	**13305.8**	**5.71E+06**	**1.00**[#]
	1.0	**9.00**	**0.50**	**12480.5**	**1.11E+07**	**1.00**[#]
	10	**3.05**	**2.46**	**10947.4**	**1.55E+07**	**1.00**[#]
	100	**-1.14**	**3.80**	**9731.32**	**1.72E+07**	**1.00**[#]
R38	0.01	16.87	-2.08	21359	1.28E+05	0.94
	0.1	11.73	-0.43	19903.2	1.43E+05	0.92
	1.0	4.71	1.83	17898.2	1.59E+05	0.90
	10	0.58	3.15	16654.3	1.62E+05	0.89
	100	-0.60	3.52	16288.5	1.62E+05	0.89
R39	0.01	21.98	-3.55	24818.8	9.59E+04	0.70
	0.1	17.01	-1.95	23403.7	1.06E+05	0.68
	1.0	10.05	0.29	21403.7	1.16E+05	0.65
	10	6.11	1.54	20211.2	1.18E+05	0.65

	100	5.04	1.88	19879.2	1.18E+05	0.65
R40	0.01	23.70	-4.10	24344.9	1.86E+05	1.36
	0.1	17.84	-2.20	22713.6	2.19E+05	1.40
	1.0	10.29	0.24	20609.3	2.58E+05	1.45
	10	5.18	1.87	19085.5	2.65E+05	1.46
	100	3.37	2.45	18525.1	2.66E+05	1.46
1, 6-H(p)-(L, L)	**0.01**	**19.86**	**-2.96**	**22898.08**	**1.37E+05**	**1.94[#]**
	0.1	**14.54**	**-1.24**	**21404.62**	**1.56E+05**	**2.07[#]**
	1.0	**7.36**	**1.08**	**19374.23**	**1.78E+05**	**2.22[#]**
	10	**2.84**	**2.52**	**18022.79**	**1.82E+05**	**2.25[#]**
	100	**1.39**	**2.98**	**17575.93**	**1.82E+05**	**2.25[#]**
R41	0.01	6.13	0.99	15067.2	8.05E+04	1.00
	0.1	2.71	2.09	14074.4	8.77E+04	1.00
	1.0	-2.46	3.75	12554.2	9.78E+04	1.00
	10	-4.63	4.44	11891.8	1.00E+05	1.00
	100	-5.03	4.56	11768.5	1.00E+05	1.00
1, 6-H(s)-(L, L)	**0.01**	**6.13**	**0.99**	**15067.2**	**8.05E+04**	**1.00[#]**
	0.1	**2.71**	**2.09**	**14074.4**	**8.77E+04**	**1.00[#]**
	1.0	**-2.46**	**3.75**	**12554.2**	**9.78E+04**	**1.00[#]**
	10	**-4.63**	**4.44**	**11891.8**	**1.00E+05**	**1.00[#]**
	100	**-5.03**	**4.56**	**11768.5**	**1.00E+05**	**1.00[#]**

[e] k_{ave} is the average rate constants of 800 K for each reaction class.

[#] The uncertainty factor values of the pressure-dependent rate rule at 800 K for each class at different pressures (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class at different pressures).

Table S10. Calculated pressure-dependent rate constants, rate rules, ratios of rate constants of reactions to the average values of the reactions and uncertainty factor values of the rate rule in subclasses of (L, R) at different pressures.

| Reaction | Pressure (atm) | Modified Arrhenius parameters | | | T=800K | |
		Log A (s^{-1})	n	E (cal/mol)	k (s^{-1})	$k/k_{ave}{}^e$
R42	0.01	7.28	0.85	22910.4	4.75E+03	0.92
	0.1	1.77	2.64	21378.9	5.55E+03	1.00
	1.0	-5.71	5.04	19221.6	6.16E+03	1.04
	10	-10.23	6.48	17852.4	6.27E+03	1.05
	100	-11.69	6.94	17397.5	6.28E+03	1.05
R43	0.01	9.66	0.22	24839.7	4.90E+03	0.95
	0.1	4.60	1.85	23397.1	5.40E+03	0.97
	1.0	-3.10	4.32	21147.1	5.82E+03	0.99
	10	-7.87	5.83	19691.6	5.88E+03	0.99
	100	-9.48	6.34	19188.3	5.89E+03	0.99
R44	0.01	4.48	1.80	22924.6	4.20E+03	0.82
	0.1	-0.08	3.26	21587.7	4.42E+03	0.79
	1.0	-7.13	5.51	19485.5	4.58E+03	0.78
	10	-10.98	6.73	18296.2	4.60E+03	0.77
	100	-12.06	7.07	17957.6	4.60E+03	0.77
R45	0.01	6.51	1.22	23046.3	9.10E+03	1.77
	0.1	1.56	2.81	21598.5	9.62E+03	1.73
	1.0	-6.16	5.28	19314.4	1.01E+04	1.70
	10	-10.78	6.74	17893.6	1.01E+04	1.70
	100	-12.26	7.21	17432.3	1.01E+04	1.70
R46	0.01	8.00	0.79	24750.1	5.47E+03	1.06
	0.1	2.81	2.46	23248.2	5.90E+03	1.06
	1.0	-5.07	4.98	20928.2	6.24E+03	1.06
	10	-9.93	6.52	19440.7	6.29E+03	1.06
	100	-11.56	7.04	18929.7	6.30E+03	1.06
R47	0.01	1.79	2.67	23040	2.45E+03	0.48
	0.1	-1.93	3.85	21932.6	2.51E+03	0.45
	1.0	-8.19	5.84	20035.4	2.55E+03	0.43
	10	-11.28	6.82	19075.5	2.56E+03	0.43

	100	-12.00	7.05	18847.5	2.56E+03	0.43
1, 6-H(p)-(L, R)	**0.01**	**5.61**	**1.46**	**23085.38**	**5.15E+03**	**3.71**[#]
	0.1	**0.86**	**2.98**	**21719.66**	**5.57E+03**	**3.84**[#]
	1.0	**-6.51**	**5.34**	**19551.59**	**5.90E+03**	**3.94**[#]
	10	**-10.92**	**6.74**	**18201.44**	**5.95E+03**	**3.96**[#]
	100	**-12.33**	**7.19**	**17760.93**	**5.96E+03**	**3.96**[#]
R48	0.01	-0.94	3.36	21959	6.51E+02	0.52
	0.1	-4.21	4.4	20985.3	6.90E+02	**0.53**
	1.0	-9.13	5.97	19489.4	9.08E+02	**0.57**
	10	-11.08	6.58	18883.7	7.41E+02	**0.54**
	100	-11.44	6.69	18770.5	7.42E+02	**0.54**
R49	0.01	2.66	2.33	22430.6	2.05E+03	1.65
	0.1	-1.42	3.64	21225	2.22E+03	1.71
	1.0	-7.83	5.68	19297.1	3.07E+03	1.91
	10	-11.02	6.69	18307.7	2.50E+03	1.81
	100	-11.80	6.94	18063.2	2.51E+03	1.82
R50	0.01	-6.35	4.94	19677.2	4.01E+02	0.32
	0.1	-7.81	5.4	19230.6	4.06E+02	0.31
	1.0	-10.38	6.21	18432.6	5.04E+02	0.31
	10	-11.11	6.44	18202.6	4.14E+02	0.30
	100	-11.20	6.47	18172.9	4.14E+02	0.30
R51	0.01	-0.42	3.22	21512.5	1.15E+03	0.93
	0.1	-3.69	4.27	20534.8	1.22E+03	0.94
	1.0	-8.94	5.93	18936.1	1.57E+03	0.98
	10	-11.16	6.64	18243	1.31E+03	0.95
	100	-11.60	6.77	18105.1	1.31E+03	0.95
R52	0.01	-0.94	3.37	20666.4	1.57E+03	1.26

	0.1	-3.54	4.2	19880.3	1.63E+03	1.25
	1.0	-8.10	5.64	18486.2	2.04E+03	1.27
	10	-9.85	6.2	17936.9	1.72E+03	1.24
	100	-10.15	6.29	17842.5	1.72E+03	1.24
R53	0.01	5.11	1.61	22329.7	2.28E+03	1.84
	0.1	1.17	2.87	21162.2	2.31E+03	1.78
	1.0	-5.27	4.92	19229.4	2.33E+03	1.45
	10	-8.46	5.93	18241.4	2.33E+03	1.69
	100	-9.21	6.16	18006.3	2.33E+03	1.69
R54	0.01	-0.53	3.26	20757	5.93E+02	0.48
	0.1	-3.26	4.12	19935.9	6.13E+02	0.47
	1.0	-7.95	5.61	18502	8.14E+02	0.51
	10	-9.78	6.19	17930.5	6.44E+02	0.47
	100	-10.09	6.29	17830.6	6.44E+02	0.47
1, 7-H(p)-(L, R)	**0.01**	**-1.79**	**3.63**	**20763.14**	**1.24E+03**	**5.70[#]**
	0.1	**-4.74**	**4.57**	**19890.69**	**1.30E+03**	**5.69[#]**
	1.0	**-9.17**	**5.99**	**18611.54**	**1.63E+03**	**6.08[#]**
	10	**-11.81**	**6.81**	**17749.60**	**1.38E+03**	**6.05[#]**
	100	**-12.26**	**6.95**	**17611.87**	**1.38E+03**	**6.06[#]**
R55	0.01	3.28	1.91	18713.7	5.26E+03	0.61
	0.1	1.22	2.57	18095.4	5.43E+03	0.61
	1.0	-2.11	3.63	17077.6	6.08E+03	0.60
	10	-3.12	3.95	16763.1	5.66E+03	0.60
	100	-3.26	3.99	16719.5	5.67E+03	0.60
R56	0.01	1.97	2.32	17866.1	6.51E+03	0.76
	0.1	0.04	2.93	17284.3	6.69E+03	0.75

Reaction	Pressure (atm)	Log A (s⁻¹)	n	E (cal/mol)	k (s⁻¹)	k/k_ave
	1.0	-3.30	3.99	16262.6	7.56E+03	0.75
	10	-4.34	4.32	15937.1	6.97E+03	0.74
	100	-4.49	4.37	15891.6	6.98E+03	0.74
R57	0.01	6.21	1.06	18781	1.45E+04	1.68
	0.1	3.78	1.84	18058.7	1.51E+04	1.69
	1.0	-0.29	3.13	16824.4	1.70E+04	1.68
	10	-1.71	3.58	16385.1	1.61E+04	1.71
	100	-1.92	3.65	16317.6	1.61E+04	1.71
R58	0.01	3.45	1.92	18714	8.13E+03	0.95
	0.1	1.07	2.68	17999.2	8.44E+03	0.95
	1.0	-3.01	3.97	16761.5	9.81E+03	0.97
	10	-4.42	4.42	16322.1	8.95E+03	0.95
	100	-4.63	4.49	16254.8	8.96E+03	0.95
1, 8-H(p)-(L, R)	**0.01**	**3.89**	**1.75**	**18415.72**	**8.59E+03**	**2.75[#]**
	0.1	**1.66**	**2.46**	**17746.11**	**8.91E+03**	**2.78[#]**
	1.0	**-2.14**	**3.67**	**16593.51**	**1.01E+04**	**2.79[#]**
	10	**-3.41**	**4.07**	**16196.35**	**9.42E+03**	**2.84[#]**
	100	**-3.60**	**4.13**	**16136.84**	**9.42E+03**	**2.84[#]**

[e] k_{ave} is the average rate constants of 800 K for each reaction class.

[#] The uncertainty factor values of the pressure-dependent rate rule at 800 K for each class at different pressures (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class at different pressures).

Table S11. Calculated pressure-dependent rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in subclasses of (R, L) at different pressures.

Reaction	Pressure (atm)	Modified Arrhenius parameters			T=800K	
		Log A (s⁻¹)	n	E (cal/mol)	k (s⁻¹)	k/k_ave^e
R59	0.01	11.98	-0.48	26492.2	3.11E+03	1.00
	0.1	6.81	1.19	25038.1	3.53E+03	1.00
	1.0	-0.29	3.46	22970.8	3.83E+03	1.00

	10	-4.22	4.71	21772.2	3.88E+03	1.00
	100	-5.34	5.07	21425.4	3.88E+03	1.00
1, 6-H(p)-(R, L)	**0.01**	**11.98**	**-0.48**	**26492.2**	**3.11E+03**	**1.00#**
	0.1	**6.81**	**1.19**	**25038.1**	**3.53E+03**	**1.00#**
	1.0	**-0.29**	**3.46**	**22970.8**	**3.83E+03**	**1.00#**
	10	**-4.22**	**4.71**	**21772.2**	**3.88E+03**	**1.00#**
	100	**-5.34**	**5.07**	**21425.4**	**3.88E+03**	**1.00#**
R60	0.01	15.33	-1.59	22777.8	4.66E+04	0.71
	0.1	9.05	0.45	21067.4	5.82E+04	0.69
	1.0	0.93	3.08	18809.3	7.00E+04	0.62
	10	-4.91	4.94	17072	7.25E+04	0.57
	100	-7.30	5.70	16335.4	7.28E+04	0.56
R61	0.01	17.18	-2.13	22692.5	6.27E+04	0.95
	0.1	10.55	0.03	20885.5	8.27E+04	0.98
	1.0	2.18	2.74	18587.4	1.15E+05	1.01
	10	-4.31	4.82	16672.9	1.30E+05	1.03
	100	-7.29	5.76	15757.6	1.34E+05	1.03
R62	0.01	19.37	-2.76	23320.7	9.73E+04	1.48
	0.1	12.54	-0.54	21451.3	1.28E+05	1.52
	1.0	4.03	2.22	19131.4	1.81E+05	1.60
	10	-2.81	4.41	17118.8	2.85E+05	1.65
	100	-6.17	5.48	16086.4	2.15E+05	1.66
R63	0.01	14.36	-1.26	21714.4	5.66E+04	0.86
	0.1	8.46	0.64	20049.7	6.85E+04	0.81
	1.0	0.46	3.22	17780.6	8.72E+04	0.77
	10	-4.94	4.94	16158.5	9.48E+04	0.75
	100	-6.91	5.56	15548.3	9.61E+04	0.74
1, 6-H(s)-(R, L)	**0.01**	**17.22**	**-2.14**	**22743.73**	**6.58E+04**	**2.09#**
	0.1	**10.77**	**-0.05**	**20972.87**	**8.44E+04**	**2.21#**

	1.0	**2.44**	**2.65**	**18671.62**	**1.13E+05**	**2.58**[#]
	10	**-3.92**	**4.69**	**16785.22**	**1.27E+05**	**2.87**[#]
	100	**-6.82**	**5.60**	**15894.64**	**1.30E+05**	**2.96**[#]
R64	0.01	-1.03	3.79	14968.5	7.84E+05	1.18
	0.1	-1.16	3.84	14928.2	7.85E+05	0.94
	1.0	-1.98	4.09	14673.5	7.89E+05	0.68
	10	-4.21	4.8	13977.5	7.98E+05	0.56
	100	-6.59	5.55	13229.5	8.03E+05	0.53
R65	0.01	22.86	-3.94	20792.5	5.41E+05	0.82
	0.1	15.70	-1.57	19025.2	8.80E+05	1.12
	1.0	8.37	0.87	17291.5	1.53E+06	1.32
	10	0.82	3.32	15204.1	2.03E+06	1.44
	100	-4.36	4.97	13662.5	2.22E+06	1.47
1, 6-H(t)-(R, L)	**0.01**	**3.50**	**2.28**	**15499.24**	**6.62E+05**	**1.45**[#]
	0.1	**4.36**	**2.05**	**15938.73**	**8.32E+05**	**1.12**[#]
	1.0	**3.68**	**2.33**	**16026.17**	**1.16E+06**	**1.95**[#]
	10	**-0.85**	**3.80**	**14789.17**	**1.41E+06**	**2.55**[#]
	100	**-5.03**	**5.14**	**13534.31**	**1.51E+06**	**2.77**[#]
R66	0.01	9.08	0.25	22478.4	1.30E+04	0.30
	0.1	6.00	1.24	21567.6	1.40E+04	0.28
	1.0	1.44	2.69	20193.4	1.47E+04	0.25
	10	-0.20	3.21	19686.4	1.48E+04	0.25
	100	-0.47	3.29	19602.6	1.48E+04	0.25
R67	0.01	13.65	-1.09	23686.5	5.49E+04	1.25
	0.1	9.34	0.30	22439.9	6.18E+04	1.25
	1.0	3.19	2.26	20625.8	6.84E+04	1.18
	10	0.29	3.18	19736.3	6.95E+04	1.18
	100	-0.35	3.39	19535.1	6.97E+04	1.17
R68	0.01	17.50	-2.21	23603.1	4.27E+04	0.97
	0.1	13.12	-0.81	22336.7	4.76E+04	0.96

	1.0	6.53	1.3	20406.6	5.84E+04	0.98
	10	3.10	2.39	19361.3	5.72E+04	0.97
	100	2.28	2.65	19103.1	5.75E+04	0.97
R69	0.01	19.32	-2.76	23764.4	6.46E+04	1.48
	0.1	14.26	-1.13	22317.5	7.47E+04	1.51
	1.0	7.08	1.17	20244.5	9.75E+04	1.63
	10	2.86	2.51	18966.2	9.49E+04	1.61
	100	1.63	2.9	18585	9.57E+04	1.61
1, 7-H(p)-(R, L)	**0.01**	**18.39**	**-2.50**	**23865.63**	**4.38E+04**	**4.96[#]**
	0.1	**13.49**	**-0.92**	**22461.84**	**4.95E+04**	**5.35[#]**
	1.0	**6.19**	**1.41**	**20317.91**	**5.98E+04**	**6.65[#]**
	10	**2.32**	**2.65**	**19154.23**	**5.91E+04**	**6.43[#]**
	100	**1.14**	**3.02**	**18785.27**	**5.94E+04**	**6.47[#]**
R70	0.01	22.15	-3.71	22457.5	2.33E+05	0.98
	0.1	16.03	-1.72	20799.9	2.92E+05	1.11
	1.0	8.63	0.69	18782.3	3.62E+05	1.24
	10	3.39	2.37	17237.6	3.77E+05	1.27
	100	1.45	2.98	16643.4	3.79E+05	1.27
R71	0.01	10.28	0.11	18678.7	3.45E+05	1.44
	0.1	9.29	0.43	18371.7	3.45E+05	1.31
	1.0	6.57	1.29	17529	3.45E+05	1.18
	10	3.52	2.25	16574.5	3.45E+05	1.16
	100	2.27	2.64	16178.8	3.45E+05	1.16
R72	0.01	11.66	-0.57	18245.5	6.04E+04	0.58
	0.1	6.89	0.96	16886.7	6.70E+04	0.58
	1.0	0.27	3.09	14989.2	7.36E+04	0.58
	10	-3.32	4.23	13903.9	7.47E+04	0.57
	100	-4.23	4.52	13623.4	7.49E+04	0.57

1, 7-H(s)-(R, L)	**0.01**	**12.61**	**-0.71**	**19180.96**	**2.39E+05**	**2.49**[#]
	0.1	**10.27**	**0.05**	**18542.93**	**2.63E+05**	**2.26**[#]
	1.0	**5.35**	**1.63**	**17144.19**	**2.92E+05**	**2.06**[#]
	10	**1.27**	**2.93**	**15913.08**	**2.98E+05**	**2.03**[#]
	100	**-0.23**	**3.41**	**15449.78**	**2.98E+05**	**2.02**[#]
R73	0.01	19.48	-3.01	17865.6	9.24E+05	1.00
	0.1	13.35	-1.00	16264.9	1.25E+06	1.00
	1.0	6.74	1.17	14568.4	1.72E+06	1.00
	10	1.60	2.82	13088.6	1.85E+06	1.00
	100	-0.42	3.46	12476.1	1.87E+06	1.00
1, 7-H(t)-(R, L)	**0.01**	**19.48**	**-3.01**	**17865.6**	**9.24E+05**	**1.00**[#]
	0.1	**13.35**	**-1.00**	**16264.9**	**1.25E+06**	**1.00**[#]
	1.0	**6.74**	**1.17**	**14568.4**	**1.72E+06**	**1.00**[#]
	10	**1.60**	**2.82**	**13088.6**	**1.85E+06**	**1.00**[#]
	100	**-0.42**	**3.46**	**12476.1**	**1.87E+06**	**1.00**[#]
R74	0.01	9.58	0.28	18388.6	2.42E+05	0.75
	0.1	8.87	0.51	18165.6	2.42E+05	0.66
	1.0	6.89	1.13	17548.2	2.42E+05	0.58
	10	4.82	1.78	16895.9	2.42E+05	0.57
	100	4.09	2.01	16663.9	2.42E+05	0.57
R75	0.01	23.11	-4.04	21077.4	4.89E+05	1.51
	0.1	17.83	-2.32	19630.6	5.86E+05	1.60
	1.0	11.39	-0.23	17869.4	7.04E+05	1.69
	10	7.39	1.04	16685.3	7.27E+05	1.70
	100	6.22	1.41	16327.8	7.29E+05	1.71
R76	0.01	21.62	-3.55	22048	2.38E+05	0.74
	0.1	16.75	-1.97	20678.3	2.69E+05	0.74
	1.0	10.28	0.12	18850.1	3.04E+05	0.73

	10	6.65	1.27	17763.5	3.10E+05	0.73
	100	5.72	1.57	17474.5	3.11E+05	0.73
1, 8-H(p)-(R, L)	**0.01**	**16.24**	**-1.87**	**19517.89**	**3.23E+05**	**2.05[#]**
	0.1	**13.89**	**-1.10**	**18905.86**	**3.66E+05**	**2.42[#]**
	1.0	**9.32**	**0.38**	**17643.51**	**4.17E+05**	**2.90[#]**
	10	**5.97**	**1.45**	**16640.60**	**4.26E+05**	**3.00[#]**
	100	**4.96**	**1.77**	**16332.07**	**4.27E+05**	**3.01[#]**
R77	0.01	12.10	-0.48	16279.2	1.89E+06	1.00
	0.1	11.60	-0.32	16124.3	1.89E+06	1.00
	1.0	9.81	0.25	15567.3	1.89E+06	1.00
	10	7.25	1.05	14765	1.89E+06	1.00
	100	5.99	1.45	14368.6	1.89E+06	1.00
1, 8-H(s)-(R, L)	**0.01**	**12.10**	**-0.48**	**16279.2**	**1.89E+06**	**1.00[#]**
	0.1	**11.60**	**-0.32**	**16124.3**	**1.89E+06**	**1.00[#]**
	1.0	**9.81**	**0.25**	**15567.3**	**1.89E+06**	**1.00[#]**
	10	**7.25**	**1.05**	**14765**	**1.89E+06**	**1.00[#]**
	100	**5.99**	**1.45**	**14368.6**	**1.89E+06**	**1.00[#]**
R78	0.01	12.50	-0.79	20922.5	3.13E+04	1.00
	0.1	9.47	0.18	20030.8	3.34E+04	1.00
	1.0	4.58	1.74	18571.5	3.75E+04	1.00
	10	2.66	2.35	17979.5	3.68E+04	1.00
	100	2.33	2.45	17876.4	3.69E+04	1.00
1, 9-H(p)-(R, L)	**0.01**	**12.50**	**-0.79**	**20922.5**	**3.13E+04**	**1.00[#]**
	0.1	**9.47**	**0.18**	**20030.8**	**3.34E+04**	**1.00[#]**
	1.0	**4.58**	**1.74**	**18571.5**	**3.75E+04**	**1.00[#]**
	10	**2.66**	**2.35**	**17979.5**	**3.68E+04**	**1.00[#]**
	100	**2.33**	**2.45**	**17876.4**	**3.69E+04**	**1.00[#]**

[e] k_{ave} is the average rate constants of 800 K for each reaction class.

[#] The uncertainty factor values of the pressure-dependent rate rule at 800 K for each class at different

pressures (The ratios of the largest rate constant to the smallest rate constant at 800 K in each class at different pressures).

9. Cartesian coordinates for all reactants, transition states and products

r1

C	0.46891	0.50782	-0.09913
O	0.80051	1.5286	0.44607
O	1.28904	-0.50151	-0.38768
C	2.63787	-0.32254	0.05176
H	3.07678	0.55776	-0.42225
H	2.66578	-0.19402	1.1353
O	-1.28498	-1.14948	-0.41388
O	-1.11637	-1.4965	0.83218
H	3.16731	-1.22594	-0.24326
C	-1.96369	1.1349	0.08576
H	-2.95811	0.95665	-0.32651
H	-1.96668	0.92025	1.15583
H	-1.68811	2.1799	-0.05917
C	-0.94984	0.24466	-0.59937
H	-0.96207	0.36746	-1.68755

r2

C	-0.03952	-0.70722	0.27277
H	-0.0507	-1.68813	-0.21464
H	-0.0328	-0.89329	1.35179
C	1.24181	-0.00699	-0.11253
O	1.31282	1.02141	-0.74027
O	2.31046	-0.68611	0.32315
C	3.572	-0.1056	-0.01485
H	3.67241	-0.01922	-1.09852
H	3.66334	0.88818	0.4281
H	4.32544	-0.77832	0.3899
C	-1.26092	0.0986	-0.13578
H	-1.221	0.34193	-1.20133
C	-1.4924	1.34523	0.69354
H	-0.67331	2.04737	0.52952
H	-2.43107	1.81394	0.39419
H	-1.54491	1.08919	1.75589
O	-2.37526	-0.82099	0.04473
O	-3.47719	-0.33253	-0.44683

r3

C	0.38003	-0.25866	-0.45055
C	1.74019	0.22214	-0.00453
O	1.96394	1.27448	0.54104
O	2.69489	-0.67312	-0.30378
C	4.01771	-0.28559	0.06794
H	4.30665	0.63049	-0.45176
H	4.07554	-0.11132	1.14429
H	0.2363	-1.28088	-0.0883
H	0.39573	-0.32368	-1.5458
H	4.66312	-1.11226	-0.22309
C	-2.08468	0.31581	-0.5472
H	-2.06131	0.37809	-1.64091
C	-3.22349	1.13761	0.02503
H	-4.17454	0.85049	-0.42829
H	-3.28185	0.9771	1.1039
H	-3.04906	2.19911	-0.16557

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C    -0.72714   0.66608   0.03788
H    -0.48944   1.70023  -0.22948
H    -0.78918   0.62717   1.12928
O    -2.36861  -1.10343  -0.33718
O    -2.34619  -1.41279   0.92796

r4
C     0.03275   0.56299  -0.27143
C    -1.23786  -0.25817  -0.16902
O    -1.28667  -1.45719  -0.03272
O    -2.32806   0.51596  -0.26236
C    -3.57207  -0.18385  -0.19279
H    -3.63817  -0.92207  -0.99437
C     1.24436  -0.35337  -0.10631
H     1.16262  -1.20322  -0.78918
C     0.01849   1.75435   0.69301
H     0.97691   2.27672   0.64845
H    -0.7764    2.44896   0.42008
H    -3.66564  -0.6964    0.76676
C     1.52186  -0.83361   1.30431
H     0.6728   -1.41906   1.66206
H     2.41247  -1.46382   1.29925
H     1.69562   0.00945   1.97745
H    -0.15306   1.43073   1.72302
H     0.06076   0.95484  -1.29704
O     2.36749   0.44936  -0.57363
O     3.44128  -0.27315  -0.71399
H    -4.34539   0.57393  -0.30159

r5
C    -0.89952  -0.23267   0.16998
C     0.56278  -0.42657  -0.24113
O     0.92185  -1.18272  -1.10641
O     1.38539   0.29924   0.51891
C     2.77023   0.17969   0.18609
H     3.10129  -0.85424   0.30258
C    -1.15715  -0.8826    1.52162
H    -0.47588  -0.47806   2.27229
H    -2.18796  -0.69176   1.82917
H    -1.00775  -1.96192   1.44325
C    -1.82883  -0.71413  -0.927
H    -2.86674  -0.57653  -0.61579
H    -1.64167  -0.14866  -1.8414
H    -1.64201  -1.76985  -1.12773
O    -1.12476   1.19071   0.3915
O    -0.7072    1.89422  -0.62246
H     2.93506   0.49154  -0.84704
H     3.29829   0.8356    0.8751

r6
C    -0.54172  -0.11246   0.28024
C     0.86705  -0.45898  -0.21312
O     1.10241  -1.31128  -1.03053
O     1.79879   0.25755   0.41958
C     3.14163  -0.00991   0.00983
H     3.39181  -1.05713   0.19139
C    -1.58123  -0.59842  -0.7246
H    -1.35876  -0.10536  -1.67587
H     3.25917   0.20435  -1.05411
H    -1.41218  -1.6673   -0.88011
O    -0.63412   1.33888   0.4002
O    -0.25234   1.92848  -0.69709
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H	3.76996	0.64731	0.60727
C	-3.01892	-0.31934	-0.29845
H	-3.30665	-0.90921	0.57594
H	-3.15802	0.73864	-0.05875
H	-3.70655	-0.57374	-1.10766
C	-0.73843	-0.62399	1.70034
H	-1.68719	-0.2583	2.09794
H	-0.75219	-1.71664	1.70011
H	0.07245	-0.273	2.34105

r7

C	-0.28236	-0.67537	-0.92692
H	-0.52387	-1.72255	-1.13086
C	1.05251	-0.64885	-0.21439
O	1.34466	-1.3497	0.7237
O	1.88467	0.2431	-0.7665
C	3.11933	0.41089	-0.07075
H	2.92588	0.77171	0.9421
C	-1.60144	-0.73431	1.2661
H	-0.68642	-0.64821	1.85084
H	-2.4277	-0.25601	1.79827
H	-1.83021	-1.79539	1.13899
H	3.65945	-0.53627	-0.01457
H	-0.20775	-0.13457	-1.87295
H	3.68488	1.14669	-0.63935
C	-1.43254	-0.08451	-0.0978
C	-2.7226	-0.08929	-0.90348
H	-3.51982	0.39992	-0.33903
H	-2.58974	0.43749	-1.85175
H	-3.02446	-1.11846	-1.11203
O	-1.16285	1.34805	0.09382
O	-0.09869	1.5566	0.81321

r8

C	0.05519	-0.14927	0.22799
C	-1.39286	0.22314	0.01592
O	-1.80127	1.33627	-0.20813
O	-2.19093	-0.85105	0.11612
C	-3.58242	-0.58464	-0.06004
H	-3.93474	0.12172	0.69464
H	-3.76634	-0.16077	-1.04948
H	0.29749	-0.9901	-0.42867
H	0.16003	-0.53456	1.24908
H	-4.08488	-1.54416	0.04695
C	2.4206	0.76937	0.34258
H	3.05238	1.6369	0.13888
H	2.54093	0.44851	1.38055
O	2.96448	-0.28095	-0.48902
O	2.69922	-1.45918	0.00369
C	0.97128	1.04339	-0.01506
H	0.62632	1.89468	0.58051
H	0.906	1.35504	-1.06217

r9

C	-1.44045	0.68184	0.10399
H	-1.31364	1.48963	0.8258
C	-0.39203	-0.40186	0.2716
H	-0.58321	-1.22066	-0.42782
H	-0.42532	-0.8265	1.28001
C	0.98503	0.15937	0.021

O	1.21693	1.31419	-0.24359
O	1.92772	-0.78456	0.1305
C	3.26431	-0.32868	-0.09011
H	3.36039	0.09723	-1.09063
H	3.53157	0.43355	0.64475
O	-2.75141	0.14167	0.37235
O	-3.0845	-0.73662	-0.53188
H	-1.43935	1.0917	-0.90783
H	3.89861	-1.20633	0.0178

r10
C	2.18613	0.09651	-0.02492
O	2.35407	1.27096	-0.24181
O	3.19201	-0.78654	0.08513
C	4.49772	-0.22981	-0.06975
H	4.60401	0.2242	-1.05713
H	4.67783	0.53495	0.68862
C	0.84507	-0.5733	0.1603
H	0.76681	-1.38383	-0.57322
H	0.84484	-1.05737	1.14404
H	5.19235	-1.05934	0.04848
C	-0.30648	0.41389	0.02529
H	-0.16442	1.2269	0.74582
H	-0.2642	0.87851	-0.96623
C	-1.66037	-0.25697	0.24101
H	-1.81104	-1.06725	-0.48037
H	-1.71206	-0.69833	1.24338
C	-2.79939	0.73289	0.08348
H	-2.74341	1.543	0.81544
H	-2.84241	1.14901	-0.92717
O	-4.06932	0.09815	0.34905
O	-4.36731	-0.75628	-0.58914

r11
C	-0.21323	-0.44854	-0.73702
H	-0.24137	-1.41781	-1.24763
H	-0.1826	0.32467	-1.50915
C	-1.48224	-0.3166	0.07617
O	-1.56148	-0.49198	1.26639
O	-2.52737	-0.00543	-0.7017
C	-3.77469	0.10365	-0.01286
H	-4.51408	0.34793	-0.77317
H	-4.02173	-0.83987	0.47822
H	-3.72141	0.89036	0.74219
C	1.024	-0.35779	0.1366
H	0.88259	-0.9337	1.05591
C	2.30668	-0.74436	-0.58287
H	2.20997	-1.79344	-0.8844
H	2.38163	-0.14836	-1.49804
C	3.54846	-0.55032	0.28184
H	3.47747	-1.12805	1.20836
H	4.44543	-0.87352	-0.25068
H	3.67216	0.50166	0.54847
O	1.12857	1.0088	0.64576
O	1.35504	1.85784	-0.31559

r12
C	0.81296	-0.52548	-0.08476
O	1.0509	-1.58689	0.43221
O	1.73016	0.38809	-0.39847
C	3.06777	0.04553	-0.02668
H	3.38194	-0.8647	-0.54146

H	3.68277	0.89171	-0.32504
H	3.12837	-0.11659	1.05103
C	-0.58962	-0.09837	-0.50926
H	-0.69744	-0.27399	-1.58639
C	-1.6675	-0.81968	0.28144
H	-1.51671	-0.58268	1.33903
H	-1.48945	-1.89209	0.16777
C	-3.07092	-0.4331	-0.17238
H	-3.22589	-0.67287	-1.22897
H	-3.82396	-0.97035	0.40751
H	-3.24185	0.63805	-0.0409
O	-0.72961	1.3352	-0.38994
O	-0.49069	1.71737	0.83461

r13

C	1.18919	-0.54795	-0.11157
O	1.25454	-1.66037	0.34513
O	2.23678	0.24813	-0.32081
C	3.49391	-0.29686	0.08751
H	3.70885	-1.21149	-0.46877
H	4.2332	0.47136	-0.12877
H	3.475	-0.52636	1.15445
C	-0.11661	0.09061	-0.57886
H	-0.18166	-0.01024	-1.66894
C	-1.32744	-0.51458	0.10753
H	-1.23386	-0.31957	1.18176
H	-1.27269	-1.59965	-0.02393
C	-2.64608	0.03686	-0.42833
H	-2.71289	-0.16282	-1.50536
H	-2.65712	1.12599	-0.31147
O	-0.06842	1.52189	-0.37832
O	0.15535	1.80064	0.87613
C	-3.84697	-0.57566	0.28629
H	-4.78715	-0.18022	-0.10514
H	-3.86168	-1.66314	0.16525
H	-3.81206	-0.36069	1.35848

r14

C	-0.34846	0.29377	-0.10203
C	1.03664	-0.30371	0.02139
O	1.27663	-1.40243	0.46183
O	1.98133	0.54069	-0.41424
C	3.31842	0.04384	-0.32578
H	3.56856	-0.18988	0.71088
C	-0.45506	1.61996	0.65741
H	0.26558	2.34034	0.26883
H	-1.46046	2.03084	0.54799
H	-0.25802	1.47132	1.72367
H	3.42675	-0.8614	-0.92667
H	-0.53652	0.47659	-1.16655
H	3.95694	0.83822	-0.70705
O	-2.699	-0.22142	0.25619
O	-3.0092	-0.04135	-0.99755
C	-1.35649	-0.73684	0.38633
H	-1.23869	-0.94256	1.45248
H	-1.29251	-1.66941	-0.17736

r15

C	0.40737	-0.80933	0.16905
H	0.54886	-1.25753	1.15924
C	1.64221	-0.00326	-0.16821
O	1.6481	1.0913	-0.67398

O	2.75861	-0.6774	0.14875
C	3.9774	-0.00548	-0.17356
H	4.04123	0.17239	-1.24907
C	-0.86808	0.02838	0.10947
H	4.03079	0.95413	0.34463
C	-0.91051	1.07832	1.21837
H	-0.85904	0.60041	2.20389
H	-0.07067	1.76864	1.12013
H	-1.83658	1.65516	1.16895
H	0.37232	-1.64314	-0.54425
H	-0.90526	0.53184	-0.863
H	4.7775	-0.66602	0.15514
C	-2.06911	-0.90298	0.18885
H	-2.07288	-1.63896	-0.6209
H	-2.12667	-1.41133	1.157
O	-3.30564	-0.1627	0.10514
O	-3.47298	0.32636	-1.09186

r16
C	1.23664	-0.77367	-0.77596
C	0.34445	0.29586	-0.17582
O	1.51797	-1.7951	0.21952
O	1.91048	-1.26811	1.3421
H	0.74939	-1.31673	-1.58642
H	2.1991	-0.37286	-1.10334
H	0.52489	0.2667	0.90476
C	-1.10873	-0.1112	-0.29275
O	-1.51569	-1.1403	-0.77415
O	-1.89606	0.78049	0.32595
C	-3.26598	0.39915	0.44283
H	-3.71377	0.26961	-0.54426
H	-3.34906	-0.54042	0.99322
H	-3.755	1.20684	0.98403
C	0.70818	1.72619	-0.59895
H	0.7726	1.80306	-1.69069
H	-0.09287	2.39653	-0.27699
C	2.02686	2.1466	0.05391
H	2.86121	1.51277	-0.25919
H	2.282	3.17809	-0.19929
H	1.95386	2.0701	1.14268

r17
C	0.48761	0.30749	0.54308
C	-0.92365	-0.26082	0.54823
O	-1.28074	-1.05729	1.37991
O	-1.66934	0.1627	-0.46955
C	-2.9881	-0.38948	-0.51095
H	-2.93863	-1.47588	-0.61087
H	-3.52918	-0.14191	0.40402
H	0.68498	0.71763	1.53818
O	0.62633	1.38078	-0.40437
O	-0.01848	2.44267	-0.00507
C	2.92603	-0.22416	0.26916
H	3.6537	-1.01588	0.07429
H	3.07908	0.56877	-0.46801
H	3.1296	0.18864	1.26163
H	-3.46828	0.05845	-1.37816
C	1.50411	-0.77706	0.17715
H	1.36818	-1.5601	0.93211
C	1.21399	-1.3617	-1.20704
H	1.95442	-2.12681	-1.45353
H	0.22468	-1.82705	-1.25162

| H | 1.25939 | -0.58241 | -1.97314 |

r18

C	-0.34458	0.30937	-0.07686
C	1.03729	-0.28841	0.05892
O	1.28711	-1.32315	0.61942
O	1.96719	0.48778	-0.50739
C	3.31326	0.01462	-0.40334
H	3.60394	-0.06842	0.64414
C	-0.44365	1.61707	0.71786
H	0.27356	2.34634	0.34235
H	-1.44734	2.0336	0.62645
H	-0.2399	1.43869	1.77693
H	3.40763	-0.96166	-0.87904
H	3.92447	0.75296	-0.91471
O	-2.70188	-0.20778	0.2082
O	-3.00622	-0.09027	-1.04839
C	-1.36365	-0.72187	0.38478
H	-1.28202	-0.92206	1.45308
H	-1.28633	-1.65409	-0.17478
C	-0.58546	0.60189	-1.56951
H	-0.78645	-0.31419	-2.08458
H	-1.42233	1.2605	-1.67336
H	0.28504	1.06261	-1.98768

r19

C	-0.03309	-0.14022	0.13206
C	1.4029	0.31313	-0.05187
O	1.79229	1.45394	0.01259
O	2.21896	-0.72749	-0.28932
C	3.5951	-0.38578	-0.45372
H	3.71814	0.30798	-1.28791
C	-0.93202	1.09545	0.19822
H	-0.63005	1.71278	1.052
C	-0.13938	-1.04297	1.36854
H	-1.13106	-1.49596	1.41908
H	0.59946	-1.84442	1.31705
H	3.98207	0.08437	0.45295
C	-2.41257	0.79003	0.33907
H	-2.64786	0.19667	1.22511
H	-3.00246	1.70937	0.34086
H	0.03624	-0.46732	2.28362
H	-0.28955	-0.74071	-0.74888
H	-0.77545	1.70988	-0.69367
O	-2.89417	0.0519	-0.80766
O	-2.72437	-1.23186	-0.65339
H	4.11322	-1.32229	-0.65183

r20

C	0.44996	0.60589	0.00274
O	1.2255	1.45209	0.3663
O	0.75884	-0.65971	-0.25904
C	2.13356	-0.99546	-0.04659
H	2.77163	-0.40447	-0.70639
H	2.41255	-0.79669	0.98966
O	-1.82175	-0.2345	-0.46664
O	-1.94943	-0.92589	0.63425
H	2.21615	-2.05587	-0.27388
C	-1.01687	0.92229	-0.23822
H	-1.10436	1.5336	-1.13932
H	-1.40105	1.47123	0.62338

r21

C	-1.23203	0.15144	-0.02819
O	-1.20041	1.28475	-0.41939
O	-0.19188	-0.428	0.6476
C	0.94356	0.37254	0.80584
H	0.68166	1.41813	0.96743
H	1.53855	-0.06786	1.60376
C	-2.36163	-0.82323	-0.18573
H	-2.01983	-1.67798	-0.77374
H	-2.66754	-1.19604	0.79388
H	-3.19336	-0.3305	-0.68444
O	1.72087	0.36557	-0.39583
O	2.36655	-0.76609	-0.51467

r22

C	-1.24425	0.15072	-0.03028
O	-1.23278	1.27484	-0.43229
O	-0.19078	-0.40141	0.64871
C	0.9439	0.40152	0.79023
H	0.68572	1.45172	0.91075
H	1.52962	-0.01234	1.60677
C	-2.35351	-0.84528	-0.1718
H	-1.99426	-1.69922	-0.74822
H	-2.64807	-1.20976	0.81288
O	1.73158	0.35021	-0.40524
O	2.38515	-0.77302	-0.49075
C	-3.54662	-0.18172	-0.88439
H	-4.34881	-0.88497	-0.96693
H	-3.87262	0.66652	-0.31948
H	-3.24739	0.13435	-1.86187

r23

C	-0.18517	0.38655	0.16419
O	-0.07221	1.41226	-0.44896
O	0.86285	-0.20684	0.81427
C	2.10073	0.42544	0.6691
H	2.00078	1.5104	0.63969
H	2.74526	0.05796	1.46559
C	-1.44426	-0.41722	0.34074
H	-1.25627	-1.41443	-0.07564
H	-1.59753	-0.56867	1.41595
O	2.68865	0.07506	-0.58822
O	3.10246	-1.16581	-0.56491
C	-2.65199	0.24217	-0.31326
H	-2.78724	1.24106	0.11334
H	-2.44211	0.39325	-1.37653
C	-3.91721	-0.58999	-0.13188
H	-4.15067	-0.72715	0.92856
H	-4.77634	-0.10852	-0.60422
H	-3.80253	-1.58293	-0.57756

r24

C	0.35309	0.35677	0.24651
O	0.41728	1.41641	-0.31376
O	1.44532	-0.25552	0.79951
C	2.66344	0.40699	0.62179
H	2.54224	1.48971	0.65027
H	3.35543	0.01475	1.3645
C	-0.88318	-0.47573	0.44936
H	-0.70896	-1.44145	-0.04088
H	-0.96659	-0.69715	1.51995

O	3.19046	0.1257	-0.67889
O	3.67853	-1.08773	-0.71782
C	-2.13576	0.20464	-0.08628
H	-2.26254	1.17208	0.41324
H	-1.99498	0.43067	-1.14921
C	-3.38615	-0.64926	0.1058
H	-3.51279	-0.87555	1.17208
H	-3.24807	-1.61399	-0.39842
C	-4.64037	0.03642	-0.42781
H	-4.54284	0.24897	-1.49674
H	-5.52775	-0.58577	-0.28807
H	-4.8122	0.9879	0.08473

r25

C	-0.10227	-0.24631	0.01893
O	-0.16693	-1.08657	-0.837
O	-1.16201	0.06372	0.82677
C	-2.34966	-0.62129	0.55353
H	-2.16235	-1.65453	0.26109
H	-2.98979	-0.51414	1.42747
C	1.08736	0.61384	0.35248
H	0.82209	1.63632	0.05393
H	1.19901	0.63849	1.44327
O	-3.0124	-0.03384	-0.57077
O	-3.53328	1.11947	-0.23813
C	2.37583	0.15461	-0.32914
H	2.15999	0.03771	-1.39779
C	3.4625	1.21406	-0.15091
H	3.68094	1.36709	0.91218
H	4.39024	0.90509	-0.6401
H	3.15959	2.17651	-0.5742
C	2.83613	-1.196	0.21946
H	3.04975	-1.11934	1.29213
H	2.07584	-1.96576	0.06896
H	3.7523	-1.5231	-0.27997

r26

C	0.42071	-0.64722	-0.07397
O	0.33025	-1.39817	0.85563
O	-0.62161	-0.39793	-0.93963
C	-1.89	-0.73258	-0.48837
H	-2.50984	-1.02503	-1.33431
H	-1.84841	-1.4847	0.30076
C	1.63254	0.15785	-0.47254
H	1.76397	0.01939	-1.55244
O	-2.53018	0.45016	0.04021
O	-1.78164	1.00103	0.95502
C	2.86226	-0.32588	0.28525
H	3.73802	0.25777	-0.00829
H	2.71006	-0.21101	1.36132
H	3.0629	-1.38123	0.0883
C	1.32968	1.64093	-0.20666
H	2.17981	2.25296	-0.51752
H	0.44084	1.96625	-0.75068
H	1.15695	1.80628	0.86076

r27

C	-0.00532	-0.16798	-0.41114
O	0.15987	-1.12677	-1.11494
O	1.00813	0.70366	-0.10963
C	2.26195	0.37856	-0.63427
H	2.18174	-0.08011	-1.61954

H	2.86565	1.28397	-0.6112
C	-1.29877	0.25979	0.24476
H	-1.08417	0.31559	1.32109
O	2.89646	-0.60994	0.18379
O	3.2982	-0.07576	1.30855
C	-2.3809	-0.79123	-0.01029
H	-2.54418	-0.87005	-1.09109
H	-2.00188	-1.76686	0.30915
C	-1.68912	1.6649	-0.23508
H	-2.56125	2.02307	0.31509
H	-0.87394	2.37347	-0.08071
H	-1.94217	1.64782	-1.30011
C	-3.69391	-0.48298	0.70381
H	-4.16447	0.42391	0.31496
H	-4.40476	-1.30233	0.57507
H	-3.53536	-0.3444	1.7785

r28

C	-0.21107	-0.6122	-0.2347
O	0.01466	-1.25511	-1.22131
O	0.70343	-0.47707	0.78675
C	2.01917	-0.79968	0.48635
H	2.50087	-1.2154	1.37036
H	2.08181	-1.44755	-0.38865
C	-1.4807	0.15893	0.07448
O	2.75021	0.41471	0.21257
O	2.17049	1.08803	-0.74224
C	-2.52749	-0.18332	-0.98384
H	-3.43877	0.39196	-0.79699
H	-2.16051	0.0515	-1.98527
H	-2.7766	-1.24751	-0.9592
C	-1.11829	1.65327	0.01376
H	-2.00888	2.24943	0.23427
H	-0.34174	1.89798	0.74256
H	-0.75497	1.92715	-0.98076
C	-1.98781	-0.20196	1.47743
H	-2.90628	0.3564	1.68124
H	-2.21705	-1.26928	1.55272
H	-1.25108	0.05061	2.24255

TS1

C	-0.77177	0.52235	-0.19653
C	-1.33535	0.62741	1.21809
H	-1.10042	1.36361	-0.81422
H	-0.887	-0.05509	1.93953
C	0.74717	0.46268	-0.2333
O	1.43887	1.37805	-0.59799
O	1.2041	-0.69765	0.23981
C	2.62941	-0.81472	0.25911
H	3.06265	-0.04607	0.90248
H	2.83896	-1.80887	0.64796
H	3.03094	-0.7	-0.74934
O	-1.30928	-0.70813	-0.66801
O	-2.65196	-0.61271	-0.29303
H	-2.43133	-0.02964	0.74181
H	-1.58435	1.61325	1.60129

TS2

| C | 1.27991 | 0.30625 | 0.30071 |
| C | 2.57139 | 1.0778 | 0.05429 |

H	1.19055	0.03174	1.35803
H	2.66107	1.54178	-0.92897
C	0.01162	0.98141	-0.18393
O	2.76727	-1.2562	-0.17771
O	1.46015	-0.87076	-0.48896
H	3.18829	-0.12873	-0.07042
H	2.99151	1.65934	0.87142
H	-0.0585	1.98249	0.25665
H	0.02852	1.09117	-1.27063
C	-1.21758	0.208	0.24839
O	-1.31442	-0.39633	1.28636
O	-2.20137	0.30498	-0.65456
C	-3.40736	-0.37521	-0.29919
H	-4.09872	-0.20462	-1.12207
H	-3.21436	-1.44189	-0.17018
H	-3.80928	0.02569	0.63347

TS3

C	1.94425	0.21576	0.41704
C	3.08845	1.16589	0.07855
H	2.01006	-0.07284	1.47602
H	3.01425	1.65431	-0.89405
O	-2.14803	1.27171	-0.39444
O	-2.82129	-0.78466	0.20557
C	-4.16042	-0.3793	-0.07841
H	-4.25987	-0.10489	-1.13083
H	-4.78738	-1.23762	0.15549
H	-4.4373	0.48028	0.53532
O	2.22771	-0.92432	-0.39757
O	3.60205	-1.11151	-0.21425
H	3.85845	0.07136	-0.12987
H	3.49453	1.79164	0.86974
C	-1.89076	0.16024	-0.00238
C	-0.50806	-0.35153	0.32058
H	-0.50386	-0.67773	1.36719
H	-0.32029	-1.24939	-0.2768
C	0.55562	0.70945	0.06182
H	0.33434	1.61045	0.64281
H	0.53904	1.00162	-0.99278

TS4

C	1.25052	0.10955	0.23306
C	2.63236	0.50883	-0.273
H	1.20045	0.21321	1.32513
H	2.71842	0.63575	-1.35346
C	0.07283	0.83055	-0.41517
O	2.40961	-1.77442	0.25326
O	1.16196	-1.26934	-0.12741
H	3.02023	-0.7683	-0.03088
H	3.21981	1.20939	0.31538
H	0.09658	0.63424	-1.49096
C	-1.20277	0.24819	0.16762
O	-1.51617	0.35484	1.32821
O	-1.9327	-0.3969	-0.74786
C	-3.12256	-1.00636	-0.24248
H	-3.60127	-1.47793	-1.09836
H	-2.87054	-1.74877	0.51726
H	-3.77634	-0.2531	0.20175
C	0.13249	2.33069	-0.12012
H	0.0642	2.49978	0.95741
H	1.06685	2.76086	-0.49051
H	-0.69714	2.85257	-0.60182

TS5

C	0.65925	0.11719	0.23274
C	1.54139	1.30998	-0.12699
H	1.21736	1.89017	-0.98885
C	-0.81694	0.40441	-0.02459
O	-1.26484	1.50507	-0.22622
O	-1.54532	-0.71108	0.03107
C	-2.94303	-0.53034	-0.2122
H	-3.10025	-0.11572	-1.20968
H	-3.38835	-1.51948	-0.13037
H	-3.3698	0.151	0.52637
O	1.04471	-0.87954	-0.72825
O	2.44288	-0.76324	-0.75773
H	2.46213	0.43483	-0.58225
H	1.95428	1.89731	0.68989
C	0.88671	-0.37647	1.65628
H	0.29433	-1.27596	1.83069
H	1.94579	-0.61168	1.7812
H	0.60083	0.39113	2.38057

TS6

C	0.41193	-0.15223	-0.16773
C	1.09335	-1.27488	-0.94669
H	0.49885	-2.17621	-1.08069
C	-1.10591	-0.22161	-0.33025
O	-1.6638	-0.85035	-1.19463
O	-1.72927	0.52619	0.58064
C	-3.15696	0.50733	0.50178
H	-3.5268	-0.51394	0.61024
H	-3.50646	1.13332	1.32002
H	-3.48772	0.90431	-0.46005
O	0.67052	-0.4739	1.21201
O	1.96753	-1.0139	1.20863
H	1.90587	-1.48492	0.09513
H	1.68946	-0.99633	-1.81256
C	0.8996	1.25282	-0.54132
H	0.31818	1.96302	0.05453
H	0.63783	1.42283	-1.59345
C	2.39132	1.48645	-0.31653
H	3.00741	0.78516	-0.88669
H	2.65767	2.49775	-0.63328
H	2.64599	1.37343	0.73801

TS7

C	-1.1692	0.28182	0.18157
C	-2.44104	0.09566	1.0158
H	-2.31921	-0.44797	1.95329
C	0.06604	0.56724	1.04366
O	-2.24861	-1.42309	-0.76948
O	-0.96807	-1.04069	-0.35158
H	-2.82755	-0.84498	0.12421
H	-3.1517	0.9186	1.05697
H	-0.0118	1.58333	1.43985
H	0.10692	-0.1476	1.86715
C	1.34313	0.47586	0.2335
O	1.69656	1.28155	-0.59282
O	2.03704	-0.62729	0.5365
C	3.22649	-0.81533	-0.23169
H	3.66213	-1.74833	0.12015
H	2.98249	-0.8784	-1.2939
H	3.91564	0.01738	-0.0759

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C      -1.38638   1.29426  -0.93506
H      -1.5797    2.28545  -0.51549
H      -0.50132   1.35397  -1.56878
H      -2.24549   0.98761  -1.53519


TS8
C       1.68956   0.64619   0.66711
C       0.47109  -0.25291   0.83348
O       2.23709   0.27284  -0.60075
O       2.16957  -1.10248  -0.59101
H       1.44038   1.70632   0.58948
H       2.41143   0.45829   1.46792
H       1.13716  -1.15523   0.00899
C      -0.76498   0.21762   0.16337
O      -0.84161   1.23493  -0.48591
O      -1.78557  -0.63384   0.34793
C      -3.00078  -0.25807  -0.30161
H      -3.35407   0.70286   0.07836
H      -2.84525  -0.1747   -1.37919
H       0.32048  -0.77903   1.77365
H      -3.71533  -1.0471   -0.07533


TS9
C      -2.50389  -0.69562   0.45143
C      -1.11033  -0.1895    0.80968
O      -2.74297  -0.09138  -0.81432
O      -2.36689   1.23709  -0.58744
H      -2.57852  -1.77876   0.30569
H      -3.24057  -0.35756   1.18814
H      -1.4501    0.95289   0.18963
H      -0.89046   0.02672   1.85372
C       0.01768  -0.78482   0.01687
H      -0.23628  -0.808    -1.0495
H       0.20261  -1.82958   0.30658
C       1.30496  -0.01476   0.20066
O       1.43224   0.96239   0.89506
O       2.30224  -0.56058  -0.50914
C       3.55637   0.11565  -0.40027
H       3.89626   0.12125   0.63736
H       4.24894  -0.43992  -1.02954
H       3.4625    1.14716  -0.74558


TS10
C      -3.10917  -0.75027   0.20312
C      -1.82998  -0.24886   0.87112
O      -3.24208   0.10725  -0.92376
O      -3.02843   1.37274  -0.36864
H      -3.04717  -1.77327  -0.18312
H      -3.96831  -0.6449    0.87484
H      -2.19441   0.9768    0.44928
C       1.92648  -0.16441   0.01129
O       2.09366  -1.18509  -0.60855
O       2.90482   0.7204    0.25995
C       4.1823    0.36675  -0.27105
H       4.52389  -0.57934   0.15424
H       4.12724   0.2636   -1.35673
H      -1.80561  -0.25795   1.96241
H       4.85426   1.17725   0.00493
C       0.61742   0.28379   0.61738
H       0.73948   0.27616   1.70762
H       0.44528   1.32829   0.33732
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C          -0.5419   -0.60402   0.18294
H          -0.68164  -0.53347  -0.90149
H          -0.28763  -1.65353   0.38995

TS11
C          -1.27576   0.00548  -0.64387
C          -0.33354   0.8449    0.22673
O          -1.41931  -1.2183    0.10002
O          -1.58418  -0.79214   1.40281
H          -0.83386   0.14424   1.30404
H          -0.81287  -0.30026  -1.58672
H          -0.58411   1.89023   0.39629
C          -2.61477   0.69215  -0.85356
H          -3.2862    0.03763  -1.41227
H          -3.06851   0.91818   0.11441
H          -2.48707   1.62318  -1.41137
C           1.13195   0.61971   0.1643
O           1.95604   1.37667   0.62227
O           1.43692  -0.54401  -0.43304
C           2.83153  -0.84637  -0.47363
H           2.91259  -1.80926  -0.97403
H           3.37211  -0.07475  -1.02584
H           3.23576  -0.90225   0.53913

TS12
C          -1.56818   0.53455  -0.32756
C          -0.83441  -0.16679   0.82203
O          -2.18975  -0.56933  -0.99965
O          -2.75197  -1.30668   0.04977
H          -1.85335  -1.0502    0.83974
H          -0.87363   0.96716  -1.0561
H          -0.77857   0.37286   1.76761
C           1.55509   0.01143   0.14377
C           0.402    -0.93073   0.43607
H           0.72146  -1.63162   1.2124
H           0.21     -1.51806  -0.47036
O           1.46488   1.21249   0.06064
O           2.70156  -0.66002  -0.02229
C           3.8361    0.15321  -0.33061
H           4.00209   0.88882   0.45859
H           4.67949  -0.5303   -0.40603
H           3.68003   0.67835  -1.2752
C          -2.57567   1.56009   0.15618
H          -3.13986   1.95822  -0.68947
H          -3.27441   1.09745   0.8569
H          -2.06061   2.38508   0.65489

TS13
C          -1.262     0.23854   0.51842
O          -1.47233   1.04493  -0.64898
O          -0.8743    2.24292  -0.32349
H          -1.86411   0.65024   1.3409
H           0.01971   1.7472    0.31407
C          -1.68349  -1.18501   0.20004
H          -1.12518  -1.51707  -0.67736
H          -1.38059  -1.8191    1.04162
C           0.21124   0.49354   0.86141
H           0.47594   0.62643   1.9083
C           1.2621   -0.15852   0.04218
O           1.08222  -0.75268  -0.99585
O           2.4785    0.03198   0.58424
C           3.55988  -0.5035   -0.17837
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H	4.46443	-0.25548	0.37354
H	3.45457	-1.58577	-0.28078
H	3.58029	-0.05769	-1.17519
C	-3.19033	-1.28474	-0.02855
H	-3.49337	-0.65642	-0.86952
H	-3.4821	-2.31388	-0.24896
H	-3.74675	-0.95749	0.85531

TS14

C	-0.98102	-0.36643	-0.07127
C	-2.31296	-0.31696	0.68388
O	-1.08506	0.75518	-0.95312
O	-1.55657	1.77412	-0.11369
H	-2.25168	1.01413	0.57422
H	-0.87313	-1.24042	-0.72369
H	-2.28607	-0.59251	1.73945
C	-3.51615	-0.77818	-0.08922
H	-4.44851	-0.50427	0.4088
H	-3.50504	-0.34399	-1.09276
H	-3.50282	-1.87108	-0.19629
C	1.50797	-0.36437	0.04773
O	1.62145	-0.995	-0.97386
O	2.5207	0.28588	0.63591
C	3.77205	0.18692	-0.0464
H	4.47829	0.76928	0.54224
H	4.0895	-0.85599	-0.1107
H	3.68406	0.59132	-1.05655
C	0.22739	-0.23293	0.84107
H	0.22284	-1.02465	1.59945
H	0.20475	0.72841	1.35921

TS15

C	-0.52623	-0.06071	-0.57671
C	-1.61708	-0.66694	0.3049
O	-0.73263	1.33453	-0.45051
O	-0.85846	1.48131	0.93986
H	-1.4573	0.39779	1.09499
H	-0.62637	-0.30119	-1.64357
H	-1.33155	-1.56618	0.84792
C	-3.00988	-0.61431	-0.25459
H	-3.75802	-0.82959	0.51086
H	-3.21289	0.37047	-0.6845
H	-3.12563	-1.36191	-1.05074
C	0.86255	-0.48441	-0.09809
O	1.08827	-1.5315	0.45681
O	1.78562	0.42125	-0.40886
C	3.11207	0.09134	0.0083
H	3.44373	-0.83028	-0.47478
H	3.73408	0.93167	-0.29236
H	3.14291	-0.04538	1.09086

TS16

C	0.0401	0.09214	0.67549
C	1.24601	-0.48049	-0.06507
O	0.13947	1.48649	0.44591
O	0.37426	1.53704	-0.93771
H	1.0685	0.49968	-0.95392
H	0.072	-0.05282	1.76359
H	1.08798	-1.44243	-0.55268
C	2.58717	-0.26005	0.57805
H	2.61968	0.75456	0.99175
H	2.67516	-0.94949	1.43212

C	-1.26444	-0.49368	0.13451
O	-1.35565	-1.60187	-0.33383
O	-2.28296	0.3479	0.2876
C	-3.53848	-0.13967	-0.19057
H	-3.82156	-1.04776	0.34577
H	-4.2554	0.65776	-0.00719
H	-3.47336	-0.36379	-1.25695
C	3.74685	-0.48385	-0.38939
H	4.70851	-0.35337	0.11131
H	3.71721	-1.49336	-0.80973
H	3.69709	0.22806	-1.21805

TS17

C	0.48206	-0.21023	0.29785
C	1.52853	-0.20678	-0.82501
O	0.655	1.07006	0.89325
O	0.68887	1.91825	-0.2244
H	1.28317	1.0955	-0.95071
H	1.22943	-0.72419	-1.73515
C	2.96412	-0.34707	-0.40503
H	3.63899	-0.0822	-1.22159
H	3.1809	0.29265	0.45536
H	3.18397	-1.38517	-0.1219
C	-0.91915	-0.32718	-0.31738
O	-1.15533	-0.87057	-1.36843
O	-1.84672	0.1933	0.48483
C	-3.18305	0.11153	-0.01355
H	-3.47255	-0.93184	-0.15658
H	-3.8095	0.58759	0.73793
H	-3.26027	0.6338	-0.96905
C	0.65917	-1.25925	1.3849
H	-0.11477	-1.13368	2.14504
H	0.57654	-2.25934	0.95194
H	1.63949	-1.14763	1.85192

TS18

C	1.40146	0.29705	0.16158
O	1.62155	-0.45283	-1.05434
O	1.32794	-1.75431	-0.70363
H	0.45053	-1.46599	0.067
C	1.3719	1.7623	-0.23998
H	2.36587	2.06582	-0.57901
H	0.64472	1.92449	-1.0339
H	1.10427	2.37377	0.62632
C	0.06827	-0.28749	0.67121
H	-0.02423	-0.47157	1.74021
C	-1.20503	0.09197	0.01127
O	-1.3145	0.67014	-1.04523
O	-2.25947	-0.33545	0.731
C	-3.53012	-0.06433	0.14012
H	-4.27032	-0.46761	0.82849
H	-3.66796	1.01146	0.01136
H	-3.60696	-0.54622	-0.83693
C	2.504	-0.0032	1.17236
H	3.46907	0.29644	0.75741
H	2.33312	0.55223	2.09842
H	2.53489	-1.07106	1.39876

TS19

C	1.67307	-0.06455	-0.83583
C	0.47791	0.60489	-0.14808
O	2.0872	-1.06993	0.08355

O	2.05696	-0.41786	1.30099
H	1.41726	-0.5773	-1.76541
H	2.46904	0.67387	-0.98628
H	1.05104	0.23567	1.02462
C	-0.78172	-0.18932	-0.25886
O	-0.8788	-1.23114	-0.86345
O	-1.79658	0.37693	0.41512
C	-3.01845	-0.36233	0.38587
H	-3.37123	-0.4743	-0.64141
H	-2.87101	-1.35435	0.81749
H	-3.72809	0.21374	0.97662
C	0.36277	2.1039	-0.19057
H	0.12537	2.44745	-1.20594
H	-0.43272	2.45022	0.47062
H	1.30866	2.56548	0.10486

TS20
C	2.42614	0.08131	-0.68245
C	1.08792	0.59874	-0.14508
O	2.45109	-1.26548	-0.23843
O	2.0843	-1.14456	1.10651
H	2.50983	0.06397	-1.77511
H	3.2545	0.65209	-0.24477
H	1.28752	-0.19575	0.90302
C	0.9978	2.05029	0.23071
H	0.98569	2.67819	-0.67162
H	0.0834	2.24789	0.79366
H	1.85647	2.3529	0.8356
C	-0.10703	-0.00127	-0.84661
H	0.10576	-1.04266	-1.11752
H	-0.32901	0.52885	-1.78329
C	-1.35302	0.00097	0.01118
O	-1.38903	0.2518	1.19072
O	-2.43278	-0.33636	-0.70797
C	-3.65113	-0.40559	0.03554
H	-4.42237	-0.6792	-0.682
H	-3.57184	-1.15729	0.82334
H	-3.8727	0.56111	0.49227

TS21
C	1.26811	-0.90931	-0.86861
C	0.36794	0.1731	-0.26142
O	1.46282	-1.84608	0.18856
O	1.68423	-1.04459	1.29178
H	0.79464	-1.45685	-1.68585
H	2.2236	-0.47325	-1.17967
H	0.86456	-0.19092	0.94576
C	-1.07486	-0.21484	-0.25356
O	-1.50595	-1.2416	-0.7243
O	-1.84412	0.69409	0.3688
C	-3.22532	0.34236	0.45975
H	-3.65564	0.2281	-0.53719
H	-3.34072	-0.59834	1.00196
H	-3.70572	1.1586	0.99573
C	0.71267	1.62734	-0.48799
H	0.7266	1.81541	-1.57239
H	-0.08909	2.24619	-0.07845
C	2.05445	2.03775	0.1224
H	2.88177	1.43104	-0.2542
H	2.27282	3.08285	-0.10734
H	2.03348	1.92416	1.20946

TS22

C	1.43306	-0.20552	-0.61594
O	1.56953	-1.4029	0.16435
O	1.48247	-0.95406	1.47128
H	0.62513	-0.10736	1.21462
C	0.24579	0.50358	0.07012
C	-1.06665	-0.12139	-0.28593
O	-1.20495	-1.01436	-1.08813
O	-2.0862	0.41669	0.40503
C	-3.36223	-0.16196	0.12838
H	-4.0746	0.37883	0.74857
H	-3.60822	-0.05193	-0.9298
H	-3.3585	-1.22438	0.38013
C	2.72012	0.59937	-0.61982
H	3.51461	0.00547	-1.07538
H	2.60553	1.5233	-1.19271
H	3.01406	0.84712	0.40274
C	0.24731	1.998	0.25276
H	0.15917	2.5054	-0.71759
H	-0.60093	2.30557	0.86539
H	1.1723	2.33759	0.72256
H	1.1603	-0.55501	-1.61629

TS23

C	0.28683	-0.3148	-0.55672
C	1.53769	0.42203	-0.05225
O	0.5119	-1.65038	-0.10944
O	0.89791	-1.47537	1.22552
H	1.47673	-0.37552	1.01026
H	0.20513	-0.36587	-1.64842
C	-1.03428	0.17494	0.03287
O	-1.17532	0.71964	1.09777
O	-2.0458	-0.14585	-0.78296
C	-3.34553	0.16564	-0.27687
H	0 -3.43956	1.24097	-0.1113
H	-4.04887	-0.17114	-1.0357
H	-3.51638	-0.35356	0.66805
C	2.77959	-0.01319	-0.79614
H	3.68106	0.29271	-0.25957
H	2.79638	-1.09627	-0.93562
H	2.80622	0.46245	-1.7865
C	1.4669	1.89226	0.26216
H	1.30266	2.4627	-0.66388
H	0.6618	2.12595	0.95696
H	2.41816	2.23198	0.68033

TS24

C	-1.02294	0.39997	0.10398
O	-1.41331	1.53199	-0.03581
O	-1.80785	-0.67526	0.10924
C	-3.1977	-0.40338	-0.08837
H	-3.35411	0.07517	-1.05704
H	-3.6953	-1.37004	-0.0503
H	-3.56993	0.25729	0.69719
C	0.43653	0.04197	0.3468
C	1.37921	1.16197	-0.13135
H	1.11702	1.39629	-1.1657
C	2.81298	0.71982	-0.01887
H	3.47489	0.97498	-0.84354
H	3.27389	0.82101	0.96343
H	2.63414	-0.64727	-0.08823
H	1.17328	2.05417	0.47114

H	0.57638	-0.15372	1.41938
O	0.74122	-1.13606	-0.37239
O	1.9701	-1.58692	0.09653

TS25

C	-0.32647	0.20684	0.55229
H	-0.27622	-0.11781	1.59533
C	-1.15595	1.45162	0.40657
H	-1.39883	1.98889	1.32044
H	-0.88331	2.08807	-0.43343
H	-2.35861	0.888	0.00834
O	-2.31259	-1.07391	0.11225
O	-2.9693	0.01986	-0.44478
C	1.09544	0.3954	0.04598
O	1.50676	1.34152	-0.57448
O	1.84468	-0.67678	0.35099
C	3.19857	-0.61466	-0.10451
H	3.70672	0.24439	0.33788
H	3.66314	-1.54451	0.21773
H	3.23014	-0.52199	-1.19177
C	-0.95826	-0.97251	-0.25011
H	-0.48779	-1.91976	0.02017
H	-0.87168	-0.79088	-1.3278

TS26

C	-0.9433	-0.27896	0.2107
C	-2.21544	-1.12395	-0.01839
H	-2.16259	-1.5431	-1.02797
C	-3.45708	-0.28906	0.14416
H	-4.25314	-0.43695	-0.58231
H	-3.81122	-0.14544	1.16438
H	-2.92424	0.95928	-0.13137
H	-2.20244	-1.95787	0.69621
H	-0.88206	0.06891	1.24819
O	-1.02869	0.85177	-0.64446
O	-2.02236	1.68487	-0.14712
C	0.32855	-1.00405	-0.18568
H	0.35849	-1.16166	-1.26656
H	0.35646	-1.98642	0.29877
C	1.55428	-0.23633	0.26159
O	1.6338	0.38821	1.28915
O	2.56012	-0.36246	-0.61423
C	3.76385	0.31192	-0.24342
H	4.47122	0.12294	-1.04862
H	3.57853	1.38218	-0.13441
H	4.14289	-0.07839	0.70331

TS27

C	-1.07498	0.42789	-0.03437
O	-1.45492	1.56319	-0.17432
O	-1.8782	-0.63682	-0.02108
C	-3.26392	-0.34563	-0.21633
H	-3.41626	0.12596	-1.18905
H	-3.77698	-1.30381	-0.16785
H	-3.62353	0.32838	0.56385
C	0.38322	0.03347	0.20825
C	1.30761	1.23321	-0.11069
H	0.97088	1.66348	-1.05558
C	2.74724	0.80392	-0.19518
H	3.3341	1.2194	-1.01166
H	3.29567	0.73351	0.74361
H	2.56597	-0.52668	-0.52129

H	1.15353	1.99083	0.66738
O	0.6604	-0.97614	-0.76085
O	1.92407	-1.49476	-0.50463
C	0.53276	-0.48933	1.63451
H	0.19303	0.26953	2.34445
H	-0.07255	-1.38994	1.75222
H	1.57387	-0.73548	1.84386

TS28

C	-1.28196	0.62948	0.1503
C	-0.17327	-0.30215	-0.40504
C	-0.42604	-1.74605	-0.03413
H	-0.23865	-2.49071	-0.80373
H	-0.09975	-2.04197	0.96321
H	-1.80626	-1.68399	0.14987
O	-2.52052	0.08837	-0.28039
O	-2.74624	-1.08796	0.42318
C	-1.20595	2.04008	-0.39755
H	-2.03361	2.63528	-0.00772
H	-0.26563	2.50271	-0.0937
H	-1.26964	2.0279	-1.48921
H	-1.24199	0.61809	1.24537
C	1.1818	0.12465	0.1339
H	-0.15768	-0.20319	-1.49537
O	1.35969	0.85973	1.07381
O	2.17554	-0.4563	-0.5524
C	3.49062	-0.14293	-0.08773
H	4.17184	-0.69777	-0.72981
H	3.67472	0.9305	-0.16561
H	3.60769	-0.44604	0.95461

TS29

C	1.27757	0.9694	0.29993
C	0.28122	-0.21391	0.189
C	0.64846	-1.05278	-1.0159
H	0.52614	-2.12984	-0.91336
H	0.34506	-0.65995	-1.98686
H	2.01441	-0.79119	-1.04963
O	2.5801	0.43324	0.38439
O	2.901	-0.07544	-0.8705
H	1.19264	1.63593	-0.56348
C	-1.11083	0.37965	0.00649
O	-1.36457	1.55875	-0.01992
O	-2.03853	-0.58036	-0.12057
C	-3.37597	-0.1052	-0.29035
H	-3.99877	-0.99381	-0.37243
H	-3.67567	0.4992	0.56791
H	-3.44925	0.50417	-1.19336
H	1.11332	1.5309	1.22292
C	0.32605	-1.05862	1.46922
H	0.0594	-0.45799	2.34379
H	-0.36964	-1.89674	1.39659
H	1.33952	-1.44139	1.6103

TS30

C	0.29148	-0.21176	0.26399
C	2.7343	0.04802	-0.18329
H	3.37427	0.11285	-1.06133
H	3.26997	0.16934	0.7599
H	2.3551	-1.27012	-0.1066
O	0.41888	-1.47757	-0.35733
O	1.56143	-2.07736	0.15899

H	0.37064	-0.338	1.35291
C	1.39139	0.73527	-0.26247
H	1.13923	0.93967	-1.30734
C	1.38269	2.0499	0.5301
H	2.16093	2.72113	0.16013
H	0.41843	2.55223	0.43147
H	1.58069	1.85817	1.59015
O	-1.35888	1.25915	-0.7401
O	-2.03615	-0.53984	0.41982
C	-3.38612	-0.1861	0.10997
H	-4.00653	-0.94534	0.58129
H	-3.61745	0.80513	0.50541
H	-3.53522	-0.18025	-0.97137
C	-1.11245	0.2747	-0.08924

TS31

C	1.03138	-0.31125	0.09091
O	1.05637	-0.92375	-0.95414
O	2.0708	0.3945	0.56376
C	3.22758	0.38891	-0.27273
H	2.99183	0.81332	-1.25097
H	3.96949	0.99681	0.24167
H	3.59355	-0.63072	-0.41085
C	-1.28464	-1.14262	0.62769
H	-0.89364	-2.11462	0.30497
C	-2.11263	-0.56769	-0.54472
H	-1.50225	-0.5157	-1.45067
H	-3.02418	-1.14391	-0.71665
H	-1.94197	-1.28617	1.48732
O	-2.53935	0.72887	-0.17073
O	-1.43529	1.55038	-0.18727
C	-0.15643	-0.21312	0.97194
H	-0.69981	0.96194	0.52489
H	0.05516	-0.00628	2.01879

TS32

C	-2.1058	-1.20445	0.33096
H	-1.98866	-2.19719	-0.12603
C	-2.84129	-0.29058	-0.66893
H	-2.31699	-0.24325	-1.63092
H	-3.87368	-0.61325	-0.82478
H	-2.73538	-1.31373	1.21726
O	-2.91936	1.00398	-0.10936
O	-1.63229	1.52677	-0.10407
C	-0.76992	-0.61353	0.70837
H	-1.06106	0.70143	0.52474
H	-0.48654	-0.67042	1.75896
C	0.36631	-0.84317	-0.25264
H	0.1146	-0.49507	-1.26172
H	0.59961	-1.9133	-0.35345
C	1.63157	-0.1395	0.18343
O	1.76849	0.46642	1.21617
O	2.60432	-0.28333	-0.72942
C	3.84072	0.34695	-0.39152
H	4.51915	0.13236	-1.2151
H	3.6995	1.4238	-0.27866
H	4.23066	-0.05644	0.54518

TS33

C	-0.23591	0.03411	0.34099
C	-0.64534	-1.41608	-0.00165
H	-0.51284	-1.61969	-1.07091

H	-0.08152	-2.13716	0.59198
H	-0.3042	0.13047	1.43324
O	-2.00136	-1.57376	0.35478
O	-2.7544	-0.82759	-0.54893
C	-1.16502	1.03249	-0.31039
H	-2.26589	0.23812	-0.4161
C	1.21297	0.30981	-0.02866
O	1.62243	1.33369	-0.51489
O	2.00226	-0.73351	0.27393
C	3.38919	-0.54319	-0.01823
H	3.88631	-1.46151	0.288
H	3.52938	-0.36404	-1.08594
H	3.7784	0.31232	0.53717
H	-0.93971	1.18869	-1.36832
C	-1.46565	2.29278	0.45434
H	-0.54467	2.88409	0.54726
H	-2.20939	2.90802	-0.05586
H	-1.82884	2.0706	1.46202

TS34

C	-0.98971	-0.69043	0.93513
H	-0.74329	-1.75093	0.80354
C	-1.83696	-0.26671	-0.29338
H	-1.25752	-0.45392	-1.20402
H	-1.60322	-0.57221	1.83211
O	-2.05366	1.13362	-0.16976
O	-0.86256	1.77624	-0.41126
C	0.26497	0.12637	1.03385
H	-0.15528	1.24804	0.37183
H	0.56924	0.51133	2.0048
C	1.37137	-0.31027	0.14987
O	1.2519	-1.1191	-0.74448
C	3.60851	-0.00447	-0.43714
H	4.45165	0.59377	-0.09696
H	3.83889	-1.06978	-0.36754
H	3.35915	0.23369	-1.47325
O	2.52055	0.32744	0.42489
C	-3.20021	-0.92379	-0.33018
H	-3.75989	-0.594	-1.2073
H	-3.08758	-2.00938	-0.37404
H	-3.7698	-0.66638	0.5668

TS35

C	1.08929	-0.90861	-0.19696
H	0.93225	-1.76167	-0.86709
C	-0.01058	0.12933	-0.46993
H	0.00092	0.44375	-1.52334
H	0.95856	-1.27026	0.82811
O	0.23084	1.26128	0.34216
O	1.34921	1.89875	-0.18395
C	2.4588	-0.29431	-0.37217
H	2.13467	1.00263	-0.17677
C	-1.39152	-0.42225	-0.14713
O	-1.64388	-1.60105	-0.11894
O	-2.28277	0.54636	0.05373
C	-3.60906	0.09184	0.33257
H	-4.20164	0.99074	0.48915
H	-3.99574	-0.48659	-0.50904
H	-3.61379	-0.5361	1.22542
C	3.52469	-0.69025	0.61655
H	3.75208	-1.76128	0.52846
H	4.45326	-0.1393	0.45341

| H | 3.18953 | -0.51119 | 1.6423 |
| H | 2.79304 | -0.24794 | -1.4122 |

TS36

C	1.20932	-0.8841	0.30733
H	0.851	-1.48663	1.15305
C	1.77157	0.41759	0.93975
H	1.02207	0.88609	1.58351
O	2.12352	1.29298	-0.11531
O	0.95494	1.75835	-0.67536
C	0.03608	-0.53006	-0.56728
H	0.39199	0.74493	-0.9101
H	-0.05834	-1.03051	-1.5303
C	-1.24176	-0.2709	0.13735
O	-1.34487	-0.11696	1.33487
C	-3.52804	0.12952	-0.10079
H	-4.2547	0.16636	-0.91022
H	-3.79939	-0.63828	0.62692
H	-3.46995	1.093	0.41004
O	-2.27731	-0.18356	-0.71309
H	2.69809	0.22219	1.48589
C	2.2953	-1.62057	-0.47323
H	3.14106	-1.87096	0.17292
H	1.90727	-2.54854	-0.90078
H	2.66585	-0.99309	-1.2885

TS37

C	1.28391	0.33986	-1.15417
H	0.87765	0.00128	-2.114
C	2.11739	-0.81366	-0.56097
H	1.51514	-1.72324	-0.48516
O	2.54952	-0.4114	0.72776
O	1.44787	-0.42225	1.55244
C	0.1648	0.73724	-0.2181
H	0.68952	0.28137	0.92676
C	-1.01275	-0.17538	-0.30819
O	-1.00873	-1.23384	-0.89747
C	-3.2008	-0.59822	0.38493
H	-3.96569	-0.0957	0.97403
H	-3.55152	-0.77353	-0.63425
H	-2.93411	-1.55701	0.83449
O	-2.07358	0.27792	0.3799
H	3.02719	-0.99378	-1.13786
H	1.94272	1.19504	-1.32761
C	-0.09444	2.21217	-0.0139
H	-0.45184	2.6702	-0.94492
H	-0.84776	2.37994	0.75591
H	0.82944	2.71994	0.27397

TS38

O	0.38538	-1.14422	0.32724
O	1.44955	-1.77259	-0.30968
C	0.10212	0.06985	-0.35969
H	0.18659	-0.12873	-1.43787
C	3.13513	-0.14197	0.46197
H	4.14139	-0.42492	0.15468
H	2.99194	-0.13241	1.54403
H	2.36849	-1.20419	0.11141
C	2.4969	0.99533	-0.29492
H	3.04752	1.92258	-0.0838
H	2.59882	0.81856	-1.37281
C	1.01992	1.21377	0.05663

H	0.65053	2.12282	-0.4257
H	0.90744	1.36508	1.13676
C	-1.35785	0.41749	-0.07131
O	-1.75296	1.54041	0.12218
O	-2.14346	-0.65802	-0.1051
C	-3.52801	-0.39524	0.12973
H	-4.0265	-1.36021	0.0657
H	-3.66641	0.04727	1.11822
H	-3.91727	0.29414	-0.62231

TS39

O	-1.69459	-0.99337	-0.75846
O	-2.61415	0.05028	-0.82012
C	-0.94265	1.81602	-0.40992
H	-1.39173	2.80762	-0.45439
H	-0.18163	1.64268	-1.17094
H	-1.93995	0.98417	-0.82053
C	-0.62437	1.30228	0.9715
H	0.18263	1.90533	1.40576
H	-1.49993	1.43068	1.61799
C	-0.20947	-0.17942	1.01898
H	0.03129	-0.41968	2.06484
C	-1.29621	-1.16931	0.5939
H	-0.89403	-2.18392	0.6346
H	-2.17625	-1.08403	1.23959
C	1.06767	-0.49331	0.24938
O	1.38611	-1.59701	-0.11538
O	1.83813	0.59102	0.06108
C	3.07321	0.33517	-0.6115
H	2.8857	-0.11242	-1.58922
H	3.56169	1.3023	-0.71468
H	3.6892	-0.3487	-0.02401

TS40

O	-3.02776	-0.0439	0.31623
O	-2.67641	-1.24931	-0.28086
C	-0.34793	-1.2729	0.55078
H	0.17151	-2.18564	0.26609
H	-0.44796	-1.12472	1.62745
H	-1.65986	-1.48131	0.18123
C	0.00081	-0.03381	-0.2446
H	-0.08719	-0.28018	-1.31243
C	-0.89713	1.16301	0.08747
H	-0.48099	2.05677	-0.38819
H	-0.86574	1.34431	1.16774
C	-2.34699	1.01034	-0.35535
H	-2.91351	1.90814	-0.09141
H	-2.42465	0.844	-1.43634
C	1.46273	0.33703	-0.01867
O	1.85905	1.41285	0.35249
O	2.27496	-0.69683	-0.29077
C	3.66714	-0.42882	-0.11465
H	4.18438	-1.34676	-0.38724
H	3.97945	0.39663	-0.75751
H	3.87397	-0.16293	0.92402

TS41

O	2.32406	-1.31984	-0.16672
O	1.19762	-1.51091	0.60325
C	-0.13272	0.25991	-0.48781
H	-0.06196	-0.04447	-1.53395
H	0.38662	-0.84555	0.0823

C	2.25869	1.11808	-0.44319
H	2.84741	2.00526	-0.18472
H	2.31803	1.00307	-1.53213
C	2.93282	-0.08327	0.20798
H	3.96633	-0.17642	-0.13798
H	2.92144	-0.01091	1.30115
C	0.80135	1.34892	-0.02394
H	0.4522	2.30851	-0.42753
H	0.71953	1.43472	1.06547
C	-1.51831	0.32671	0.03928
O	-1.87528	1.04417	0.94557
O	-2.33496	-0.53053	-0.59737
C	-3.67653	-0.54745	-0.11183
H	-4.2011	-1.28883	-0.71167
H	-3.69578	-0.82262	0.94481
H	-4.13602	0.43665	-0.22644

TS42

C	-1.07575	-0.13044	-0.01829
O	-2.22778	-0.41566	-0.17247
O	-0.7144	1.17949	-0.07695
O	1.28275	-0.90107	0.45035
O	1.79261	-0.21724	-0.64681
C	-0.05169	-1.25356	0.16291
H	-0.09922	-1.85953	-0.74811
H	-0.38687	-1.85997	1.00768
C	0.5464	1.64484	0.26279
H	0.63051	2.6867	-0.03589
H	0.85506	1.41297	1.28504
H	1.42131	0.89065	-0.38612

TS43

C	-0.39361	0.93543	-0.19741
O	-1.21448	1.7598	-0.48413
O	0.85527	1.36359	0.13445
O	0.22089	-1.48458	0.11452
O	1.30826	-1.36608	-0.74177
C	-0.77355	-0.55267	-0.27595
H	-1.02134	-0.72321	-1.33073
C	1.84767	0.53811	0.63661
H	2.78575	1.08691	0.66046
H	1.5783	0.00513	1.5516
H	1.91439	-0.50075	-0.18552
C	-1.98045	-0.82024	0.61075
H	-2.77975	-0.12835	0.3458
H	-2.3183	-1.84742	0.46772
H	-1.71884	-0.67796	1.66212

TS44

C	0.64189	1.03601	-0.19097
O	0.48559	2.18935	-0.47603
O	1.87969	0.64063	0.21661
C	2.16563	-0.61876	0.71638
H	1.58051	-0.90522	1.59348
H	1.66242	-1.48432	-0.15283
H	3.24372	-0.7273	0.80534
C	-0.53575	0.06145	-0.35009
C	-1.72181	0.53803	0.48584
H	-1.45091	0.45943	1.54517
C	-2.98444	-0.2666	0.1944
H	-3.81808	0.09509	0.80007
H	-3.26708	-0.17468	-0.8586

H	-2.83305	-1.32541	0.41289
H	-1.86653	1.59779	0.26349
H	-0.78701	0.09108	-1.4187
O	-0.29807	-1.28441	0.0261
O	0.70066	-1.81148	-0.78214

TS45

C	1.06005	1.04774	-0.1948
O	0.88105	2.18928	-0.5121
O	2.26578	0.71748	0.34602
C	2.56195	-0.52219	0.88747
H	1.90947	-0.82972	1.70837
H	2.18742	-1.41991	-0.01377
H	3.63049	-0.57725	1.08058
C	-0.04513	0.01428	-0.4646
C	-1.34089	0.44777	0.21521
H	-1.20205	0.39034	1.30249
C	-2.53692	-0.4025	-0.20747
H	-2.64766	-0.34452	-1.29732
H	-2.33908	-1.45183	0.03159
H	-1.50417	1.49968	-0.0367
H	-0.17041	0.0116	-1.55565
O	0.21202	-1.31156	-0.03277
O	1.30902	-1.80704	-0.72504
C	-3.82349	0.06029	0.46962
H	-4.04468	1.10275	0.22076
H	-4.67642	-0.54785	0.15962
H	-3.73928	-0.01102	1.55845

TS46

C	0.07899	1.03419	-0.16559
O	-0.46948	2.04918	-0.49227
O	1.43648	1.06027	-0.05428
C	2.21103	-0.00532	0.36974
H	1.97305	-0.37836	1.36895
H	1.78526	-1.0513	-0.33452
H	3.25711	0.21853	0.17613
C	-0.76991	-0.22232	0.12663
O	-0.01557	-1.40627	0.39244
O	0.82985	-1.67491	-0.67569
C	-1.70714	-0.45506	-1.05404
H	-2.37476	-1.2849	-0.81143
H	-2.28918	0.44508	-1.25233
H	-1.12962	-0.71431	-1.94327
C	-1.53199	0.0285	1.42618
H	-2.16912	-0.83255	1.63944
H	-0.84083	0.16965	2.26134
H	-2.14805	0.92198	1.31652

TS47

C	-0.72647	1.02186	0.01577
O	-0.59045	2.19051	0.24799
O	-1.95153	0.60455	-0.41162
C	-2.25213	-0.69171	-0.79068
H	-1.64539	-1.08313	-1.61098
H	-1.77951	-1.46346	0.18403
H	-3.32948	-0.78744	-0.90118
C	0.47456	0.06998	0.20394
O	0.17828	-1.31161	-0.01076
O	-0.82801	-1.72068	0.85368
C	1.01664	0.27484	1.61598
H	1.86509	-0.39288	1.7744

H	1.32538	1.31222	1.75001
H	0.24459	0.03317	2.34858
C	1.49051	0.41364	-0.89803
H	1.01082	0.2217	-1.86559
H	1.67614	1.48956	-0.8378
C	2.79385	-0.37484	-0.80117
H	2.59975	-1.44901	-0.76406
H	3.41823	-0.16871	-1.6734
H	3.36624	-0.09682	0.08691

TS48

C	1.13203	-0.42277	0.00394
O	1.92849	-0.31966	-0.87957
O	0.80402	0.62559	0.8386
C	0.53603	1.83082	0.21186
H	-0.7543	1.6264	-0.14506
H	0.5464	2.64477	0.93275
H	1.09622	1.98751	-0.7108
C	-1.17388	-1.13746	0.37349
H	-1.39387	-0.60698	1.30009
O	-1.77554	1.02035	-0.253
O	-1.36764	-0.21956	-0.7149
C	0.28055	-1.62418	0.33893
H	0.56585	-2.04006	1.31052
H	0.45128	-2.3762	-0.43226
H	-1.87454	-1.96763	0.24639

TS49

C	0.95392	-1.01969	0.00325
O	1.64888	-1.44622	-0.86902
O	1.36654	-0.02133	0.86352
C	1.96638	1.0754	0.26879
H	0.86618	1.76915	-0.11169
H	2.48881	1.67257	1.01222
H	2.5157	0.84128	-0.64386
C	-1.27993	-0.06415	0.31734
H	-1.07998	0.47521	1.24524
C	-2.76654	-0.26637	0.09932
H	-3.2855	0.69287	0.14644
H	-2.94517	-0.71174	-0.88292
H	-3.18002	-0.9308	0.86333
O	-0.29765	1.96966	-0.28003
O	-0.76047	0.75515	-0.75455
C	-0.48167	-1.37938	0.29737
H	-0.56512	-1.88622	1.26396
H	-0.82628	-2.05516	-0.48843

TS50

C	1.50791	-0.88325	0.02483
O	2.28442	-1.18546	-0.83034
O	1.71594	0.18398	0.87675
C	2.11296	1.36555	0.2754
H	0.91287	1.84491	-0.12686
H	2.5087	2.05564	1.01663
H	2.70825	1.22631	-0.62802
C	-0.86824	-0.35269	0.28404
H	-0.79949	0.22472	1.20985
C	-2.29313	-0.81782	0.03347
H	-2.32698	-1.30191	-0.94974
H	-2.54502	-1.58479	0.77602
O	-0.26635	1.82557	-0.31852
O	-0.4821	0.54094	-0.78555

C	0.15781	-1.49744	0.30115
H	0.15111	-1.99588	1.27565
H	0 -0.03944	-2.23768	-0.47727
C	-3.28298	0.34101	0.08992
H	-2.99808	1.11421	-0.6278
H	-4.29594	0.00709	-0.14529
H	-3.29713	0.79503	1.08535

TS51

C	-0.32614	-1.01505	0.13024
O	-0.52154	-1.79062	-0.75753
O	0.86927	-0.95555	0.81505
C	2.00876	-0.96497	0.02807
H	2.05547	0.33969	-0.33495
H	2.88779	-1.16496	0.63592
H	1.90972	-1.5422	-0.892
C	-0.42978	1.37094	0.563
H	0.26867	1.43804	1.39701
O	1.69036	1.47355	-0.39019
O	0.33557	1.3671	-0.65404
C	-1.26159	0.07711	0.61146
H	-1.08196	2.25064	0.55003
H	-1.52991	-0.12693	1.65575
C	-2.5029	0.13295	-0.27093
H	-3.01423	-0.83097	-0.2887
H	-3.1953	0.89386	0.09666
H	-2.21962	0.38114	-1.29706

TS52

C	-0.1664	-0.9768	-0.19221
O	-0.17462	-1.69111	-1.15069
O	0.83538	-1.02622	0.75706
C	2.1263	-1.05178	0.25609
H	2.30812	0.265	-0.00379
H	2.83079	-1.32756	1.03705
H	2.22359	-1.57348	-0.69673
C	-0.26862	1.37714	0.36469
H	0.21786	1.35207	1.34109
O	2.01575	1.41963	-0.065
O	0.75639	1.40857	-0.6401
C	-1.1515	0.1341	0.1394
H	-0.86888	2.28999	0.27149
C	-2.08848	0.33189	-1.04953
H	-2.62283	-0.59262	-1.27855
H	-2.81805	1.11385	-0.81983
H	-1.52365	0.62488	-1.93799
C	-1.92443	-0.18934	1.42354
H	-2.53049	0.67395	1.71527
H	-2.59766	-1.03603	1.26594
H	-1.24315	-0.42832	2.24396

TS53

C	-0.71584	1.07723	0.17411
O	-1.16212	1.81719	-0.65162
O	-1.5071	0.20352	0.89068
C	-2.42152	-0.52423	0.14795
H	-1.61745	-1.51012	-0.3233
H	-3.15826	-0.98561	0.80107
H	-2.80512	0.00383	-0.7259
C	0.99028	-0.63892	0.39958
H	0.51034	-1.15395	1.23322
O	-0.59296	-2.08815	-0.51836

O	0.29682	-1.06605	-0.79706
C	0.74495	0.88385	0.53398
C	1.61761	1.75189	-0.36486
H	1.2911	2.79216	-0.31998
H	2.66462	1.70075	-0.05952
H	1.53481	1.42211	-1.40399
H	0.88331	1.15609	1.58837
C	2.44861	-1.03782	0.28504
H	3.01876	-0.66981	1.14327
H	2.52576	-2.12643	0.2511
H	2.8904	-0.63304	-0.6283

TS54

C	1.11341	-1.02228	0.15169
O	1.82831	-1.57976	-0.62668
O	1.4988	0.1143	0.83108
C	2.13356	1.07746	0.06524
H	1.04564	1.65758	-0.50354
H	2.61169	1.81614	0.70383
H	2.73116	0.67345	-0.75251
C	-1.21329	-0.14918	0.08294
O	-0.10514	1.80115	-0.74829
O	-0.54916	0.52516	-1.03357
C	-0.31593	-1.35906	0.48082
H	-0.42052	-1.56965	1.54992
H	-0.5781	-2.25509	-0.08464
C	-2.51975	-0.65551	-0.51587
H	-3.03416	-1.31127	0.19276
H	-3.1711	0.18666	-0.76075
H	-2.31807	-1.21867	-1.43072
C	-1.46849	0.79026	1.24974
H	-2.06271	0.25578	1.99643
H	-0.5366	1.12193	1.70698
H	-2.02661	1.66622	0.91468

TS55

C	-0.01398	-1.29091	0.07765
O	-0.39485	-1.76236	1.1104
O	-0.85691	-0.72788	-0.85073
C	-2.08184	-0.27279	-0.3995
H	-2.78142	-0.18972	-1.22757
H	-2.43597	-0.77041	0.50256
H	-1.76399	0.99358	-0.02471
C	2.00422	0.1923	-0.0036
H	2.20926	0.19719	1.07177
C	1.08504	1.36781	-0.30983
H	1.61902	2.32241	-0.24243
H	0.61929	1.28306	-1.29578
H	2.95969	0.33006	-0.51748
O	0.0625	1.32906	0.68907
O	-1.09204	1.93198	0.2297
C	1.40923	-1.17481	-0.40496
H	1.41805	-1.2787	-1.49303
H	1.99047	-1.98343	0.04057

TS56

C	-1.40791	-0.75619	0.05294
O	-2.04707	-0.72475	1.06489
O	-1.41812	0.25727	-0.87693
C	-1.77045	1.51876	-0.43531
H	-2.07966	2.13707	-1.27441
H	-2.41193	1.51911	0.44503

H	-0.56876	1.99479	-0.0164
C	0.97864	-1.52875	0.0474
H	1.06886	-1.68349	1.12851
C	1.41785	-0.09761	-0.25021
H	1.06301	0.22519	-1.23536
H	1.66238	-2.23027	-0.43993
O	0.73082	0.69188	0.73655
O	0.57318	1.99054	0.29237
C	-0.46513	-1.84234	-0.39981
H	-0.50968	-1.90938	-1.49001
H	-0.79719	-2.78699	0.03369
C	2.91458	0.11929	-0.11982
H	3.45496	-0.42506	-0.89901
H	3.1378	1.18409	-0.21647
H	3.26419	-0.22349	0.85817

TS57

C	0.53634	-0.92385	0.03031
O	0.62083	-1.53635	1.05685
O	-0.49374	-1.08891	-0.862
C	-1.67721	-1.61448	-0.37703
H	-2.26484	-2.03136	-1.19142
H	-1.55898	-2.22727	0.5159
H	-2.31382	-0.4827	0.02635
C	0.9664	1.52967	-0.06259
H	1.15509	1.67383	1.00803
C	-0.51876	1.75009	-0.31292
H	-0.83507	1.37274	-1.28936
H	1.5449	2.28983	-0.5973
O	-1.20032	1.01648	0.70863
O	-2.46637	0.65833	0.28764
C	1.49075	0.1349	-0.47726
H	1.47836	0.07715	-1.57127
H	-0.78442	2.81032	-0.23261
C	2.8952	-0.10622	0.06433
H	3.30137	-1.05413	-0.29577
H	3.56641	0.69851	-0.24644
H	2.87148	-0.14398	1.1559

TS58

C	0.33772	-1.28585	0.01323
O	0.47604	-1.7182	-1.09624
O	1.35618	-0.70047	0.72599
C	2.41682	-0.18198	0.00724
H	3.29328	-0.08739	0.64371
H	2.55881	-0.64145	-0.97013
H	1.96855	1.07575	-0.23622
C	-1.69711	0.07883	0.55303
C	-0.78227	1.29998	0.65759
H	-0.12024	1.24495	1.52678
O	0.01684	1.32696	-0.5277
O	1.21089	1.98183	-0.29496
C	-0.9302	-1.24105	0.82461
H	-0.67078	-1.31283	1.88366
H	-1.37287	2.22288	0.71017
H	-1.55181	-2.0936	0.54303
C	-2.4077	0.03413	-0.80174
H	-3.16341	-0.75565	-0.81019
H	-2.90273	0.98634	-1.01245
H	-1.69372	-0.16471	-1.60426
H	-2.44826	0.18037	1.34541

TS59

C	1.21631	-0.00825	0.03099
O	2.3372	-0.18328	-0.35738
O	0.41019	-1.08416	0.28676
C	-0.94337	-1.1405	-0.12466
H	-1.34774	-2.04099	0.33722
H	-1.00256	-1.1738	-1.21604
O	-1.73132	-0.08312	0.34233
O	-1.57424	0.98944	-0.52712
C	0.68206	1.33611	0.37998
H	0.33653	1.42599	1.40998
H	-0.53709	1.39688	-0.20993
H	1.28624	2.15667	0.00418

TS60

C	-0.53273	0.83634	0.09422
O	-1.02613	1.57824	-0.70613
O	0.71904	1.08079	0.64113
C	1.79095	0.50763	-0.06761
H	2.71132	0.90117	0.36256
H	1.70168	0.71336	-1.13955
O	1.83692	-0.88456	0.14207
O	0.84038	-1.46341	-0.61835
C	-1.10963	-0.44604	0.56885
H	-0.89076	-0.65737	1.61662
H	-0.16683	-1.21211	-0.00571
C	-2.46138	-0.81981	0.03597
H	-2.71271	-1.85327	0.27955
H	-3.22773	-0.1693	0.47425
H	-2.49986	-0.67967	-1.04613

TS61

C	0.26417	1.10741	0.10719
O	0.15533	2.02332	-0.65672
O	1.48089	0.78929	0.69507
C	2.25016	-0.15164	-0.01434
H	3.23086	-0.19002	0.45898
H	2.30206	0.11071	-1.07619
C	-2.17074	0.36813	-0.10781
H	-2.59636	1.28401	0.32653
C	-3.10478	-0.81475	0.13241
H	-4.08865	-0.63079	-0.30387
H	-2.70092	-1.72725	-0.31602
H	-3.23936	-0.99891	1.2023
H	-2.05882	0.57294	-1.17738
O	1.71071	-1.44491	0.12533
O	0.59929	-1.5363	-0.68979
C	-0.8091	0.15774	0.4911
H	-0.75684	-0.16322	1.53415
H	-0.24006	-0.90994	-0.09094

TS62

C	0.81954	1.11573	0.10537
O	0.73297	2.02107	-0.67378
O	2.04162	0.7253	0.63605
C	2.70668	-0.27518	-0.09669
H	3.70798	-0.37055	0.32183
H	2.71452	-0.03374	-1.16466
O	2.09329	-1.52764	0.09874
O	0.93305	-1.5579	-0.65037
C	-0.29256	0.24944	0.56788
H	-0.20367	-0.05457	1.61345

H	0.17261	-0.86378	-0.01933
C	-1.66748	0.53702	0.03762
H	-2.02621	1.47295	0.49294
H	-1.60112	0.73818	-1.03777
C	-2.66354	-0.58773	0.31698
H	-2.29508	-1.51474	-0.13916
H	-2.70914	-0.77179	1.39724
C	-4.05675	-0.26489	-0.21354
H	-4.75869	-1.07681	-0.01014
H	-4.4504	0.64488	0.2501
H	-4.03357	-0.10299	-1.29534

TS63

C	-0.35486	-1.03839	-0.00703
O	-0.09836	-1.87232	-0.82854
O	-1.58417	-1.00914	0.63621
C	-2.553	-0.18166	0.03756
H	-3.49696	-0.37265	0.54708
H	-2.60892	-0.36705	-1.04029
O	-2.26553	1.17727	0.26603
O	-1.24208	1.54713	-0.58554
C	0.52404	0.08443	0.40539
H	0.45896	0.31786	1.47191
H	-0.26675	1.05038	-0.07846
C	1.88196	0.19069	-0.23785
H	1.75416	0.01383	-1.31246
C	2.47975	1.57959	-0.01452
H	3.4592	1.65921	-0.49316
H	1.83465	2.3631	-0.42297
H	2.61232	1.77354	1.0555
C	2.80074	-0.90911	0.31697
H	2.93699	-0.78611	1.3968
H	2.38105	-1.89887	0.12479
H	3.78473	-0.85012	-0.15715

TS64

C	-0.39549	0.98276	0.10551
O	-0.87979	1.97622	-0.35549
O	0.83132	1.02405	0.74827
C	1.9393	0.50375	0.05016
H	2.81284	0.68939	0.6747
H	2.02444	0.96566	-0.93864
O	1.86217	-0.89183	-0.10005
O	1.0094	-1.16356	-1.15338
C	-1.02125	-0.37884	0.06901
H	-0.10031	-0.95579	-0.65799
C	-2.31964	-0.4303	-0.69542
H	-2.62941	-1.46451	-0.8612
H	-3.10558	0.07423	-0.12034
H	-2.23631	0.0841	-1.6543
C	-0.95416	-1.1594	1.36424
H	-1.58271	-0.67978	2.12529
H	-1.32737	-2.17442	1.21102
H	0.06704	-1.20579	1.74573

TS65

C	0.34346	1.16271	0.02018
O	0.17528	2.19629	-0.56097
O	1.58836	0.8336	0.53234
C	2.33133	-0.13955	-0.16601
H	3.29763	-0.20765	0.33326
H	2.42243	0.1303	-1.22306

O	1.75676	-1.41869	-0.06639
O	0.71594	-1.49464	-0.97349
C	-0.71535	0.13115	0.27232
H	-0.16606	-0.82994	-0.41929
C	-2.04033	0.45222	-0.38407
H	-2.47408	1.31683	0.13883
H	-1.84833	0.79251	-1.40608
C	-0.73452	-0.44763	1.6712
H	-1.14545	0.28718	2.37553
H	-1.36164	-1.34035	1.71127
H	0.27228	-0.71124	1.99707
C	-3.02543	-0.71409	-0.38103
H	-3.34619	-0.97213	0.63148
H	-3.91874	-0.46057	-0.95563
H	-2.5775	-1.60622	-0.83079

TS66

C	1.30928	-0.31123	0.0403
O	2.40357	-0.48074	-0.41753
C	0.13776	1.87955	-0.30253
H	-1.11601	1.34683	-0.31618
H	-0.06764	2.88896	0.05195
H	0.46554	1.83391	-1.34088
C	-0.92444	-1.25941	0.39571
O	-2.02014	0.71451	0.01349
O	-1.75086	-0.55404	-0.48963
O	0.41142	-1.33029	-0.04887
H	-1.26761	-2.29436	0.37857
H	-1.01656	-0.8237	1.39407
C	0.89513	1.00707	0.67211
H	1.83539	1.49191	0.95373
H	0.30858	0.86501	1.5856

TS67

C	0.78533	-0.88477	-0.1044
O	1.6822	-1.55334	-0.53539
C	0.40523	1.49266	-0.71035
H	-0.93198	1.48976	-0.47571
H	0.63723	2.54589	-0.54782
H	0.51044	1.17668	-1.74898
C	-1.58966	-0.88417	0.55962
O	-1.92942	1.32391	0.0798
O	-2.28741	0.02072	-0.24765
O	-0.46051	-1.43591	-0.08245
H	-2.26098	-1.73157	0.70395
H	-1.33866	-0.40386	1.50938
C	0.98157	0.56129	0.33813
H	0.45412	0.73919	1.28379
C	2.47661	0.82721	0.54589
H	2.62828	1.85253	0.89054
H	2.88937	0.13851	1.2861
H	3.01879	0.67659	-0.38893

TS68

C	-0.2318	-0.83567	-0.17654
O	-0.17363	-1.56071	-1.12694
C	-0.5814	1.52141	0.35745
H	0.60545	1.47061	-0.31617
H	-1.07178	2.41353	-0.03299
H	-0.17058	1.63933	1.36105
C	2.05042	-0.7272	0.33978
O	1.61557	1.14982	-0.82652

O	2.38159	0.63226	0.21145
O	0.72415	-0.82058	0.8107
H	2.71839	-1.11963	1.1062
H	2.1472	-1.24469	-0.61797
C	-1.30941	0.20907	0.10089
C	-2.09353	-0.20819	1.36029
H	-2.83344	0.56001	1.60192
H	-2.62017	-1.15142	1.18662
H	-1.42248	-0.33033	2.21356
C	-2.22816	0.30348	-1.11473
H	-2.67927	-0.66714	-1.33149
H	-3.02372	1.02913	-0.92378
H	-1.6677	0.61681	-1.9992

TS69

C	-0.10162	0.95893	0.15867
O	-0.12711	1.78837	-0.70311
C	0.55877	-1.37829	0.46121
H	-0.51685	-1.39469	-0.37861
H	1.23162	-2.10926	0.01331
H	0.05417	-1.7305	1.36013
C	-2.38806	0.45913	0.24284
O	-1.4712	-1.15779	-1.02723
O	-2.47371	-0.90026	-0.10038
O	-1.18256	0.66101	0.94796
H	-3.22058	0.64336	0.92138
H	-2.41336	1.09073	-0.64834
C	1.07256	0.05268	0.50373
H	1.35643	0.29091	1.54062
C	2.24897	0.31632	-0.43488
H	2.39662	1.39719	-0.51227
H	1.97244	-0.02432	-1.43964
C	3.53609	-0.35895	0.02826
H	4.35245	-0.15958	-0.66952
H	3.83913	0.01138	1.01268
H	3.42426	-1.44483	0.10347

TS70

C	0.82389	1.25114	0.03846
O	1.1165	2.31954	-0.41881
C	-1.46955	0.31789	-0.38832
H	-1.00957	-0.92978	-0.43454
H	-1.34073	0.68573	-1.4093
C	1.53981	-1.06062	0.44355
O	-0.51302	-1.93522	-0.06046
O	0.81236	-1.83751	-0.46673
O	1.75162	0.25629	-0.01476
H	2.53889	-1.4956	0.48679
H	1.04532	-1.09342	1.4182
C	-0.54937	0.9747	0.6228
H	-0.50797	0.36365	1.53072
H	-0.94659	1.95758	0.89908
C	-2.8978	0.14446	0.05938
H	-3.37248	1.1225	0.21085
H	-3.48472	-0.40356	-0.68019
H	-2.94365	-0.39728	1.00931

TS71

C	0.11277	-1.36846	-0.16078
O	0.63744	-2.30073	-0.70298
C	0.87597	0.95816	-0.57035
H	-0.353	1.42858	-0.42992

H	0.93305	0.65043	-1.61856
C	-2.03719	-0.38686	0.54777
O	-1.35978	1.7473	0.11539
O	-2.26609	0.75304	-0.22886
O	-1.24856	-1.34755	-0.11977
H	-3.00903	-0.86706	0.66705
H	-1.61363	-0.0912	1.51141
C	0.91518	-0.20536	0.413
H	0.47087	0.13795	1.3561
C	1.71227	2.16304	-0.21836
H	2.78127	1.94922	-0.33782
H	1.47059	3.00863	-0.8663
H	1.5422	2.46424	0.82036
C	2.34899	-0.6771	0.68037
H	2.83618	-0.9547	-0.25649
H	2.92279	0.11402	1.16716
H	2.34669	-1.55701	1.32684

TS72

C	0.8101	1.40761	0.03271
O	0.76658	2.51566	-0.42211
C	-1.07553	-0.18598	-0.41739
H	-0.2519	-1.2264	-0.4484
H	-1.05508	0.20852	-1.43779
C	2.20228	-0.56862	0.46021
O	0.52098	-2.0324	-0.04992
O	1.76188	-1.54534	-0.44103
O	1.9972	0.74286	-0.01581
H	3.28668	-0.67105	0.51263
H	1.73607	-0.74125	1.43396
C	-0.41877	0.72383	0.60393
H	-0.20194	0.15397	1.51403
H	-1.09512	1.54202	0.87213
C	-2.39099	-0.80709	-0.00669
H	-2.65749	-1.58678	-0.72761
H	-2.26704	-1.30113	0.96463
C	-3.52811	0.21998	0.07255
H	-4.47144	-0.27248	0.32036
H	-3.33523	0.97522	0.83905
H	-3.65438	0.73474	-0.88391

TS73

C	-0.76562	1.31928	-0.24205
O	-0.84044	2.47387	0.0728
C	1.36102	-0.03311	0.02488
H	0.77815	-1.19184	0.06195
C	-1.90041	-0.85601	-0.28267
O	0.01029	-2.10762	-0.14095
O	-1.13838	-1.70966	0.52813
O	-1.79825	0.49819	0.09838
H	-2.94537	-1.10806	-0.09827
H	-1.62586	-1.02017	-1.32804
C	0.45787	0.74592	-0.92972
H	0.19578	0.11466	-1.78592
H	1.00049	1.61778	-1.31087
C	2.71673	-0.33238	-0.57417
H	3.29586	0.59609	-0.67084
H	3.28586	-1.01653	0.05997
H	2.62458	-0.77489	-1.57024
C	1.36704	0.45401	1.45573
H	2.06634	-0.12787	2.06011
H	1.66588	1.51014	1.4962

| H | 0.37283 | 0.37617 | 1.90711 |

TS74

C	-1.82115	1.57994	0.10728
H	-2.55138	1.85056	0.87015
H	-2.03813	2.01154	-0.87108
H	-2.10947	0.25305	-0.097
C	-0.10205	-1.54417	0.50615
H	-0.04409	-2.61893	0.69356
H	-0.5277	-1.02848	1.37121
O	-0.94343	-1.29812	-0.61035
O	-2.19165	-0.8974	-0.14979
O	1.21665	-1.15885	0.23699
C	1.61665	0.10805	-0.1016
O	2.79038	0.34285	-0.05469
C	0.59046	1.11812	-0.57571
H	1.17753	1.94641	-0.97209
H	0.02683	0.67033	-1.39707
C	-0.37623	1.61968	0.52744
H	-0.11048	2.65417	0.78169
H	-0.24487	1.06375	1.46198

TS75

C	-1.03792	2.11076	0.36043
H	-1.63051	2.62681	1.11588
H	-0.85815	2.7093	-0.53443
H	-1.9197	1.15831	-0.08777
C	-1.18122	-1.50136	0.29953
H	-1.66049	-2.48287	0.27383
H	-1.42732	-0.97922	1.22736
O	-1.65776	-0.71888	-0.78443
O	-2.56221	0.22176	-0.30654
O	0.18721	-1.7805	0.17889
C	1.20145	-0.8622	0.08436
O	2.31765	-1.26364	0.25471
C	0.87569	0.57519	-0.29078
H	0.20652	0.52296	-1.15383
C	0.13854	1.31655	0.85769
H	0.85784	1.99138	1.34411
H	-0.18565	0.63515	1.65216
C	2.15551	1.3066	-0.68423
H	2.63557	0.83151	-1.54159
H	1.92292	2.34392	-0.94277
H	2.86761	1.29954	0.14396

TS76

C	0.94368	-2.01944	0.17755
H	1.19166	-2.79667	-0.54693
H	1.21004	-2.28102	1.20372
H	-0.42987	-2.06067	0.17895
C	-1.84473	0.25243	-0.6172
H	-2.86652	0.53175	-0.88278
H	-1.34564	-0.23018	-1.46132
O	-1.88329	-0.67591	0.45611
O	-1.56342	-1.94239	-0.01929
O	-1.23738	1.46298	-0.25137
C	0.05341	1.59904	0.19161
O	0.56544	2.67809	0.09107
C	1.25461	-0.60472	-0.23663
H	0.75766	-0.42168	-1.19868
C	0.73623	0.40678	0.82191
H	1.57805	0.81149	1.38749

H	0.0446	-0.07268	1.51568
C	2.7584	-0.40364	-0.47411
H	2.95541	0.63583	-0.75361
H	3.32061	-0.62542	0.4382
H	3.12358	-1.05564	-1.27162

TS77

C	-1.9044	-0.72215	0.34137
H	-2.10617	-1.01365	1.37662
H	-1.62188	0.58141	0.48259
C	0.74283	1.51024	-0.61787
H	1.15391	2.46122	-0.96449
H	0.02027	1.12067	-1.3396
O	0.06911	1.70353	0.61555
O	-1.2998	1.71596	0.38634
O	1.85975	0.67982	-0.46108
C	1.83264	-0.60176	0.02448
O	2.83356	-1.25037	-0.08835
C	0.58841	-1.11795	0.71897
H	0.88952	-2.06619	1.16385
H	0.3366	-0.42512	1.52542
C	-0.63207	-1.31732	-0.21299
H	-0.78573	-2.39285	-0.37474
H	-0.44845	-0.90998	-1.21446
C	-3.108	-0.73556	-0.56436
H	-3.4138	-1.76706	-0.78394
H	-3.95956	-0.22446	-0.11043
H	-2.8821	-0.24854	-1.51816

TS78

C	-0.12942	-1.34829	-0.09265
O	-0.52363	-1.91951	0.88757
H	-0.03753	1.51644	0.44604
C	-2.13914	-0.14777	-0.35446
O	-0.93645	-0.62769	-0.92217
H	-2.9081	-0.15292	-1.12747
H	-2.40448	-0.74825	0.51642
C	2.23984	1.06645	-0.01281
H	2.72393	1.63817	0.78512
H	2.9257	1.10551	-0.87441
C	1.31789	-1.30779	-0.51883
H	1.69398	-2.33004	-0.43904
H	1.40843	-0.9777	-1.55711
C	2.11374	-0.39327	0.4411
H	3.12163	-0.80059	0.55988
H	1.64194	-0.43915	1.42856
C	0.9595	1.74398	-0.43027
H	0.46379	1.32776	-1.30879
H	0.99246	2.83366	-0.44709
O	-1.97642	1.20192	-0.00662
O	-1.03802	1.26369	1.01941

P1

C	-0.50932	-0.19075	0.15371
O	-0.49617	-1.36823	-0.11709
O	-1.61307	0.55795	0.17892
H	1.52089	-1.5533	-0.55178
C	0.73203	0.6427	0.50017
H	0.54905	1.093	1.48515
C	0.97497	1.69399	-0.52727
H	0.32864	2.55909	-0.56866

H	1.6612	1.47826	-1.33312
O	2.16215	-0.82092	-0.53791
O	1.82927	-0.21851	0.70868
C	-2.82251	-0.13042	-0.15674
H	-3.00357	-0.94068	0.55194
H	-3.61282	0.61514	-0.10035
H	-2.75188	-0.54686	-1.16319

P2

C	-1.12181	-0.16852	0.22618
O	-1.09204	0.72846	1.03219
O	-2.21013	-0.48573	-0.48878
C	-3.35696	0.32449	-0.22749
H	-3.13579	1.37271	-0.43758
H	-4.13883	-0.04446	-0.88854
H	-3.65926	0.23131	0.81782
C	0.03545	-1.09184	-0.08908
H	-0.09194	-2.01442	0.48681
H	0.01663	-1.36226	-1.14801
C	1.36546	-0.43095	0.27321
H	1.27982	-0.02389	1.28931
C	2.53572	-1.33903	0.14928
H	2.88663	-1.9168	0.9937
H	2.98897	-1.48132	-0.8232
O	1.44926	0.65374	-0.64871
O	2.49386	1.51116	-0.2074
H	1.97894	2.21326	0.21873

P3

C	-1.20898	-0.27348	0.23139
O	-1.15729	0.69255	1.03618
O	-2.29456	-0.49414	-0.4514
C	-3.42877	0.36114	-0.2872
H	-3.09871	1.34539	-0.02794
H	-3.98172	0.39991	-1.20242
H	-4.05454	-0.0219	0.49164
C	0.01247	-1.19456	0.05455
H	-0.04752	-2.00425	0.75148
H	0.0253	-1.58244	-0.94258
C	1.30181	-0.39202	0.3098
H	1.28898	-0.00414	1.30694
H	1.3618	0.41767	-0.38712
C	2.52326	-1.3131	0.13296
H	2.53609	-1.70098	-0.86418
C	3.8126	-0.51056	0.38821
H	4.2219	-0.45546	1.37529
H	4.29913	-0.00806	-0.42153
O	2.44309	-2.39521	1.06436
O	3.49005	-3.1847	0.91279
H	3.43622	-3.91115	1.53806

P4

C	0.06352	0.86409	-0.30286
C	-1.08421	-0.00288	0.1778
O	-1.10086	-0.60567	1.22385
O	-2.11694	0.0231	-0.67664
C	-3.25826	-0.72703	-0.25936
H	-2.99408	-1.77892	-0.1333
C	1.38109	0.21517	0.141
H	1.32414	0.04572	1.22433
C	-0.10334	2.27161	0.27973
H	0.7002	2.92397	-0.06941

H	-1.05987	2.70091	-0.02695
H	-3.64007	-0.34431	0.68939
C	2.59377	0.99372	-0.22289
H	3.17946	1.51538	0.52104
H	2.91692	1.00387	-1.25655
H	-0.07335	2.23481	1.37287
H	0.03541	0.90639	-1.39636
O	1.35984	-1.04954	-0.52367
H	-3.9986	-0.60789	-1.0481
O	2.38222	-1.85385	0.04963
H	1.86038	-2.40036	0.65719

P5

C	-0.93928	-0.24733	0.20652
C	0.52987	-0.49162	-0.18832
O	0.90315	-1.40135	-0.88157
O	1.36338	0.39706	0.38718
C	2.75065	0.16033	0.1284
H	3.04144	-0.82302	0.50265
C	-1.16577	-0.9736	1.48972
H	-0.81534	-0.5303	2.41252
H	-1.49855	-2.00214	1.47082
C	-1.85808	-0.71404	-0.91395
H	-2.89476	-0.60835	-0.5889
H	-1.69248	-0.10276	-1.80232
H	-1.64846	-1.75684	-1.15661
O	-1.14227	1.12492	0.52279
H	2.94917	0.20195	-0.94443
H	3.28938	0.94693	0.65321
O	-0.72588	1.89815	-0.59807
H	0.17826	2.122	-0.32377

P6

C	-0.5719	-0.16551	0.31115
C	0.85049	-0.51548	-0.16334
O	1.12408	-1.49351	-0.80939
O	1.76993	0.36578	0.2769
C	3.11885	0.03107	-0.06385
H	3.38162	-0.9426	0.35369
C	-1.58494	-0.57413	-0.76348
H	-1.31751	-0.05798	-1.68969
H	3.23851	-0.00667	-1.14834
H	-1.46318	-1.64578	-0.94508
O	-0.66398	1.21584	0.63385
H	3.7381	0.81506	0.36794
C	-3.01121	-0.22743	-0.35318
H	-3.29966	-0.75264	0.56239
H	-3.10234	0.84537	-0.16856
H	-3.71597	-0.50441	-1.14033
C	-0.77832	-0.87344	1.60876
H	-1.0503	-1.92024	1.60177
H	-0.44584	-0.40331	2.52481
O	-0.32044	1.9621	-0.5287
H	0.62201	2.121	-0.3562

P7

C	0.99519	-0.55825	-0.48627
O	1.24556	-1.52781	0.27585
O	2.02903	0.3693	-0.82648
C	2.96615	0.45462	0.25029

H	3.3957	-0.5094	0.42651
H	3.73972	1.14865	-0.00427
H	2.46422	0.78844	1.13433
C	-0.42456	-0.37061	-1.05256
H	-0.99745	0.23802	-0.38452
H	-0.36704	0.10607	-2.00879
C	-1.10259	-1.74499	-1.20406
C	-2.52234	-1.55735	-1.77035
H	-2.46482	-1.08067	-2.72658
H	-2.99344	-2.51228	-1.87562
H	-3.09523	-0.94872	-1.10231
C	-0.27806	-2.62096	-2.16554
H	0.78137	-2.48799	-2.23507
H	-0.76459	-3.36256	-2.76404
O	-1.17947	-2.38204	0.07389
O	-1.76063	-3.56009	-0.05598
H	-1.81224	-3.98776	0.80195

P8

C	-0.09627	-0.21246	-0.34291
C	-1.55709	-0.08688	0.12811
O	-2.08731	1.04906	0.23799
O	-2.31102	-1.26111	0.44062
C	-3.69518	-1.02489	0.17006
H	-4.04148	-0.20875	0.76914
H	-3.82045	-0.78565	-0.8653
H	-0.07126	-0.29517	-1.40942
H	0.34531	-1.08423	0.09289
H	-4.25932	-1.90351	0.40389
C	2.19939	0.9278	0.39501
H	2.67581	1.85897	0.16952
H	2.34047	0.69644	1.43013
O	2.77294	-0.10768	-0.40732
C	0.693	1.03571	0.09381
H	0.19473	1.97793	0.18796
O	4.06414	-0.20018	-0.14915
H	4.49158	0.63527	-0.35146

P9

C	-1.0613	0.55248	-0.07267
O	-1.76492	1.54255	-0.09016
O	-1.55283	-0.70421	0.0592
C	-2.97114	-0.77377	0.18132
H	-3.45181	-0.34762	-0.70215
H	-3.21197	-1.83111	0.27758
H	-3.30605	-0.22056	1.06159
C	0.47379	0.55019	-0.1954
H	0.76197	-0.01711	-1.05565
C	0.97921	1.99748	-0.34203
H	0.55221	2.43725	-1.21906
H	0.69075	2.56486	0.51807
O	2.40469	1.99538	-0.45556
O	2.8385	3.23567	-0.5816
H	3.79547	3.23426	-0.65784

P10

C	1.99352	0.09795	-0.01377
O	1.91514	1.2807	0.20898
O	3.16077	-0.56128	-0.10249
C	4.3215	0.2482	0.08497
H	4.30497	0.71491	1.07215
H	5.17232	-0.4243	-0.00806

H	4.3665	1.03341	-0.67281
C	-1.68215	-0.9999	-0.30409
H	-2.91983	1.6102	-0.83344
C	-2.94866	-0.84819	0.46193
H	-3.77047	-1.41015	0.00581
H	-2.83336	-1.17934	1.50462
H	-1.65938	-1.62331	-1.19209
O	-3.3342	0.51519	0.62696
O	-3.66082	1.00877	-0.67049
C	0.82188	-0.82841	-0.23683
H	0.94433	-1.70371	0.40915
H	0.88612	-1.20183	-1.26609
C	-0.51315	-0.13086	0.01092
H	-0.56784	0.21319	1.05042
H	-0.5282	0.79123	-0.5921

P11

C	1.22028	0.0582	-0.12692
O	1.48689	1.19795	-0.46549
O	2.15681	-0.84918	0.21856
C	3.49665	-0.36679	0.16105
H	3.63209	0.47041	0.84979
H	4.12809	-1.20554	0.4488
H	3.74018	-0.02982	-0.8491
C	-0.12536	-0.47108	-0.04721
H	-0.29809	-1.47734	0.31091
C	-1.30733	0.45542	-0.38802
H	-1.30417	1.29588	0.27419
C	-2.62899	-0.31878	-0.22855
H	-2.72736	-0.65186	0.78351
H	-3.44972	0.3222	-0.47445
H	-2.62821	-1.16458	-0.88392
O	-1.18185	0.9114	-1.73755
O	-2.19105	1.71107	-2.02809
H	-2.16008	1.94063	-2.95973

P12

C	-0.51619	-0.40474	0.14565
C	-1.91175	0.14514	-0.04113
O	-2.18614	1.26827	-0.38334
O	-2.83542	-0.79599	0.21219
C	-4.18687	-0.37275	0.03357
H	-4.41113	0.47375	0.68588
H	-4.35815	-0.07182	-1.00232
H	-0.37138	-1.20338	-0.59783
H	-0.47109	-0.92113	1.11438
H	-4.80444	-1.23123	0.2909
C	1.94328	0.31128	0.36246
H	2.0149	-0.05878	1.3983
C	2.90133	1.47195	0.15463
H	3.92346	1.16516	0.38493
H	2.85248	1.81297	-0.88353
H	2.63585	2.30627	0.80873
C	0.53219	0.64178	0.02906
H	0.27053	1.60366	-0.3956
O	2.28088	-0.79882	-0.48869
O	3.49559	-1.36013	0.00946
H	4.10792	-1.13805	-0.70618

P13

C	-1.59756	0.055	-0.19268
O	-1.65435	1.287	0.05739

O	-2.75512	-0.63018	-0.67795
C	-3.93198	0.00123	-0.16685
H	-3.95905	1.02069	-0.49069
H	-4.79813	-0.51146	-0.52995
H	-3.91936	-0.03309	0.90253
C	-0.28147	-0.7148	0.0239
H	-0.20709	-1.73493	-0.29027
C	1.01175	0.03293	0.39818
H	1.1914	0.81249	-0.31239
C	2.19526	-0.95238	0.38942
H	2.29868	-1.37693	-0.58729
H	2.01562	-1.73194	1.09999
C	3.48849	-0.20465	0.7637
H	3.38506	0.2199	1.74041
H	4.3108	-0.88925	0.75761
H	3.66813	0.57491	0.05313
O	0.87353	0.60031	1.7035
O	1.98201	1.24122	2.02432
H	1.88922	1.62212	2.90062

P14

C	-1.43346	-0.72567	0.16057
O	-1.81037	-1.29786	-0.89493
O	-2.25692	0.27546	0.76435
C	-3.01577	0.94248	-0.24765
H	-3.6332	0.23223	-0.75679
H	-3.63193	1.69158	0.20413
H	-2.34999	1.40273	-0.94751
C	-0.08538	-1.10356	0.80206
H	0.68722	-0.48114	0.40135
H	-0.14274	-0.96358	1.86131
C	0.23327	-2.57877	0.49572
H	0.29063	-2.71875	-0.56353
C	1.58134	-2.95666	1.1372
H	1.90183	-2.47013	2.03469
C	2.46814	-4.0348	0.48698
H	3.49634	-3.82395	0.69494
H	2.21314	-4.99445	0.88566
H	2.31111	-4.03511	-0.57143
O	-0.79928	-3.41061	1.03124
O	-0.52615	-4.67507	0.76867
H	-1.21933	-5.23351	1.12818

P15

C	-0.98618	-0.42859	-0.00777
O	-1.33649	-1.48696	-0.46183
O	-1.82691	0.541	0.36702
C	-3.20933	0.2424	0.16531
H	-3.49488	-0.64057	0.74076
H	-3.75599	1.11932	0.50642
H	-3.40476	0.05242	-0.89185
C	0.4671	-0.01949	0.24226
H	0.57155	0.24347	1.30578
C	1.42212	-1.08336	-0.14761
H	1.13907	-1.71903	-0.97832
C	2.81876	-1.08965	0.36313
H	2.87247	-0.6871	1.37973
H	3.23902	-2.09936	0.36292
H	3.47166	-0.45911	-0.25654
O	0.61896	1.19214	-0.52103
O	1.8808	1.7432	-0.15476
H	1.59623	2.54715	0.3041

P16

C	0.88143	-0.48974	-0.20288
O	1.2369	-1.43506	-0.85871
O	1.71479	0.48583	0.2028
H	0.37017	2.15971	-0.06994
C	-0.55142	-0.30234	0.30533
C	-1.51943	-0.5951	-0.79652
H	-1.18631	-1.21357	-1.61952
O	-0.57176	1.95361	-0.18371
O	-0.74647	0.99449	0.8543
C	3.07658	0.30745	-0.20026
H	3.15106	0.29642	-1.28935
H	3.62299	1.15072	0.21781
H	3.46311	-0.63562	0.18954
C	-2.88133	-0.00133	-0.74652
H	-3.32564	-0.09164	0.25248
H	-2.84562	1.07382	-0.96885
H	-3.55016	-0.47863	-1.46505
C	-0.73921	-1.23361	1.5137
H	-1.7648	-1.14331	1.87743
H	-0.55247	-2.26319	1.20465
H	-0.04971	-0.95771	2.31626

P17

C	1.33105	0.03267	-0.00565
O	1.57418	1.16408	0.3776
O	2.29626	-0.88307	-0.23784
C	3.62138	-0.4233	0.01162
H	3.73517	-0.13161	1.0584
H	4.27659	-1.25939	-0.22669
H	3.85379	0.43963	-0.6166
C	0.00955	-0.50117	-0.27018
H	-2.66853	-2.24656	-0.36045
C	-1.22658	0.32704	-0.08737
H	-0.0802	-1.53062	-0.59133
O	-2.36296	-0.41969	-0.53121
O	-2.47116	-1.57639	0.30813
C	-1.22418	1.53878	-1.02294
H	-0.38164	2.18213	-0.76701
H	-1.13341	1.21641	-2.06302
H	-2.16024	2.08906	-0.90205
C	-1.40644	0.75579	1.37121
H	-2.33536	1.325	1.46129
H	-1.46373	-0.11954	2.02056
H	-0.56178	1.37728	1.67327

P18

C	-0.98126	0.4779	-0.01969
O	-1.66556	1.31315	-0.57941
O	-1.43553	-0.75795	0.28306
C	-2.78268	-1.00606	-0.10783
H	-2.89426	-0.89486	-1.18875
H	-2.99846	-2.02881	0.19654
H	-3.46018	-0.30526	0.3856
C	0.39965	0.68511	0.4064
H	2.01256	-0.69973	-1.71763
C	1.19135	-0.45222	0.97251
H	2.08455	-0.08268	1.48892
H	0.58995	-1.05773	1.6559
O	1.5819	-1.38487	-0.03135
O	2.50107	-0.69745	-0.88171

C	1.03434	2.00664	0.16781
H	1.39246	2.44056	1.11003
H	1.91766	1.88078	-0.47019
H	0.33224	2.69635	-0.30034

P19

C	1.15309	0.21945	-0.01092
O	0.89384	-0.53169	0.90463
O	2.38537	0.35098	-0.50624
C	3.38043	-0.47841	0.10098
H	3.11142	-1.53079	-0.00673
H	4.30773	-0.26055	-0.42485
H	3.4727	-0.24268	1.16288
C	0.17348	1.1387	-0.72362
H	0.25431	0.91327	-1.79337
H	0.55998	2.15744	-0.58887
C	-1.2754	1.00678	-0.21869
C	-2.18499	1.962	-1.01354
H	-2.14917	1.70695	-2.05208
H	-1.84701	2.96862	-0.88163
C	-1.75731	-0.4427	-0.41457
H	-1.21412	-0.89357	-1.21866
H	-1.59056	-0.99856	0.48438
H	-2.80209	-0.44307	-0.64553
O	-3.52917	1.84458	-0.53996
O	-4.25794	2.82799	-1.03413
H	-5.16052	2.7487	-0.71686

P20

C	-0.93769	-0.55312	0.18848
O	-1.09887	-1.63499	0.72069
O	-1.92353	0.08581	-0.48172
C	-3.1655	-0.61292	-0.51271
H	-3.55001	-0.75623	0.49968
H	-3.84283	0.00802	-1.09655
H	-3.04106	-1.59259	-0.97911
C	0.31224	0.20098	0.20253
H	2.48312	-0.59544	-1.74471
C	1.47697	-0.44069	0.88664
H	2.12379	0.31355	1.35079
H	1.13276	-1.16048	1.63312
O	2.25599	-1.23765	-0.00249
O	2.896	-0.33799	-0.90778
C	0.40703	1.56343	-0.40089
H	1.45836	1.78878	-0.59855
H	-0.13349	1.58268	-1.35283
C	-0.19695	2.62967	0.53112
H	-1.2553	2.42241	0.70561
H	0.31742	2.64049	1.49628
H	-0.10613	3.62326	0.0857

P21

C	-1.32363	0.51084	0.0209
O	-2.06199	1.44515	0.27052
O	-1.79364	-0.74215	-0.22012
C	-3.2121	-0.86028	-0.16414
H	-3.68031	-0.20274	-0.89996
H	-3.43477	-1.90311	-0.38488
H	-3.5808	-0.58958	0.82787
C	0.21168	0.59102	-0.06864
C	0.66827	2.03267	0.22251
H	0.35004	2.31625	1.20395

C	0.83674	-0.36407	0.96513
H	1.89807	-0.38918	0.83153
H	0.60958	-0.01937	1.95228
H	0.43688	-1.34729	0.82984
C	2.20391	2.11174	0.13794
H	2.49774	3.11688	-0.08174
H	2.62852	1.81238	1.07334
H	2.55245	1.46091	-0.63655
O	0.09159	2.91893	-0.74024
O	0.58022	4.13323	-0.56957
H	0.26477	4.70717	-1.27148

P22

C	-0.96206	-0.41132	-0.52069
O	-1.37011	-1.49504	-0.84761
O	-1.7027	0.48689	0.15562
H	-0.32421	1.89042	0.9083
C	0.45405	0.0777	-0.8051
H	0.6192	-0.075	-1.88088
C	1.4825	-0.67334	-0.0153
O	0.62365	1.81387	0.71093
O	0.57716	1.49329	-0.67583
C	-3.0363	0.05857	0.44939
H	-3.01592	-0.83744	1.07271
H	-3.5068	0.88624	0.97634
H	-3.57094	-0.16497	-0.47518
C	2.89879	-0.28399	-0.27813
H	3.06978	-0.06813	-1.33718
H	3.15685	0.6276	0.28101
H	3.5899	-1.07196	0.03605
C	1.1324	-1.30039	1.29322
H	1.08253	-0.53678	2.08464
H	0.16753	-1.81527	1.25985
H	1.8918	-2.03009	1.58907

P23

C	0.76833	-0.58659	0.15175
O	1.08702	-1.71588	-0.11909
O	1.63437	0.44261	0.17501
H	0.3377	2.01097	-0.565
C	-0.65496	-0.17969	0.52463
H	-0.8324	-0.55384	1.5422
C	-1.66506	-0.81478	-0.4356
H	-1.47341	-0.43198	-1.44237
O	-0.60942	1.80375	-0.61754
O	-0.80691	1.21385	0.66411
C	2.98529	0.08697	-0.13682
H	3.04225	-0.34227	-1.13889
H	3.55745	1.01063	-0.07671
H	3.35629	-0.64503	0.58243
C	-3.06616	-0.53487	-0.0245
H	-3.34675	-0.55084	1.0218
H	-3.84382	-0.38667	-0.76027
H	-1.44236	-1.89189	-0.45998

P24

C	-0.61373	0.68959	0.0006
O	-1.10588	1.45316	0.7893
O	-1.28857	-0.35156	-0.53592
H	0.05793	-1.91316	-0.71437
C	1.65101	-0.14825	0.50144
H	1.70958	0.34731	1.47569

O	0.97156	-2.11298	-0.44533
O	1.03737	-1.38765	0.7794
C	0.82401	0.7243	-0.47976
H	0.87513	0.2457	-1.46272
C	-2.62921	-0.50564	-0.05734
H	-3.21197	0.38868	-0.28335
H	-3.03445	-1.37147	-0.5777
H	-2.6255	-0.66766	1.02193
C	1.34772	2.11607	-0.51917
H	0.93752	2.85387	0.15713
H	2.23819	2.34575	-1.08799
H	2.65899	-0.29315	0.0972

P25

C	-1.39845	-0.68537	0.19126
O	-1.828	-1.35206	-0.78577
O	-2.24528	0.27363	0.83009
C	-3.16588	0.80769	-0.12498
H	-3.76314	0.01571	-0.52617
H	-3.79952	1.52527	0.35303
H	-2.62384	1.28171	-0.91643
C	0.03918	-0.90227	0.69897
H	0.70298	-0.2393	0.18444
H	0.0802	-0.70362	1.74956
C	0.46242	-2.35928	0.43513
H	-0.20138	-3.02225	0.94966
C	1.90005	-2.57618	0.94283
H	1.94107	-2.37752	1.99342
H	2.56385	-1.9132	0.4283
C	2.32329	-4.03318	0.67899
H	2.14004	-4.78559	1.41737
H	2.8006	-4.2931	-0.2427
O	0.4076	-2.62477	-0.96894
O	0.77037	-3.87363	-1.19509
H	0.73357	-4.05186	-2.13768

P26

C	0.83939	-0.51288	-0.15925
O	1.14169	-1.51185	-0.76065
O	1.73625	0.4096	0.23909
H	0.54555	2.16586	-0.23648
C	-0.59028	-0.18778	0.27792
C	-1.55783	-0.51103	-0.87231
H	-1.22952	0.06874	-1.74802
O	-0.39719	2.00701	-0.4056
O	-0.70814	1.16135	0.69737
C	3.09199	0.10291	-0.10109
H	3.19834	0.00497	-1.1831
H	3.68834	0.93223	0.27462
H	3.395	-0.83441	0.36901
C	-2.96645	-0.18373	-0.52291
H	-3.18639	0.76604	-0.05143
H	-3.78549	-0.76072	-0.93095
H	-1.43454	-1.56596	-1.13216
C	-0.89355	-0.99637	1.53797
H	-0.78033	-2.06086	1.32277
H	-0.21046	-0.71299	2.34211
H	-1.92108	-0.79849	1.84993

P27

| C | -1.00113 | 0.6369 | -0.05756 |
| O | -1.38426 | 1.13598 | 1.03226 |

O	-1.94285	-0.00854	-0.91865
C	-2.9928	-0.57988	-0.13374
H	-3.48579	0.19249	0.41881
H	-3.69744	-1.06282	-0.77805
H	-2.58077	-1.29681	0.54535
C	0.48189	0.72121	-0.46393
H	0.55819	0.75199	-1.53076
C	1.10582	1.99666	0.13234
H	0.58521	2.85505	-0.23785
C	2.58884	2.08098	-0.27403
H	2.66513	2.11176	-1.34086
H	3.02235	2.96717	0.14027
H	3.10945	1.2226	0.09617
C	1.23118	-0.51422	0.06888
H	1.68093	-0.48975	1.03946
H	1.30205	-1.39706	-0.53151
O	1.00385	1.95554	1.55811
O	1.53865	3.04878	2.0692
H	1.47019	3.02117	3.02635

P28

C	0.79573	-0.20801	-0.21188
O	0.44453	-1.29994	-0.72948
O	1.96698	-0.09863	0.34454
C	-0.16057	0.99883	-0.23692
C	2.85498	-1.21926	0.3678
H	3.46837	-1.20652	-0.50883
H	3.47526	-1.16481	1.23796
H	2.28574	-2.12496	0.39167
C	0.08473	1.82172	-1.51531
H	-0.4609	1.59839	-2.40824
H	0.80078	2.61679	-1.51062
C	0.09464	1.88175	0.99876
H	1.10684	2.22844	0.98649
H	-0.56981	2.72027	0.98136
H	-0.0758	1.31	1.88699
C	-1.61739	0.49985	-0.21926
H	-1.78782	-0.0719	0.66897
H	-1.79471	-0.11361	-1.07782
O	-2.50539	1.62048	-0.24252
O	-3.75408	1.19279	-0.22739
H	-4.35022	1.9451	-0.243

P29

C	1.00681	0.26583	0.20643
O	0.77565	-0.80389	0.75438
O	2.19692	0.54852	-0.34658
C	3.15765	-0.50411	-0.27769
H	2.78023	-1.39672	-0.78105
H	4.04749	-0.12655	-0.77783
H	3.37652	-0.75314	0.76283
C	0.06724	1.36387	0.09245
H	0.38607	2.24659	-0.44909
C	-1.36868	1.21379	0.62837
H	-1.33854	1.02495	1.68114
H	-1.85065	0.39687	0.13314
C	-2.1543	2.51123	0.36185
H	-2.19438	2.6939	-0.69168
H	-1.66589	3.33008	0.84749
O	-3.48299	2.37754	0.87333
O	-4.15688	3.48942	0.64529
H	-5.04883	3.39971	0.98876

P30

C	1.45873	0.20314	-0.07453
O	0.93281	-0.88711	-0.03514
O	2.78208	0.36678	-0.00032
C	3.54057	-0.83872	0.13307
H	3.36656	-1.49127	-0.72456
H	4.58276	-0.52931	0.17748
H	3.25407	-1.36792	1.04382
C	0.74188	1.54041	-0.19207
H	1.23803	2.10236	-0.98903
H	0.96031	2.07881	0.74129
C	-0.77357	1.39517	-0.42428
H	-0.94514	0.82781	-1.3151
C	-1.40592	2.79124	-0.57505
H	-0.97388	3.28936	-1.41774
H	-1.22227	3.36347	0.31023
C	-2.92439	2.6468	-0.78713
H	-3.35677	2.15079	0.05662
H	-3.10803	2.07256	-1.67111
O	-3.51111	3.94301	-0.93029
O	-4.81528	3.82077	-1.09343
H	-5.20921	4.69097	-1.18918

P31

C	-0.93124	-0.42115	0.19349
O	-1.02563	-0.05297	1.34394
O	-1.98188	-0.58291	-0.61301
C	-3.24544	-0.24307	-0.03446
H	-3.24328	0.8012	0.28323
H	-3.98397	-0.40899	-0.81602
H	-3.4479	-0.87728	0.83054
H	0.63079	1.26703	1.38201
C	0.74967	0.67573	-1.20789
H	1.80574	0.66956	-1.50137
H	0.1236	0.82707	-2.09274
O	0.4596	1.79602	-0.40086
O	1.25782	1.70298	0.77473
C	1.42393	-1.17121	0.43178
H	1.17145	-1.21877	1.48438
C	0.3841	-0.66734	-0.5166
H	0.21411	-1.39107	-1.32755
C	2.84562	-1.28239	0.00659
H	3.36858	-0.31923	0.10806
H	3.38815	-2.00946	0.61624
H	2.93357	-1.58844	-1.04272

P32

C	1.38857	-0.27654	-0.20299
O	1.21127	0.80811	-0.74234
O	2.56861	-0.62653	0.33355
C	3.58271	0.37421	0.26035
H	3.26372	1.27787	0.78407
H	4.46028	-0.05788	0.73754
H	3.79474	0.62717	-0.78063
H	-0.44507	1.622	-0.54771
C	-1.89079	-0.43505	0.46322
H	-1.86323	-1.01731	1.39325
O	-1.33693	0.80566	0.87143
O	-1.37125	1.69526	-0.24291
C	0.39276	-1.32238	-0.08192
H	0.67233	-2.21978	0.4573

C	-0.98564	-1.11709	-0.58916
H	-1.43666	-2.07443	-0.86755
H	-0.96945	-0.47138	-1.47319
C	-3.32367	-0.28965	-0.02315
H	-3.76606	-1.27101	-0.21448
H	-3.91712	0.22346	0.73648
H	-3.35071	0.30036	-0.94092

P33

C	1.33417	-0.23126	0.47444
O	1.80799	-0.80134	1.42499
O	2.01756	-0.05238	-0.79631
C	3.34127	-0.58794	-0.84422
H	3.32137	-1.66458	-0.66314
H	3.7135	-0.37081	-1.84339
H	3.96911	-0.11514	-0.08629
C	-0.10396	0.3184	0.4391
H	-0.67653	-0.22674	-0.28193
C	-0.74736	0.16264	1.82956
H	-0.79843	-0.87524	2.0847
H	-0.15614	0.67985	2.5561
C	-2.16817	0.75627	1.80716
H	-2.7563	0.24619	1.07311
C	-2.81728	0.58667	3.19334
H	-2.22823	1.09531	3.92765
H	-3.80383	1.00066	3.17826
H	-2.87078	-0.45379	3.43724
O	-0.07672	1.70199	0.07877
O	-0.84719	1.89814	-0.97494
H	-0.82636	2.82641	-1.21882

P34

C	-1.80604	-0.02733	-0.12931
O	-1.98342	0.83799	-0.94604
O	-2.80983	-0.74168	0.41496
C	-4.11475	-0.4053	-0.05263
H	-4.18526	-0.56287	-1.12964
H	-4.7975	-1.06463	0.47695
H	-4.34018	0.63896	0.16747
C	-0.50905	-0.42351	0.38293
H	-0.47009	-1.20068	1.13785
C	0.71493	0.29896	-0.05681
H	0.61147	0.53453	-1.1213
C	1.9324	-0.59555	0.13908
H	2.09561	-0.80628	1.20388
H	1.81984	-1.54234	-0.40059
C	0.8535	1.62702	0.71275
H	-0.02091	2.2532	0.53206
H	0.93887	1.43794	1.78627
H	1.74569	2.16013	0.38269
O	3.04438	0.10559	-0.37315
O	4.16185	-0.76153	-0.15791
H	4.87268	-0.21672	-0.51465

P35

C	-1.12784	-0.166	0.34811
O	-1.63993	0.41171	1.34189
O	-1.96525	-0.82313	-0.60678
C	-3.23163	-0.16151	-0.66534
H	-3.0884	0.85762	-0.95817
H	-3.85823	-0.65321	-1.37984
H	-3.69585	-0.19389	0.29817

C	0.40066	-0.16532	0.16031
H	0.68904	0.69007	-0.41418
C	1.0871	-0.11366	1.53789
H	0.79872	-0.96905	2.11239
C	2.6156	-0.11297	1.35009
H	3.15102	-1.0388	1.31737
H	3.1422	0.81333	1.25231
C	0.66008	1.16845	2.27644
H	0.94846	2.02384	1.70195
H	-0.40194	1.16797	2.40693
H	1.13701	1.20435	3.2336
O	0.79719	-1.35585	-0.52549
O	2.10733	-1.35526	-0.68647
H	2.37353	-2.15449	-1.14686

P36

C	1.14707	0.05423	0.54545
O	0.82468	-0.99869	1.15454
O	2.49443	0.24099	0.10425
C	3.08155	-1.03024	-0.18583
H	2.51843	-1.51599	-0.95514
H	4.08971	-0.8905	-0.51596
H	3.07584	-1.63544	0.69655
C	0.09061	1.14163	0.27518
C	0.45265	2.38904	-0.55217
H	1.26156	2.15641	-1.21282
H	-0.39769	2.69685	-1.12407
H	0.74564	3.18055	0.10552
C	-1.38188	0.90826	0.66108
H	-1.88116	0.39267	-0.13251
H	-1.42774	0.31949	1.55335
C	-2.06976	2.26434	0.90495
H	-2.02389	2.8531	0.01268
H	-1.57048	2.77993	1.69854
O	-3.43707	2.04763	1.26329
O	-4.02668	3.20998	1.47232
H	-4.94459	3.0645	1.71288

P37

C	1.10099	-0.26282	0.4681
O	1.18886	-1.17405	1.33152
O	2.17995	-0.03371	-0.44199
C	2.86921	-1.26318	-0.68332
H	2.19132	-1.97513	-1.1058
H	3.67654	-1.09175	-1.36429
H	3.25551	-1.6426	0.23956
C	-0.16849	0.6056	0.39155
H	-0.87129	0.15191	-0.27564
C	-0.79455	0.72429	1.79354
H	-1.05028	-0.2503	2.15363
H	-0.09175	1.17798	2.46074
C	-2.06403	1.59271	1.717
H	-1.8083	2.56731	1.35691
H	-2.76683	1.13903	1.0498
C	-2.69009	1.71141	3.11899
H	-2.39924	2.5101	3.76891
H	-3.41591	0.99518	3.44317
O	0.17328	1.90809	-0.08969
O	-0.91485	2.65245	-0.1553
H	-0.68541	3.52685	-0.47837

P38

C	-1.34786	0.39135	0.03966
O	-1.82692	1.30106	0.66806
O	-2.073	-0.66311	-0.38288
H	3.14066	-1.66769	1.053
C	0.60177	-1.13885	0.00773
H	0.02953	-1.89847	-0.53113
O	2.78352	-0.8496	0.67717
O	1.95008	-1.38149	-0.35284
C	-3.45827	-0.61412	-0.03975
H	-3.93069	0.25986	-0.493
H	-3.89456	-1.53218	-0.429
H	-3.58067	-0.55586	1.04367
H	0.48456	-1.30472	1.08589
C	0.10657	0.26185	-0.38279
H	0.11386	0.31721	-1.48012
C	0.94492	1.4161	0.17884
H	0.30964	2.30703	0.22817
H	1.20616	1.18358	1.224
C	2.16635	1.70083	-0.62728
H	2.71036	2.6219	-0.4583
H	2.66086	0.91156	-1.17772

P39

C	-0.86568	0.00093	0.44587
O	-1.49176	-0.30786	1.49289
O	-0.45116	-1.01921	-0.46648
C	-1.37222	-2.11165	-0.41057
H	-2.34939	-1.76841	-0.67931
H	-1.06206	-2.87497	-1.09324
H	-1.3944	-2.50899	0.58267
C	-0.54592	1.47744	0.14708
H	-1.34564	1.9082	-0.41841
C	-0.38215	2.24545	1.47182
H	-1.29026	2.18395	2.03436
H	0.41757	1.81469	2.03731
C	-0.06238	3.72196	1.17303
H	-0.86211	4.15273	0.60754
H	0.84573	3.78346	0.61049
C	0.76108	1.56595	-0.66256
H	1.39331	2.42375	-0.56579
H	1.03697	0.76965	-1.32187
O	0.08969	4.43512	2.40315
O	0.36377	5.7007	2.14704
H	0.46586	6.17946	2.97285

P40

C	1.44709	0.26493	0.12793
O	0.86959	-0.85249	0.16587
O	2.84041	0.36049	0.43524
C	3.49305	-0.85942	0.07361
H	3.37017	-1.03236	-0.97515
H	4.5356	-0.78793	0.30355
H	3.06172	-1.67079	0.62183
C	0.65333	1.5295	-0.24945
H	1.12069	2.48926	-0.17641
C	-0.8745	1.47042	-0.43343
H	-1.10791	0.87012	-1.28787
H	-1.32229	1.04008	0.43788
C	-1.42191	2.8947	-0.64171
H	-1.1885	3.495	0.21273
H	-0.97412	3.32504	-1.51302
C	-2.94974	2.83563	-0.82569

H	-3.18315	2.23533	-1.68012
H	-3.39753	2.40529	0.04563
O	-3.45805	4.15817	-1.01908
O	-4.76762	4.10754	-1.17678
H	-5.10886	4.9954	-1.30661

P41

C	0.54186	0.62303	0.01674
O	1.39857	1.39478	0.34749
O	0.76621	-0.69429	-0.23766
H	-1.19235	-1.5614	0.40578
O	-1.86243	-0.89098	0.61548
O	-1.75714	-0.05165	-0.52927
C	2.05948	-1.13878	-0.14286
H	2.14423	-2.2122	-0.18937
H	2.78176	-0.47986	0.31343
C	-0.91403	1.00925	-0.17791
H	-0.96525	1.71971	-1.00886
H	-1.25392	1.50993	0.73489

P42

C	0.51798	-0.51454	-0.27352
O	1.09272	-1.43487	-0.78756
O	1.15164	0.49578	0.38273
C	2.51591	0.41902	0.48784
H	2.96406	1.32633	0.85902
H	3.02348	-0.32154	-0.11069
C	-1.01497	-0.36907	-0.25136
H	-1.29126	0.56323	-0.69787
C	-1.65192	-1.5262	-1.04316
H	-2.71624	-1.41607	-1.04163
H	-1.29299	-1.5088	-2.05101
H	-1.38908	-2.45772	-0.58698
O	-1.47773	-0.40549	1.10121
O	-2.6671	0.16222	1.17542
H	-3.00138	0.08972	2.07241

P43

C	-0.9132	0.15935	0.07164
O	-1.38708	1.10765	0.64454
O	-1.64205	-0.89252	-0.36588
C	-2.99758	-0.8589	-0.17086
H	-3.47854	-1.79675	-0.397
H	-3.38614	-0.11835	0.5112
C	0.57647	-0.02028	-0.27508
H	0.68958	-0.09075	-1.33675
C	1.37448	1.18893	0.24703
H	1.0106	2.0828	-0.21499
H	1.25702	1.26257	1.30802
C	2.86527	1.00562	-0.0929
H	2.98254	0.9303	-1.15378
H	3.41949	1.84658	0.26839
H	3.22958	0.11263	0.37051
O	1.06755	-1.21572	0.33701
O	1.69378	-1.94765	-0.56551
H	2.03756	-2.74243	-0.1511

P44

C	-1.12582	-0.61988	0.32158
O	-1.28206	-1.67447	0.87399
O	-2.05449	-0.06061	-0.50354
C	-3.20481	-0.77168	-0.72613

H	-3.95933	-0.20529	-1.24747
H	-3.40128	-1.6185	-0.08687
C	0.15194	0.23112	0.44302
H	-0.09989	1.20117	0.81783
C	1.13485	-0.45383	1.41066
H	1.39642	-1.41882	1.02952
H	0.67361	-0.5623	2.37003
C	2.40513	0.4062	1.54608
H	2.8642	0.51796	0.58605
H	2.14407	1.36985	1.93094
C	3.39041	-0.28156	2.5093
H	3.65196	-1.24495	2.12412
H	4.27274	0.3163	2.60389
H	2.9311	-0.3939	3.46916
O	0.76226	0.36094	-0.84366
O	0.82861	1.63744	-1.17311
H	1.22888	1.72393	-2.04138

P45

C	0.59101	-0.51704	-0.19991
O	0.96398	-1.45737	-0.84675
O	1.44314	0.38055	0.37235
H	0.27393	2.18608	-0.26616
O	-0.62272	1.95683	-0.55795
O	-1.03658	1.1326	0.52727
C	2.78623	0.15714	0.21894
H	3.39322	0.98764	0.5413
H	3.09175	-0.58795	-0.49949
C	-0.87041	-0.22204	0.14136
C	-1.22543	-1.0118	1.40127
H	-2.26157	-0.79983	1.67415
H	-1.11478	-2.08077	1.20849
H	-0.57361	-0.72171	2.22845
C	-1.75862	-0.58539	-1.04031
H	-1.59615	-1.62585	-1.32526
H	-2.80319	-0.43977	-0.75645
H	-1.52893	0.05599	-1.89243

P46

C	0.89767	-0.53685	-0.19906
O	1.16612	-1.52497	-0.82651
O	1.83859	0.35609	0.22303
H	0.67742	2.18352	-0.30272
O	-0.26056	1.99975	-0.47129
O	-0.56883	1.1972	0.66398
C	3.14317	0.09775	-0.10781
H	3.84169	0.74119	0.40313
H	3.37707	-0.88762	-0.48105
C	-0.50697	-0.16674	0.27828
C	-0.76639	-0.92316	1.58207
H	-1.72538	-0.60987	1.99831
H	-0.78734	-1.99726	1.38657
H	0.01778	-0.70148	2.30961
C	-1.51579	-0.49547	-0.82777
H	-1.39572	-1.55086	-1.08797
H	-1.23681	0.08613	-1.71086
C	-2.95293	-0.17686	-0.42985
H	-3.61695	-0.28601	-1.2901
H	-3.31821	-0.84599	0.35411
H	-3.02868	0.85171	-0.06787

P47

O	-1.24663	1.34211	0.02912
O	-2.24661	-0.6805	-0.00444
C	-3.48626	-0.10109	0.0216
H	-3.54749	0.96198	-0.1542
H	-4.28247	-0.80204	-0.17034
C	-1.16648	0.14196	0.01479
C	0.11058	-0.65434	0.01592
H	0.12463	-1.29443	0.90424
H	0.11577	-1.32304	-0.85031
C	1.31754	0.26616	-0.00856
H	1.3292	0.87576	-0.91767
H	1.31468	0.94032	0.85674
O	2.44507	-0.58931	0.02199
O	3.58879	0.24256	-0.1327
H	3.96842	0.2063	0.75733

P48
C	0.98881	-0.67677	-0.21831
O	1.41908	-1.35982	0.74702
O	1.84816	0.26358	-0.86804
C	2.80003	0.76827	0.07225
H	3.18751	1.75949	-0.03839
H	3.12478	0.15468	0.88647
C	-0.46322	-0.85354	-0.69995
H	-1.09983	-0.17651	-0.16961
H	-0.5187	-0.64798	-1.74855
C	-0.91915	-2.30056	-0.43567
H	-0.28254	-2.97759	-0.96601
C	-2.37118	-2.47733	-0.91731
H	-2.68796	-3.48274	-0.73369
H	-3.00779	-1.80031	-0.38697
H	-2.42665	-2.27178	-1.96592
O	-0.84501	-2.57527	0.96573
O	-1.23581	-3.81558	1.19225
H	-1.18603	-4.	2.13306

P49
C	1.21652	-0.84534	-0.08268
O	1.65172	-1.69319	0.64588
O	1.9796	0.19643	-0.54525
C	3.27718	0.27136	-0.10876
H	3.86746	0.98747	-0.65788
H	3.67781	-0.58713	0.40793
C	-0.23657	-0.73217	-0.57999
H	-0.67004	0.17411	-0.21167
H	-0.24775	-0.72379	-1.6499
C	-1.0497	-1.93542	-0.06754
H	-0.60569	-2.8425	-0.42103
C	-2.49626	-1.8358	-0.58631
H	-2.49274	-1.84294	-1.65628
H	-2.93854	-0.9262	-0.23716
C	-3.31134	-3.03507	-0.06765
H	-4.31618	-2.96636	-0.42888
H	-2.86851	-3.9447	-0.41603
H	-3.31566	-3.0274	1.00231
O	-1.0549	-1.93295	1.36245
O	-1.26978	-3.15806	1.80441
H	-1.33985	-3.14568	2.76177

P50
| C | 0.8675 | -0.36028 | -0.25013 |
| O | 0.65275 | -1.31592 | -0.94955 |

O	2.02643	-0.19992	0.44225
C	2.96104	-1.1941	0.35771
H	3.90897	-0.92207	0.7933
H	2.82566	-1.94799	-0.40227
C	-0.05465	0.8412	-0.08347
C	0.3931	1.89823	-1.10705
H	-0.25361	2.77776	-1.03868
H	1.42032	2.21081	-0.90268
H	0.34373	1.50567	-2.12683
C	0.00173	1.41492	1.33632
H	1.00104	1.79104	1.56197
H	-0.71047	2.24177	1.41662
H	-0.26769	0.6602	2.07746
C	-1.48162	0.38017	-0.43389
H	-1.74963	-0.45131	0.18396
H	-1.51932	0.08713	-1.46229
O	-2.39811	1.45491	-0.21059
O	-3.62066	1.0622	-0.51644
H	-4.23538	1.78495	-0.37032

P51

C	-0.85793	-0.17499	0.15795
O	-0.64699	-0.90909	1.08746
O	-2.0034	-0.2074	-0.57194
C	-2.94539	-1.13951	-0.23322
H	-3.88264	-1.00041	-0.74736
H	-2.8323	-1.64671	0.71259
C	-0.42536	2.27048	0.26294
H	0.20773	3.08787	-0.08985
H	-1.45431	2.47451	-0.03964
H	-0.38334	2.24662	1.35581
C	0.05476	0.93473	-0.32038
H	-0.001	0.97148	-1.41311
C	1.49802	0.61732	0.11303
H	1.76878	-0.35752	-0.23522
H	1.56426	0.64582	1.1806
O	2.38779	1.58731	-0.44582
O	3.63603	1.21617	-0.23009
H	4.23337	1.86605	-0.60753

P52

C	-1.04643	-0.11754	0.06038
O	-0.96225	-1.1612	0.66419
O	-2.22303	0.34381	-0.42587
C	-3.3405	-0.4258	-0.24972
H	-4.25012	0.08058	-0.52859
H	-3.28009	-1.25188	0.44145
C	-0.16353	2.17847	0.50122
H	0.56437	2.92739	0.18422
H	-1.16267	2.56119	0.28647
H	-0.06796	2.04192	1.58312
C	1.4139	0.19689	0.12215
H	1.40413	-0.09595	1.17699
O	1.5098	-0.99734	-0.6586
O	1.65484	-2.11391	0.20657
H	0.72617	-2.24996	0.46794
C	0.07842	0.85311	-0.23288
H	0.05666	1.0357	-1.31509
C	2.6219	1.07153	-0.17357
H	2.61816	1.38821	-1.22113
H	2.64476	1.95993	0.46241
H	3.52917	0.49207	0.00656

P53

C	1.35726	-0.51768	-0.03129
O	1.64628	-0.97805	1.04359
O	2.1302	0.39198	-0.67753
C	3.26267	0.82202	-0.04733
H	3.89731	1.42231	-0.67872
H	3.59559	0.27418	0.82073
C	0.09914	-0.86323	-0.84941
H	-0.47883	0.02344	-1.00648
H	0.3895	-1.27183	-1.79473
C	-0.74506	-1.89683	-0.0809
C	-1.16289	-1.30878	1.27969
H	-0.50061	-1.66516	2.0408
H	-1.1148	-0.24073	1.23653
H	-2.16355	-1.61186	1.50708
O	-1.91335	-2.21764	-0.84055
O	-2.67336	-1.14441	-0.95439
H	-3.46414	-1.36312	-1.45283
C	0.08675	-3.17301	0.14509
H	0.83943	-3.24686	-0.61183
H	0.55198	-3.12971	1.10768
H	-0.55321	-4.02915	0.09643

P54

C	-1.14444	-0.48335	0.13406
O	-1.26013	-0.45358	1.33056
O	-1.86924	0.29985	-0.70633
C	-2.777	1.15419	-0.14566
H	-3.17411	1.86691	-0.85098
H	-2.71095	1.32321	0.91855
C	-0.21807	-1.43407	-0.64669
H	-0.8079	-2.08321	-1.25958
H	0.44133	-0.86154	-1.26499
C	0.60815	-2.27454	0.34455
H	-0.05047	-2.86206	0.94949
H	1.18291	-1.62456	0.97071
C	1.55506	-3.20492	-0.43606
H	0.98062	-3.85066	-1.06688
H	2.21781	-2.61718	-1.03625
O	2.31631	-3.99132	0.48426
O	3.12715	-4.79005	-0.1843
H	3.63805	-5.31813	0.43353

P55

C	-1.4423	-0.56301	0.12616
O	-1.50468	-0.63017	1.32528
O	-2.25606	0.22806	-0.62032
C	-3.18351	0.98192	0.04254
H	-3.66113	1.7124	-0.59113
H	-3.07145	1.08392	1.11153
C	-0.48813	-1.38307	-0.76191
H	-1.05851	-2.02248	-1.40279
H	0.10476	-0.71952	-1.35612
C	0.43363	-2.23787	0.12763
H	0.99094	-1.59957	0.78098
H	-0.15817	-2.91387	0.70874
C	1.40503	-3.03842	-0.75956
H	2.00078	-2.36229	-1.33648
C	2.32134	-3.89944	0.12962
H	2.99686	-4.455	-0.48676
H	2.87814	-3.26539	0.78753

H	1.72566	-4.57618	0.70589
O	0.66002	-3.88588	-1.638
O	1.47979	-4.4534	-2.50304
H	0.9974	-5.09733	-3.02673

P56

C	-0.69688	0.86595	0.0701
O	-0.8731	1.3725	1.14636
O	0.2384	1.29228	-0.8185
C	1.13729	2.22612	-0.37967
H	1.95562	2.36796	-1.06811
H	1.22571	2.35579	0.68915
C	-1.45597	-0.35626	-0.47909
H	-0.77074	-1.16454	-0.62752
C	-2.54107	-0.78147	0.52757
H	-3.21456	0.03366	0.69154
H	-2.08064	-1.05554	1.45374
C	-3.31951	-1.98538	-0.03477
H	-2.64514	-2.79876	-0.20368
H	-3.78427	-1.70973	-0.9583
C	-2.11617	0.01008	-1.8213
H	-2.60389	-0.85206	-2.22594
H	-2.83577	0.78633	-1.66471
H	-1.36755	0.35052	-2.50583
O	-4.32249	-2.38464	0.90306
O	-4.89738	-3.49741	0.48636
H	-5.57105	-3.76518	1.11571

P57

C	-1.13135	-0.72149	0.16662
O	-1.3125	-0.70936	1.35547
O	-2.06963	-0.33163	-0.7352
C	-3.26975	0.10203	-0.24569
H	-3.89444	0.55026	-1.00218
H	-3.321	0.34322	0.80533
C	1.38694	-0.78485	0.23034
H	1.191	-0.89936	1.30238
C	0.12044	-1.2135	-0.51842
H	0.1329	-0.86806	-1.55626
H	0.05777	-2.30869	-0.53453
C	2.58544	-1.64414	-0.16865
H	2.41501	-2.69119	0.09433
H	2.76015	-1.59127	-1.24868
C	1.70467	0.69443	-0.05666
H	1.50127	0.90995	-1.08481
H	1.09625	1.31712	0.56542
H	2.73727	0.88404	0.14998
O	3.77712	-1.21136	0.49277
O	4.75137	-2.06856	0.25099
H	5.55192	-1.77693	0.69334

P58

C	-1.56593	0.11348	0.002
O	-1.64576	1.31847	0.01585
O	-0.37988	-0.53652	0.02191
C	-2.68815	-0.79973	-0.02047
H	-2.52671	-1.86658	-0.05224
H	-3.68105	-0.37851	-0.04116
C	0.75242	0.30305	0.01396
H	0.77577	0.91382	-0.89282
H	0.78579	0.93654	0.90351
O	1.81259	-0.61913	0.01131

O	2.97126	0.21079	-0.09117
H	3.59056	-0.29503	0.44654

P59

C	0.60909	0.49296	0.12655
O	-0.15503	1.44088	0.24446
O	0.21365	-0.79577	0.17169
C	2.04243	0.63529	-0.07773
H	2.31818	0.17514	-1.00354
C	2.4092	2.13042	-0.11831
H	2.12714	2.59204	0.80486
H	3.46438	2.23506	-0.26163
H	1.89091	2.603	-0.92636
C	-1.16553	-1.05387	0.44765
H	-1.7705	-0.61741	-0.31943
H	-1.42599	-0.62686	1.39355
O	-1.38809	-2.46596	0.48463
O	-2.66263	-2.70482	0.73144
H	-2.81212	-3.6528	0.75586

P60

C	0.45452	0.3578	-0.00453
O	0.38984	1.56687	0.02235
O	-0.64928	-0.42883	-0.01766
C	1.67791	-0.41331	-0.02365
H	1.60326	-1.49344	-0.05403
C	2.99013	0.2808	-0.01548
H	3.0115	0.97805	0.83101
H	3.04802	0.92783	-0.901
C	4.17654	-0.67697	0.03196
H	5.11846	-0.12842	0.03627
H	4.1434	-1.2961	0.93042
H	4.17786	-1.3405	-0.83491
C	-1.8698	0.27096	-0.00818
H	-1.9736	0.89089	-0.9021
H	-1.96273	0.88303	0.89346
O	-2.81966	-0.76893	-0.01284
O	-4.07711	-0.10885	-0.0698
H	-4.4924	-0.41905	0.74379

P61

C	0.3524	-0.38192	-0.29396
O	0.56204	0.75391	-0.69893
O	1.3262	-1.2251	0.10237
C	-0.96313	-0.97498	-0.18878
H	-1.03089	-1.98566	0.19863
C	-2.22977	-0.18732	-0.57194
H	-2.30719	0.68476	0.04319
H	-2.17072	0.10511	-1.59951
C	-3.46998	-1.07569	-0.36149
H	-3.53294	-1.36232	0.66748
H	-3.38921	-1.95119	-0.97132
C	-4.73579	-0.29148	-0.75431
H	-5.59749	-0.90873	-0.60811
H	-4.81657	0.58401	-0.14447
H	-4.67282	-0.00483	-1.78327
C	2.67948	-0.78322	-0.03278
H	2.82964	0.09317	0.56244
H	2.87967	-0.55598	-1.05903
O	3.56452	-1.81628	0.40811
O	4.81307	-1.40036	0.30547
H	5.40714	-2.09323	0.60312

P62

C	-0.14945	0.2207	-0.08432
O	-0.46791	-0.83141	-0.6233
O	-1.03383	1.17367	0.27205
C	2.35672	-0.31642	-0.05929
H	1.94716	-1.24816	-0.46214
C	3.14768	-0.62045	1.2214
H	3.98438	-1.28856	0.99881
H	3.55579	0.30106	1.64997
H	2.51691	-1.09797	1.97506
C	1.21174	0.58459	0.2417
H	1.38106	1.55004	0.70885
C	3.26935	0.32508	-1.1172
H	3.68261	1.26957	-0.74803
H	4.10423	-0.34233	-1.34876
H	2.72367	0.52745	-2.04203
C	-2.4068	0.96295	-0.06775
H	-2.76173	0.07649	0.41507
H	-2.49896	0.85285	-1.12807
O	-3.18225	2.08409	0.36425
O	-4.45365	1.87806	0.0753
H	-4.9745	2.62984	0.3671

P63

C	-0.75562	-0.50943	-0.0102
O	-0.6673	-1.71258	-0.00745
O	0.34469	0.2879	-0.00534
C	-1.98784	0.24911	-0.01832
C	-1.97083	1.73903	-0.00167
H	-1.18835	2.13911	-0.64822
H	-2.93863	2.13781	-0.30932
H	-1.76047	2.11084	1.00911
C	-3.27621	-0.4916	0.01231
H	-3.88074	-0.23885	-0.86619
H	-3.11387	-1.56753	0.03578
H	-3.86404	-0.19738	0.8896
C	1.56836	-0.40309	-0.0004
H	1.68036	-1.01674	-0.89853
H	1.67148	-1.01654	0.89909
O	2.50702	0.64421	0.00518
O	3.76204	-0.03835	0.02822
H	4.35542	0.69572	-0.16656

P64

C	-0.3428	-0.45845	-0.21966
O	-0.28678	-1.66997	-0.26117
O	0.77294	0.30514	-0.06363
C	-1.54661	0.34094	-0.321
C	-1.48208	1.82538	-0.19734
H	-2.43255	2.27886	-0.48226
H	-1.25418	2.12435	0.83355
H	-0.6833	2.24014	-0.81575
C	-2.85564	-0.36034	-0.44344
H	-3.43525	0.11014	-1.24668
H	-2.68739	-1.40341	-0.71218
C	-3.65866	-0.27953	0.8663
H	-4.63013	-0.76295	0.74925
H	-3.121	-0.78092	1.67384
H	-3.82872	0.75886	1.16078
C	1.97389	-0.41777	0.02672
H	1.9791	-1.06313	0.91034

H	2.15122	-1.00597	-0.87732
O	2.93538	0.60729	0.14307
O	4.18593	-0.06635	0.12642
H	4.55377	0.1938	0.97939

P65

C	0.72406	-0.11217	-0.09514
O	0.36163	1.02219	-0.31341
O	-0.1001	-1.16573	-0.04648
C	2.1535	-0.52802	0.15983
H	2.1639	-1.0338	1.13756
H	2.39295	-1.32358	-0.5607
C	3.10898	0.60612	0.09451
H	2.74522	1.6113	-0.06221
H	4.16551	0.43016	0.23816
C	-1.48377	-0.9489	-0.33518
H	-1.89319	-0.2623	0.37606
H	-1.58329	-0.5435	-1.32039
O	-2.18728	-2.19147	-0.25773
O	-3.46736	-1.98946	-0.50869
H	-3.93982	-2.82347	-0.45571

P66

C	-0.41468	0.13063	-0.02815
O	0.08892	1.12274	0.45139
O	0.25904	-1.00073	-0.27384
C	-1.87683	-0.00858	-0.40209
H	-1.89079	-0.39951	-1.43001
C	-2.58229	1.29921	-0.32289
H	-2.10721	2.15304	0.13831
H	-3.61401	1.36377	-0.64196
C	-2.52894	-1.08247	0.4996
H	-3.57862	-1.20188	0.22309
H	-2.02353	-2.04398	0.38926
H	-2.48707	-0.77238	1.54707
C	1.63137	-1.06743	0.12259
H	2.19037	-0.31966	-0.40015
H	1.70688	-0.89761	1.17632
O	2.15571	-2.36043	-0.19063
O	3.44876	-2.38733	0.07334
H	3.80238	-3.25281	-0.14459

P67

C	-0.53256	0.60939	-0.01842
O	-0.40632	1.80276	-0.02057
O	0.53041	-0.22261	-0.00343
C	-1.84261	-0.16561	-0.00875
C	-2.98594	0.78664	-0.13079
H	-2.83324	1.85488	-0.09717
H	-3.98816	0.38349	-0.19395
C	-1.92599	-0.93801	1.32878
H	-2.86911	-1.48744	1.36296
H	-1.10114	-1.64764	1.41649
H	-1.90021	-0.25087	2.17716
C	-1.85064	-1.1737	-1.17583
H	-1.7507	-0.66105	-2.13482
H	-1.03885	-1.89505	-1.07305
H	-2.80183	-1.71058	-1.17397
C	1.78676	0.41452	0.00451
H	1.91433	1.0399	-0.88226
H	1.91761	1.0061	0.91523
O	2.67973	-0.67464	-0.02321

| O | 3.96796 | -0.07849 | -0.08055 |
| H | 4.38295 | -0.44721 | 0.70847 |

P68

C	0.02934	0.22005	-0.07278
O	0.59061	1.08978	0.55791
O	0.61452	-0.92348	-0.45093
C	-1.45598	0.2567	-0.47784
H	-1.98053	-0.53307	0.01815
C	-2.06537	1.61161	-0.0723
H	-1.99948	1.72891	0.98921
H	-1.52797	2.40245	-0.55257
C	-3.54306	1.65946	-0.5033
H	-4.07875	0.8636	-0.02944
H	-3.9687	2.59762	-0.21421
H	-3.60841	1.5504	-1.56572
C	-1.57695	0.07512	-2.00231
H	-2.61021	0.07238	-2.28029
H	-1.12838	-0.85347	-2.2876
C	1.95267	-1.17047	-0.01133
H	2.60016	-0.40975	-0.39468
H	1.98438	-1.1602	1.05815
O	2.3831	-2.44786	-0.48872
O	3.6114	-2.68473	-0.06731
H	3.89971	-3.54304	-0.38634

P69

C	0.24345	0.76083	0.13603
O	-0.54045	1.55522	-0.33461
O	-0.03817	-0.65552	0.30477
C	1.67523	1.10407	0.58746
H	1.80045	0.83124	1.61449
H	2.37753	0.56459	-0.01307
C	1.91601	2.61644	0.42505
H	1.80113	2.88744	-0.60367
C	3.34266	2.96203	0.89071
H	3.51179	4.01198	0.77288
H	3.45587	2.69593	1.92089
H	4.05157	2.41828	0.3019
C	-1.28561	-1.15421	-0.18524
H	-2.08986	-0.66545	0.32389
H	-1.35891	-0.96186	-1.23526
O	-1.36026	-2.56314	0.04762
O	-2.5241	-3.01886	-0.37688
H	-2.57509	-3.96434	-0.21855

P70

C	-0.01389	0.02918	0.05626
O	-0.4162	-0.94823	0.64912
O	-0.81331	1.00669	-0.39274
C	2.30002	-0.87504	-0.0455
H	1.92661	-1.67109	0.58741
C	3.73833	-0.82655	-0.42754
H	4.13988	-1.82838	-0.59993
H	3.88941	-0.23783	-1.33994
H	4.3633	-0.36523	0.3532
C	1.44086	0.32979	-0.23593
H	1.48726	0.67169	-1.2802
C	1.88204	1.52005	0.65068
H	1.81575	1.24763	1.7077
H	2.92021	1.77655	0.42806
H	1.25761	2.39696	0.46607

```
C        -2.20582   0.93315  -0.07589
H        -2.62356   0.0477   -0.50759
H        -2.3288    0.90414   0.98663
O        -2.87571   2.08175  -0.60208
O        -4.17513   1.96419  -0.40188
H        -4.62549   2.73212  -0.76113
```

P71
```
C         0.29597   0.68321  -0.18801
O         1.14593   1.45565   0.19671
O         0.46651  -0.64493  -0.26299
C         1.69608  -1.19789   0.23832
H         1.81694  -0.93997   1.29315
H         1.56793  -2.26976   0.08351
O         2.80812  -0.79093  -0.4778
O         3.53344   0.18008   0.26783
H         2.93793   0.95174   0.19498
C        -1.13495   1.08886  -0.58742
H        -1.33992   0.74341  -1.57916
H        -1.8334    0.65051   0.09443
C        -1.26563   2.6226   -0.54082
H        -1.08013   2.96626   0.45537
C        -2.68812   3.0298   -0.96778
H        -3.40061   2.58425  -0.3054
H        -2.87076   2.6931   -1.96687
C        -2.82231   4.56286  -0.91014
H        -3.81095   4.84573  -1.2059
H        -2.63875   4.89965   0.08875
H        -2.11045   5.00838  -1.57322
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P72
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C         0.01346  -0.24101   0.55197
O         0.48287  -1.27906   0.13356
O         0.58659   0.95966   0.38928
C         1.78619   1.0304   -0.40092
H         1.59374   0.64192  -1.40395
H         2.02108   2.09518  -0.40352
O         2.85234   0.35618   0.16889
O         3.07774  -0.86604  -0.52468
H         2.30391  -1.38855  -0.23508
C        -1.36842  -0.13074   1.22267
H        -1.27271   0.38821   2.15349
H        -2.03436   0.40753   0.58105
C        -1.92959  -1.5421    1.47715
C        -3.284    -1.43301   2.20192
H        -3.96549  -0.86773   1.60115
H        -3.68102  -2.41309   2.36535
H        -3.14653  -0.94241   3.14283
C        -0.94213  -2.33722   2.3514
H        -0.3263   -2.95      1.72678
H        -0.32645  -1.65744   2.90251
H        -1.48756  -2.95668   3.03234
```

P73
```
C         0.52215   0.94554  -0.08668
O         0.18116   2.04641   0.26505
O        -0.35795  -0.06841  -0.24273
C        -1.6978    0.2764    0.0333
H        -2.0644    1.0235   -0.67804
H        -1.798     0.65454   1.05769
O        -2.37415  -0.9469   -0.13423
O        -3.74801  -0.61148   0.01937
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H	-3.95681	-1.06529	0.84894
C	1.95896	0.49845	-0.41423
H	2.24323	-0.29736	0.2421
H	2.00436	0.15835	-1.42773
C	2.92127	1.68621	-0.22774
H	2.87637	2.02587	0.78592
H	2.63658	2.48228	-0.88359
C	4.35794	1.23938	-0.55625
H	4.64258	0.44322	0.0995
H	4.40286	0.89984	-1.56996

P74

C	0.29517	-0.45878	0.05526
O	0.21581	-1.58193	0.4871
O	-0.79656	0.28884	-0.2161
C	-2.02474	-0.34441	0.06744
H	-2.11261	-0.56925	1.13544
H	-2.13127	-1.26572	-0.51805
O	-2.96853	0.62486	-0.32149
O	-4.22319	0.05588	0.03186
H	-4.60339	-0.1108	-0.84315
C	1.5706	0.30145	-0.23314
H	1.50676	0.63553	-1.27754
C	2.78391	-0.61798	-0.06279
H	2.60639	-1.53956	-0.63922
H	2.84002	-0.94038	0.98337
C	4.05331	0.03822	-0.48253
H	4.08014	0.63683	-1.38667
H	4.99984	-0.25256	-0.04619
C	1.6488	1.54249	0.66612
H	1.66719	1.24566	1.71963
H	2.56969	2.09103	0.45481
H	0.79468	2.20213	0.50441

P75

C	-0.17423	0.08047	-0.33123
O	-0.1707	1.14037	-0.90675
O	0.95694	-0.50889	0.1074
C	2.13894	0.20948	-0.17445
H	2.1078	1.20354	0.28754
H	2.29235	0.30448	-1.25446
O	3.135	-0.59714	0.40695
O	4.35398	0.05757	0.07491
H	4.65519	0.33882	0.95114
C	-2.70671	0.01155	-0.18556
H	-2.67162	0.49119	-1.17258
C	-3.86982	-0.92385	-0.12965
H	-4.09277	-1.58065	-0.96214
H	-4.38304	-1.10155	0.80874
C	-1.38717	-0.76655	-0.03142
H	-1.28658	-1.18209	0.97684
H	-1.35495	-1.62021	-0.71952
C	-2.81929	1.10329	0.88066
H	-2.82206	0.65699	1.88185
H	-1.98584	1.80593	0.81281
H	-3.75059	1.66195	0.75963

P76

C	-0.36566	0.64388	0.04448
O	-1.11256	1.47875	-0.41807
O	-0.73735	-0.75742	0.23943
C	1.07784	0.92192	0.5034

H	1.17079	0.69556	1.54504
H	1.75413	0.31013	-0.05628
C	1.41421	2.40629	0.26864
H	0.74456	3.01787	0.83648
H	1.31115	2.63518	-0.7715
C	2.86269	2.68101	0.71365
H	3.53242	2.0702	0.14508
C	3.19855	4.16572	0.48032
H	2.53054	4.77646	1.05098
H	4.20583	4.356	0.78703
H	3.09263	4.39627	-0.55916
C	-2.03142	-1.17638	-0.20186
H	-2.78323	-0.62895	0.3273
H	-2.12763	-0.99121	-1.25131
O	-2.19218	-2.57441	0.05221
O	-3.39494	-2.95704	-0.33425
H	-3.5035	-3.89521	-0.16206

P77

C	0.07072	0.28898	-0.00495
O	0.09196	1.49345	0.02725
O	1.19478	-0.45789	-0.02507
C	2.39294	0.28733	-0.00969
H	2.45418	0.90546	0.89403
H	2.4725	0.91969	-0.89998
O	3.37921	-0.71643	-0.01384
O	4.60842	-0.00208	-0.07049
H	4.98009	-0.20847	0.79951
C	-1.16198	-0.57801	-0.02876
H	-1.11677	-1.19429	-0.93476
H	-1.0929	-1.27872	0.81167
C	-2.4458	0.23821	0.02677
H	-2.46551	0.93839	-0.8156
H	-2.4501	0.85287	0.93254
C	-4.95666	0.13901	0.03064
H	-5.88524	-0.31363	0.35385
H	-5.00827	1.10601	-0.45663
C	-3.69277	-0.6478	-0.00554
H	-3.66663	-1.35411	0.83499
H	-3.65494	-1.27596	-0.9133

P78

C	-1.05249	-0.57263	0.32788
O	-1.2318	-1.60994	0.90198
O	-1.96041	-0.00229	-0.47902
C	-3.18371	-0.73305	-0.63012
H	-3.66523	-0.86285	0.33897
H	-3.80354	-0.13689	-1.29423
H	-2.98279	-1.71165	-1.06536
C	0.2436	0.22354	0.4306
H	0.41421	0.42056	1.49535
C	1.3988	-0.58619	-0.15234
H	1.23399	-0.71726	-1.22645
C	2.76069	0.08974	0.09428
H	2.74924	1.07958	-0.36588
H	2.87466	0.23624	1.175
O	0.20351	1.44112	-0.27555
O	-0.70226	2.31129	0.38251
H	-1.5215	2.13229	-0.10117
C	3.92665	-0.75478	-0.45247
H	4.84965	-0.24091	-0.28247
H	3.94746	-1.70036	0.04787

H   3.79294 -0.90984 -1.5027