Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

The photolysis of α-hydroperoxycarbonyls

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1. Initial generation and interconversions of 2-HPP-S1 conformers and 1,5 H-shifts

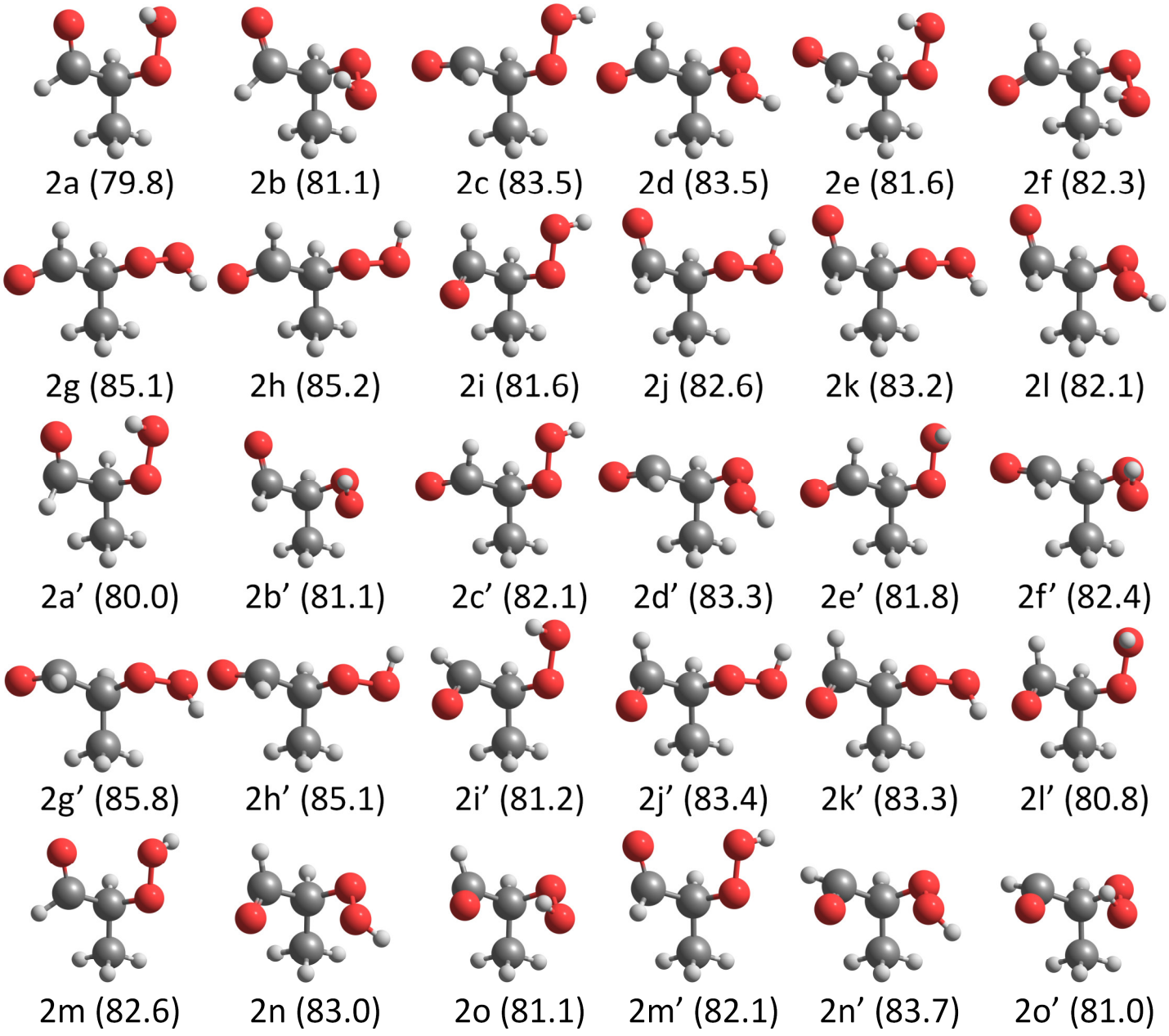


Figure S1. Geometries of the conformers (cfs) of 2-HPP(**2**) in excited S_1 state, at the TD-M06-2X-D3/6-311++G(2d,p) level of theory. 12 cfs (2a-2i) are directly generated by excitation of the 12 S_0 conformers; 18 other cfs (2m-2o, and 2a'-2o') are formed by conversions of the former. All the energies (kcal mol^{-1}, with ZPVE) are relative to the global minimum 2-HPP(1a).

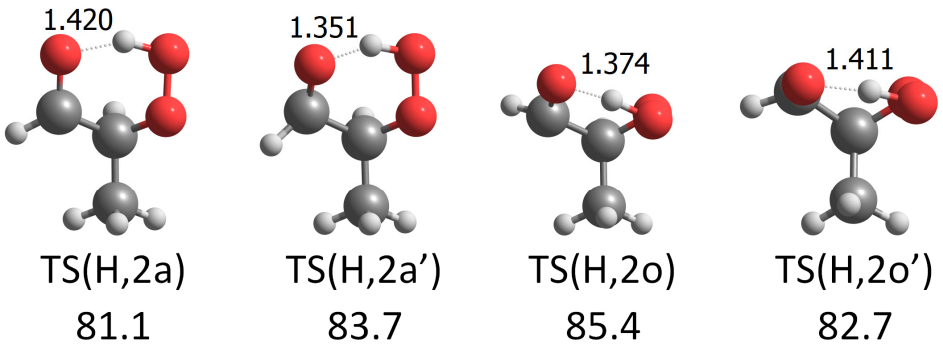


Figure S2. Geometries of the transition states of the exit channels of 2a, 2a', 2o and 2o' by 1,5 H-shifts, at the TD-M06-2X-D3/6-311++G(2d,p) level of theory. All the energies (kcal mol-1, with ZPVE) are relative to the global minimum 2-HPP(1a).

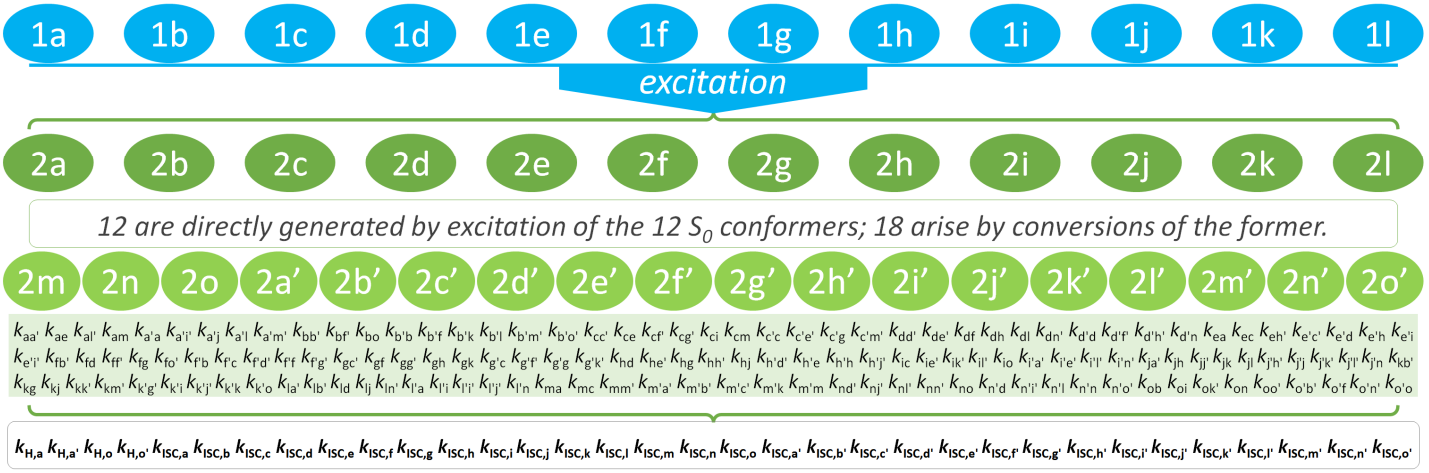


Figure S3. Schematic representation of the excitation of 2-HPP(S_0), interconversions of 2-HPP(S_1), exit channels of 2a, 2a', 2o and 2o' by 1,5 H-shifts, and exit channels of all conformers by intersystem crossing (ISC).

By taking into account the formation of 12 S_1 conformers at given fractions by direct excitation of 12 S_0 conformers, as well as 18 other S_1 conformers formed by interconversions of the former, we considered the quasi steady state for each conformer by equating the total rate of formation to the total rate of removal for each. We have located as many as 70 transition states that interconnect those 30 conformers. For each conformer we write out an algebraic equation that is linear in the concentrations of all the 30 conformers, includes the fractional formation rates U(z) of the 12 directly generated cfs, and contains the rate constants for forward-and-backward interconversions, the rate coefficient for intersystem crossing k(ISC), and the rate coefficient for the 1,5 H-shift for conformers 2a, 2a', 2o and 2o', which feature strong internal hydrogen bonds, and are determined to be the only four conformers leading to a facile direct 1,5 H-shift reaction.

We assume fractional formation rates U(z) of the 12 directly generated S_1 conformers equal to the fractional populations of their precursor S_0 conformer, for example U(2a) = 0.243, which is equal to the fractional thermal population of cf S_0-1a (see Table 1 of the paper). The fractional formation rates U(z) of all other 18 indirectly formed S_1 conformers are set equal to 0.

Solving the 30 equations, with all conformers z initially formed with their fractional rates U(z), then provides the total steady-state concentrations of all conformers, from which the overall H-shift rate and overall ISC rate and their ratio is obtained (see Table S1 and S2 below).

In addition, we can also derive the steady-state concentrations of each conformer when for example only **2a** is initially formed, i.e. with all other 29 fractional formation rates U(z) set equal to zero in the 29 other equations. From the steady-state concentration resulting from initially formed **2a** only, one can find the net removal rate constant of initially formed **2a**:

k(remove, z) ≡ U(z)/z

30 linear equations:

eqn1： u(a) - a*kisc - a*kh1 + a'*k(a'-a) + e*k(e-a) + l'*k(l'-a) + m*k(m-a) - a*k(a-a') - a*k(a-e) - a*k(a-l') - a*k(a-m) == 0
eqn2： u(a') - a'*kisc - a'*kh2 + a*k(a-a') + i'*k(i'-a') + j*k(j-a') + l*k(l-a') + m'*k(m'-a') - a'*k(a'-a) - a'*k(a'-i') - a'*k(a'-j) - a'*k(a'-l) - a'*k(a'-m') == 0
eqn3： u(b) - b*kisc + b'*k(b'-b) + f'*k(f'-b) + o*k(o-b) - b*k(b-b') - b*k(b-f') - b*k(b-o) == 0
eqn4： u(b') - b'*kisc + b*k(b-b') + f*k(f-b') + k*k(k-b') + l*k(l-b') + m'*k(m'-b') + o'*k(o'-b') - b'*k(b'-b) - b'*k(b'-f) - b'*k(b'-k) - b'*k(b'-l) - b'*k(b'-m') - b'*k(b'-o') == 0
eqn5： u(c) - c*kisc + c'*k(c'-c) + e*k(e-c) + f'*k(f'-c) + g'*k(g'-c) + i*k(i-c) + m*k(m-c) - c*k(c-c') - c*k(c-e) - c*k(c-f') - c*k(c-g') - c*k(c-i) - c*k(c-m) == 0
eqn6： u(c') - c'*kisc + c*k(c-c') + e'*k(e'-c') + g*k(g-c') + m'*k(m'-c') - c'*k(c'-c) - c'*k(c'-e') - c'*k(c'-g) - c'*k(c'-m') == 0
eqn7： u(d) - d*kisc + d'*k(d'-d) + e'*k(e'-d) + f*k(f-d) + h*k(h-d) + l*k(l-d) + n'*k(n'-d) - d*k(d-d') - d*k(d-e') - d*k(d-f) - d*k(d-h) - d*k(d-l) - d*k(d-n') == 0
eqn8： u(d') - d'*kisc + d*k(d-d') + f'*k(f'-d') + h'*k(h'-d') + n*k(n-d') - d'*k(d'-d) - d'*k(d'-f') - d'*k(d'-h') - d'*k(d'-n) == 0
eqn9： u(e) - e*kisc + a*k(a-e) + c*k(c-e) + h'*k(h'-e) - e*k(e-a) - e*k(e-c) - e*k(e-h') == 0
eqn10： u(e') - e'*kisc + c'*k(c'-e') + d*k(d-e') + h*k(h-e') + i*k(i-e') + i'*k(i'-e') - e'*k(e'-c') - e'*k(e'-d) - e'*k(e'-h) - e'*k(e'-i) - e'*k(e'-i') == 0
eqn11： u(f) - f*kisc + b'*k(b'-f) + d*k(d-f) + f'*k(f'-f) + g*k(g-f) + o'*k(o'-f) - f*k(f-b') - f*k(f-d) - f*k(f-f') - f*k(f-g) - f*k(f-o') == 0
eqn12： u(f') - f'*kisc + b*k(b-f') + c*k(c-f') + d'*k(d'-f') + f*k(f-f') + g'*k(g'-f') - f'*k(f'-b) - f'*k(f'-c) - f'*k(f'-d') - f'*k(f'-f) - f'*k(f'-g') == 0
eqn13： u(g) - g*kisc + c'*k(c'-g) + f*k(f-g) + g'*k(g'-g) + h*k(h-g) + k*k(k-g) - g*k(g-c') - g*k(g-f) - g*k(g-g') - g*k(g-h) - g*k(g-k) == 0
eqn14： u(g') - g'*kisc + c*k(c-g') + f'*k(f'-g') + g*k(g-g') + k'*k(k'-g') - g'*k(g'-c) - g'*k(g'-f') - g'*k(g'-g) - g'*k(g'-k') == 0
eqn15： u(h) - h*kisc + d*k(d-h) + e'*k(e'-h) + g*k(g-h) + h'*k(h'-h) + j*k(j-h) - h*k(h-d) - h*k(h-e') - h*k(h-g) - h*k(h-h') - h*k(h-j) == 0
eqn16： u(h') - h'*kisc + d'*k(d'-h') + e*k(e-h') + h*k(h-h') + j'*k(j'-h') - h'*k(h'-d') - h'*k(h'-e) - h'*k(h'-h) - h'*k(h'-j') == 0
eqn17： u(i) - i*kisc + c*k(c-i) + e'*k(e'-i) + k'*k(k'-i) + l'*k(l'-i) + o*k(o-i) - i*k(i-c) - i*k(i-e') - i*k(i-k') - i*k(i-l') - i*k(i-o) == 0
eqn18： u(i') - i'*kisc + a'*k(a'-i') + e'*k(e'-i') + l'*k(l'-i') + n'*k(n'-i') - i'*k(i'-a') - i'*k(i'-e') - i'*k(i'-l') - i'*k(i'-n') == 0
eqn19： u(j) - j*kisc + a'*k(a'-j) + h*k(h-j) + j'*k(j'-j) + k*k(k-j) + l*k(l-j) - j*k(j-a') - j*k(j-h) - j*k(j-j') - j*k(j-k) - j*k(j-l) == 0
eqn20： u(j') - j'*kisc + h'*k(h'-j') + j*k(j-j') + k'*k(k'-j') + l'*k(l'-j') + n*k(n-j') - j'*k(j'-h') - j'*k(j'-j) - j'*k(j'-k') - j'*k(j'-l') - j'*k(j'-n) == 0
eqn21： u(k) - k*kisc + b'*k(b'-k) + g*k(g-k) + j*k(j-k) + k'*k(k'-k) + m'*k(m'-k) - k*k(k-b') - k*k(k-g) - k*k(k-j) - k*k(k-k') - k*k(k-m') == 0
eqn22： u(k') - k'*kisc + g'*k(g'-k') + i*k(i-k') + j'*k(j'-k') + k*k(k-k') + o*k(o-k') - k'*k(k'-g') - k'*k(k'-i) - k'*k(k'-j') - k'*k(k'-k) - k'*k(k'-o) == 0
eqn23： u(l) - l*kisc + a'*k(a'-l) + b'*k(b'-l) + d*k(d-l) + j*k(j-l) + n'*k(n'-l) - l*k(l-a') - l*k(l-b') - l*k(l-d) - l*k(l-j) - l*k(l-n') == 0
eqn24： u(l') - l'*kisc + a*k(a-l') + i*k(i-l') + i'*k(i'-l') + j'*k(j'-l') + n*k(n-l') - l'*k(l'-a) - l'*k(l'-i) - l'*k(l'-i') - l'*k(l'-j') - l'*k(l'-n) == 0
eqn25： u(m) - m*kisc + a*k(a-m) + c*k(c-m) + m'*k(m'-m) - m*k(m-a) - m*k(m-c) - m*k(m-m') == 0
eqn26： u(m') - m'*kisc + a'*k(a'-m') + b'*k(b'-m') + c'*k(c'-m') + k*k(k-m') + m*k(m-m') - m'*k(m'-a') - m'*k(m'-b') - m'*k(m'-c') - m'*k(m'-k) - m'*k(m'-m) == 0
eqn27： u(n) - n*kisc + d'*k(d'-n) + j'*k(j'-n) + l'*k(l'-n) + n'*k(n'-n) + o*k(o-n) - n*k(n-d') - n*k(n-j') - n*k(n-l') - n*k(n-n') - n*k(n-o) == 0
eqn28： u(n') - n'*kisc + d*k(d-n') + i'*k(i'-n') + l*k(l-n') + n*k(n-n') + o'*k(o'-n') - n'*k(n'-d) - n'*k(n'-i') - n'*k(n'-l) - n'*k(n'-n) - n'*k(n'-o') == 0
eqn29： u(o) - o*kisc - o*kh3 + b*k(b-o) + i*k(i-o) + k'*k(k'-o) + n*k(n-o) + o'*k(o'-o) - o*k(o-b) - o*k(o-i) - o*k(o-k') - o*k(o-n) - o*k(o-o') == 0
eqn30： u(o') - o'*kisc - o'*kh4 + b'*k(b'-o') + f*k(f-o') + n'*k(n'-o') + o*k(o-o') - o'*k(o'-b') - o'*k(o'-f) - o'*k(o'-n') - o'*k(o'-o) == 0

Table S1. Relative energies (with ZPVE, kcal mol^{-1}) for all the 30 conformers of the excited 2-HPP(2)-S_1 as well as 70 transition states for the conformational interconversions, calculated at TD-M06-2X-D3/6-311++G(2d,p) level of theory. The rate constants (140 in total) for all the photo-activated interconversions are also listed.

	E + ZPVE (kcal/mol)		E + ZPVE (kcal/mol)	k (s^{-1})
2a	79.8	TS[2a-2a']	80.1	7.0×10^{12}
		TS[2a-2e]	81.5	6.7×10^{11}
		TS[2a-2l']	83.6	1.2×10^{11}
		TS[2a-2m]	82.7	7.5×10^{11}
2a'	80.0	TS[2a'-2a]	80.1	1.2×10^{13}
		TS[2a'-2i']	83.7	1.6×10^{11}
		TS[2a'-2j]	83.6	3.3×10^{11}
		TS[2a'-2l]	88.3	2.2×10^{9}
		TS[2a'-2m']	82.3	2.5×10^{12}
2b	81.1	TS[2b-2b']	81.0	5.5×10^{12}
		TS[2b-2f']	82.5	3.0×10^{11}
		TS[2b-2o]	83.8	7.6×10^{10}
2b'	81.1	TS[2b'-2b]	81.0	1.0×10^{13}
		TS[2b'-2f]	84.2	2.5×10^{11}
		TS[2b'-2k]	87.1	9.6×10^{9}
		TS[2b'-2l]	82.1	2.3×10^{12}
		TS[2b'-2m']	87.0	8.1×10^{9}
		TS[2b'-2o']	84.4	8.4×10^{10}
2c	83.5	TS[2c-2c']	83.2	5.1×10^{12}
		TS[2c-2e]	83.7	4.1×10^{12}
		TS[2c-2f']	88.9	3.4×10^{9}
		TS[2c-2g']	86.8	7.8×10^{10}
		TS[2c-2i]	83.9	1.6×10^{12}
		TS[2c-2m]	84.0	1.3×10^{12}
2c'	82.1	TS[2c'-2c]	83.2	1.7×10^{12}
		TS[2c'-2e']	82.0	3.0×10^{12}
		TS[2c'-2g]	86.0	5.8×10^{10}
		TS[2c'-2m']	83.9	3.3×10^{11}
2d	83.5	TS[2d-2d']	83.5	4.5×10^{12}
		TS[2d-2e']	88.8	4.2×10^{9}
		TS[2d-2f]	83.8	1.1×10^{13}
		TS[2d-2h]	88.3	1.1×10^{10}
		TS[2d-2l]	84.4	6.1×10^{11}

		TS[2d-2n']	84.0	2.1×10^{12}
2d'	83.3	TS[2d'-2d]	83.5	6.9×10^{12}
		TS[2d'-2f']	83.2	4.9×10^{12}
		TS[2d'-2h']	88.6	8.3×10^{9}
		TS[2d'-2n]	84.1	1.6×10^{12}
2e	81.6	TS[2e-2a]	81.5	1.6×10^{12}
		TS[2e-2c]	83.7	1.4×10^{12}
		TS[2e-2h']	85.9	6.4×10^{10}
2e'	81.8	TS[2e'-2c']	82.0	5.0×10^{12}
		TS[2e'-2d]	88.8	2.2×10^{9}
		TS[2e'-2h]	85.9	1.1×10^{11}
		TS[2e'-2i]	80.9	2.2×10^{13}
		TS[2e'-2i']	82.0	2.2×10^{12}
2f	82.3	TS[2f-2b']	84.2	1.0×10^{12}
		TS[2f-2d]	83.8	1.0×10^{13}
		TS[2f-2f']	84.2	1.0×10^{12}
		TS[2f-2g]	88.0	1.2×10^{10}
		TS[2f-2o']	82.2	2.4×10^{12}
2f'	82.4	TS[2f'-2b]	82.5	1.5×10^{12}
		TS[2f'-2c]	88.9	2.2×10^{9}
		TS[2f'-2d']	83.2	2.0×10^{12}
		TS[2f'-2f]	84.2	6.7×10^{11}
		TS[2f'-2g']	88.7	3.7×10^{9}
2g	85.1	TS[2g-2c']	86.0	1.2×10^{12}
		TS[2g-2f]	88.0	7.4×10^{10}
		TS[2g-2g']	84.7	1.1×10^{13}
		TS[2g-2h]	85.5	5.8×10^{12}
		TS[2g-2k]	85.8	1.2×10^{12}
2g'	85.8	TS[2g'-2c]	86.8	7.0×10^{11}
		TS[2g'-2f']	88.7	5.1×10^{10}
		TS[2g'-2g]	84.7	1.5×10^{13}
		TS[2g'-2k']	85.8	1.7×10^{12}
2h	85.2	TS[2h-2d]	88.3	6.4×10^{10}
		TS[2h-2e']	85.9	1.2×10^{12}
		TS[2h-2g]	85.5	5.4×10^{12}
		TS[2h-2h']	84.9	3.8×10^{12}
		TS[2h-2j]	85.6	1.3×10^{12}
2h'	85.1	TS[2h'-2d']	88.6	1.6×10^{10}

		TS[2h'-2e]	85.9	5.7×10^{11}
		TS[2h'-2h]	84.9	1.9×10^{12}
		TS[2h'-2j']	85.6	6.6×10^{11}
2i	81.6	TS[2i-2c]	83.9	5.1×10^{11}
		TS[2i-2e']	80.9	1.3×10^{13}
		TS[2i-2k']	85.4	1.3×10^{11}
		TS[2i-2l']	81.6	3.9×10^{12}
		TS[2i-2o]	88.6	2.4×10^{9}
2i'	81.2	TS[2i'-2a']	83.7	1.8×10^{11}
		TS[2i'-2e']	82.0	1.1×10^{12}
		TS[2i'-2l']	80.9	1.1×10^{13}
		TS[2i'-2n']	88.8	1.1×10^{9}
2j	82.6	TS[2j-2a']	83.6	1.1×10^{12}
		TS[2j-2h]	85.6	1.7×10^{11}
		TS[2j-2j']	88.2	8.1×10^{9}
		TS[2j-2k]	83.3	3.2×10^{12}
		TS[2j-2l]	87.4	2.0×10^{10}
2j'	83.4	TS[2j'-2h']	85.6	1.7×10^{11}
		TS[2j'-2j]	88.2	8.1×10^{9}
		TS[2j'-2k']	83.9	4.0×10^{12}
		TS[2j'-2l']	85.1	3.4×10^{11}
		TS[2j'-2n]	87.1	2.8×10^{10}
2k	83.2	TS[2k-2b']	87.1	4.7×10^{10}
		TS[2k-2g]	85.8	2.2×10^{11}
		TS[2k-2j]	83.3	4.9×10^{12}
		TS[2k-2k']	84.7	2.0×10^{12}
		TS[2k-2m']	84.8	7.1×10^{11}
2k'	83.3	TS[2k'-2g']	85.8	1.5×10^{11}
		TS[2k'-2i]	85.4	3.3×10^{11}
		TS[2k'-2j']	83.9	4.1×10^{12}
		TS[2k'-2k]	84.7	1.4×10^{12}
		TS[2k'-2o]	86.2	7.3×10^{10}
2l	82.1	TS[2l-2a']	88.3	4.9×10^{9}
		TS[2l-2b']	82.1	4.8×10^{12}
		TS[2l-2d]	84.4	3.0×10^{11}
		TS[2l-2j]	87.4	1.3×10^{10}
		TS[2l-2n']	87.4	2.0×10^{10}
2l'	80.8	TS[2l'-2a]	83.6	1.4×10^{11}

		TS[2l'-2i]	81.6	2.1×10^{12}
		TS[2l'-2i']	80.9	6.9×10^{12}
		TS[2l'-2j']	85.1	7.5×10^{10}
		TS[2l'-2n]	87.6	3.7×10^{9}
2m	82.6	TS[2m-2a]	82.7	5.2×10^{12}
		TS[2m-2c]	84.0	1.2×10^{12}
		TS[2m-2m']	82.4	1.4×10^{13}
2m'	82.1	TS[2m'-2a']	82.3	3.9×10^{12}
		TS[2m'-2b']	87.0	1.2×10^{10}
		TS[2m'-2c']	83.9	3.7×10^{11}
		TS[2m'-2k]	84.8	2.2×10^{11}
		TS[2m'-2m]	82.4	5.2×10^{12}
2n	83.0	TS[2n-2d']	84.1	1.1×10^{12}
		TS[2n-2j']	87.1	4.0×10^{10}
		TS[2n-2l']	87.6	2.4×10^{10}
		TS[2n-2n']	83.5	4.7×10^{12}
		TS[2n-2o]	83.2	4.4×10^{12}
2n'	83.7	TS[2n'-2d]	84.0	3.7×10^{12}
		TS[2n'-2i']	88.8	7.6×10^{9}
		TS[2n'-2l]	87.4	7.0×10^{10}
		TS[2n'-2n]	83.5	7.9×10^{12}
		TS[2n'-2o']	83.7	4.5×10^{12}
2o	81.1	TS[2o-2b]	83.8	1.8×10^{11}
		TS[2o-2i]	88.6	2.4×10^{9}
		TS[2o-2k']	86.2	2.9×10^{10}
		TS[2o-2n]	83.2	1.2×10^{12}
		TS[2o-2o']	81.3	8.2×10^{12}
2o'	81.0	TS[2o'-2b']	84.4	1.4×10^{11}
		TS[2o'-2f]	82.2	9.5×10^{11}
		TS[2o'-2n']	83.7	9.7×10^{11}
		TS[2o'-2o]	81.3	1.1×10^{13}

Table S2: Lists of the rate constants for 1,5 H-shift and of the net removal rate constants for the directly formed S_1 conformers (2a-2j), and the ratio of the overall H-shift rate to the rate of intersystem crossing.

	rat net removal rate constants for all the	rate s^{-1}	rate s^{-1}
k(ISC) for all cfs (estimate)	3.0×10^{9}	1.0×10^{10}	3.0×10^{10}
k(H,2a) (1,5 H-shift of 2a)	3.40×10^{11}		
k(H,2a') (1,5 H-shift of 2a')	9.69×10^{10}		
k(H,2o) (1,5 H-shift of 2o)	2.87×10^{10}		
k(H,2o') (1,5 H-shift of 2o')	2.78×10^{11}		
k(H,overall) (1,5 H-shift of pool of all cfs)	4.99×10^{10}	5.07×10^{10}	5.27×10^{10}
k(remove,2a)	4.42×10^{11}	4.81×10^{11}	5.85×10^{11}
k(remove,2b)	1.16×10^{11}	1.35×10^{11}	1.89×10^{11}
k(remove,2c)	2.03×10^{12}	2.20×10^{12}	2.64×10^{12}
k(remove,2d)	1.01×10^{12}	1.16×10^{12}	1.54×10^{12}
k(remove,2e)	7.34×10^{11}	7.91×10^{11}	9.35×10^{11}
k(remove,2f)	9.35×10^{11}	1.07×10^{12}	1.43×10^{12}
k(remove,2g)	4.55×10^{12}	4.69×10^{12}	5.01×10^{12}
k(remove,2h)	4.35×10^{12}	4.50×10^{12}	4.81×10^{12}
k(remove,2i)	6.13×10^{11}	6.73×10^{11}	8.34×10^{11}
k(remove,2j)	1.13×10^{12}	1.19×10^{12}	1.34×10^{12}
ratio of *k*(H,overall)/*k*(ISC)	94/6	84/16	64/36

2. CASSCF/CASPT2 calculations on the excited hydroperoxyacetaldehyde (HPAC).

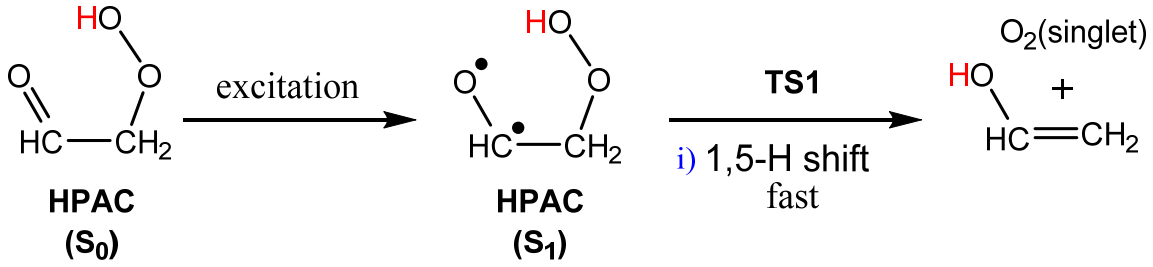
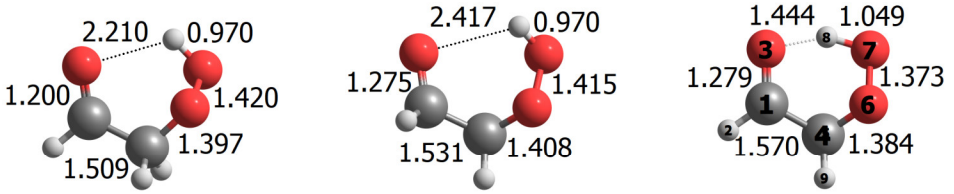


Figure S4. The 1,5 H-shift reaction of the excited hydroperoxyacetaldehyde (HPAC).



2-HPP-S_0 M06-2X-D3: 0

2-HPP-S_1 M06-2X-D3: **80.7**

2-HPP-S_1 (TS1) M06-2X-D3: **82.5**

Figure S5. Structures for the 1,5 H-shift reaction of the excited (HPAC), optimized at M06-2X-D3 level for the ground S_0 state, and TD-M06-2X-D3 level for the excited S_1 state. The relative energies (with *ZPVE*) in blue are computed at TD-M06-2X-D3/6-311++G(2d,p) level of theory. All the energies (kcal/mol) are relative to the global minimum HPAC-S_0.

The activation barrier for HPAC-S_1 is about 1.8 kcal/mol at TD-M06-2X-D3 level, which leads to a fast 1,5 H-shift with an activated rate of $\approx 2 \times 10^{11}$ s^{-1}. On the basis of TD-M06-2X-D3 structures, the CASPT2//TDDFT barrier is slightly higher (3.0 kcal/mol), and the calculated rate is $\approx 8 \times 10^{10}$ s^{-1}.

An IRC analysis of the 1,5 H-shift reaction failed at the TD-M06-2X-D3 level; this is because after TS1, there is no longer a meaningful closed-shell ground-state Kohn-Sham reference determinant such that the TD-M06-2X-D3 energies and geometries gradually lose meaning. Indeed, the biradical species produced after H atom transfer cannot be characterized precisely either. In order to elucidate the overall mechanism of the reaction (R.i, in the main text) and to establish its end products, energies were computed along approximate pathways leading from the reactant to the TS for H transfer, and then from this TS to the approximate structure corresponding to the biradical end product. These pathways were generated using relaxed scans at the TDDFT level of theory, holding the distance between the transferring hydrogen atom (H8) and the carbonyl oxygen atom (O3) fixed, but relaxing the other coordinates. Then, at the generated points, the energy was recomputed at the CASPT2 level of theory. The resulting energy curves obtained are shown in **Figure S6**, where point 1 corresponds to the S1 minimum, point 11 corresponds to the TS, and point 20 is the partially optimized minimum for the biradical (full TDDFT optimization at this point was as mentioned not possible).

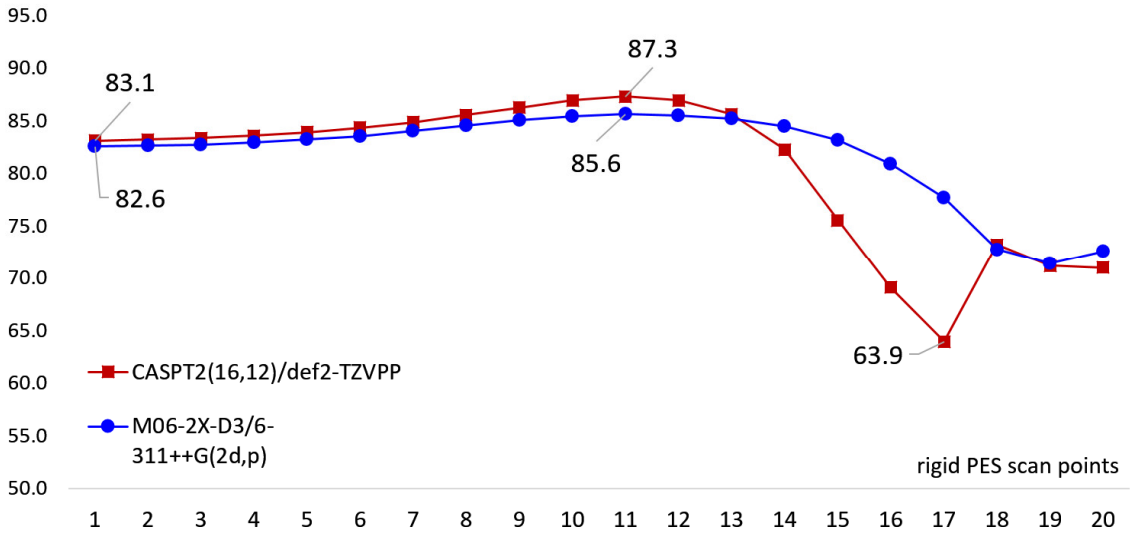


Figure S6. Single-point energies along the pathway for the 1,5 H-shift reaction of the excited HPAC. Structures for the S1 minimum (point 1) and the H-transfer TS (point 11) were obtained at the TD-M06-2X-D3 level of theory. An approximate structure for the H-transferred biradical state was also obtained at the same level (point 20), but full optimization was not possible due to wavefunction convergence problems. Intermediate structures between 1 and 11, and between 11 and 20 were generated by relaxed scans at the TD-M06-2X-D3 level. TD-M06-2X-D3 energies at these points are shown in blue; single-point CASPT2(16,12) energies of the TD-M06-2X-D3-optimized structures are in red. All the energies (kcal/mol) are relative to HPAC-S_0 without inclusion of *ZPVE*.

Up to the transition state of the 1,5 H-shift, **Figure S6** shows good agreement between CASPT2 energies and TD-M06-2X-D3 energies except for a slightly higher CAPST2 barrier. However, the agreement is less good after the TS. This is perhaps not surprising given that the end point 20 is not a fully-optimized TDDFT structure and results in this region are thus perhaps misleading. The drop in the CASPT2 energies in this region may be an artefact. Accordingly, the whole region corresponding to the 1,5 H-shift reaction of HPAC-S_1 was surveyed again using the multi-reference CASSCF method and refining the energies at the CASPT2 level of theory.

We first reoptimized the geometries of HPAC-S_1 (**A1**) and the transition state of 1,5 H-shift reaction (**TS1**) at CASSCF(16,12)/DZP level of theory. However, the CASPT2 energy of **CASSCF-TS1** is lower than that of **A1**, which motivated us to further explore the reaction pathway from **A1** to **CASSCF-TS1**. By using CASSCF, we located two S_1 conformers of **A1** with the formyl-H either above or below the OCC plane, and the corresponding transition state (**TSconf**) for the conformational change between two **A1** conformers. The conformer of the S_1 minimum that is the starting point is not the conformer that leads directly to the **CASSCF-TS1**. To construct the pathway from **A1** to **CASSCF-TS1**, 10 intermediate structures were first generated for the conformational change from **A1** to **A1'** (the second conformer that leads directly to the CASSCF-TS1) via **TSconf**, and another 10 structures generated between **A1'** and **CASSCF-TS1** both by linear interpolation using Cartesian coordinates to obtain a smoothly varying set of structures.

The energies for all the 21 points are shown in **Figure S7**, where point 1 corresponds to the S1 minimum (**A1**), point 6 corresponds to the **TSconf**, point 11 corresponds to the second conformer of A1 (**A1'**), and point 21 is the transition state **CASSCF-TS1**. The maximum along the reaction path in the rigid CASSCF scan, i.e. the H-transfer TS, corresponds to a point lying *below* the S_1 minimum (**A1**) on the CASPT2 profile. However, the maximum (point 19, referred as to CASPT2-TS1) along the CASPT2 energy profile comes a bit earlier than the CASSCF-TS1 maximum. Also, this maximum on

the CASPT2 PES is also the maximum point on the TD-M06-2X-D3 potential energy profile. It was straightforward to localize and optimize the biradical intermediate **A2** and the corresponding **TS2** for the OO elimination at CASSCF level. So, by taking the maximum (point 19) on the CASPT2 profile as the '**TS1**' for the 1,5 H-shift reaction, a complete reaction pathway is shown in **Figure S9**, which includes the starting point HPAC-S1 (**A1**), the transition state for the 1,5 H-shift (**TS1**), the biradical intermediate (**A2**), the transition state for OO elimination (**TS2**), and the final product complex (**A3**). Note that the CASPT2 energy of **TS2** lies well below that of the biradical "intermediate" **A2**, such that the biradical should be unstable and decompose spontaneously.

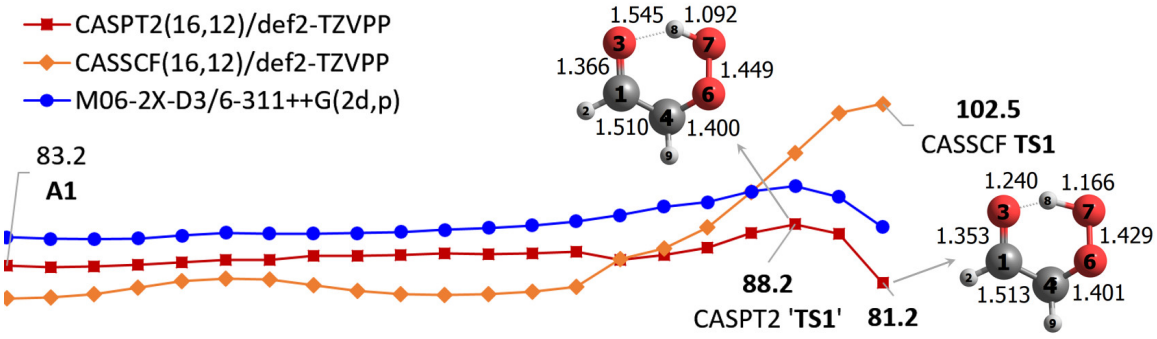


Figure S7. Potential energy surface interpolated between the HPAC-S_1 (A1) and the 1,5 H-shift transition state (TS1) optimized at CASSCF(16,12)/DZP level of theory. All the energies (kcal/mol) are relative to HPAC-S_0.

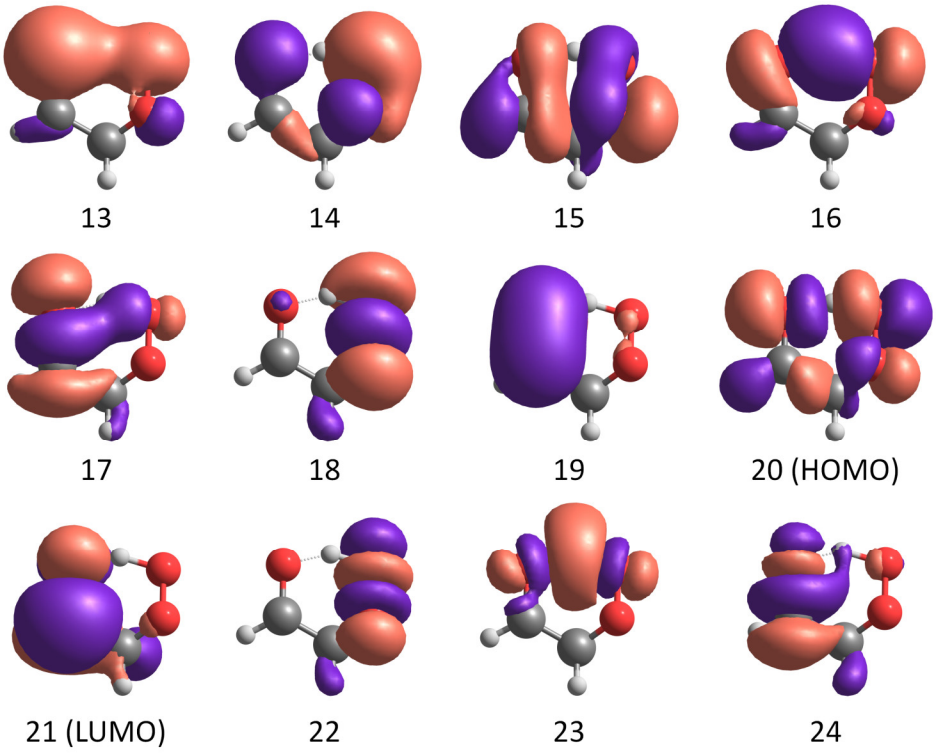


Figure S8. This active space contains all the important bonding and anti-bonding orbitals of the carbonyl and hydroperoxy groups for the 1,5 H-shift transition state with an isovalue of 0.025 $bohr^{-3/2}$.

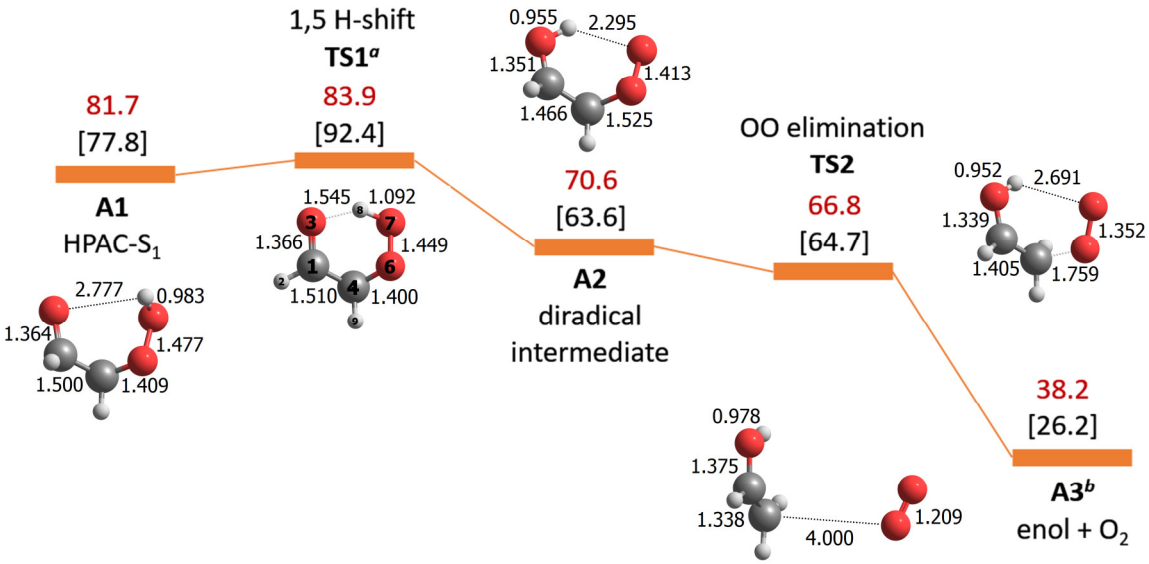


Figure S9. Potential energy surface (with CASSCF *ZPVE*) of the 1,5 H-shift reaction of the excited HPAC. Geometries were optimized at CASSCF(16,12)/DZP level of theory. The energies at CASSCF(16,12)/def2-TZVPP level of theory are in black inside the brackets, while the energies refined at the CASPT2(16,12)/def2-TZVPP level of theory are in red. All the energies (kcal/mol) are relative to HPAC-S_0. [a]TS1 refers here to the maximum on an interpolated CAPST2 potential energy surface. [b] For this bimolecular channel of A3, geometry optimization is performed using a fixed enol – O_2 distance of 4 Angstrom – at this distance, interaction between the two fragments is very small.

In **Figure S9**, The CASPT2 barrier for the 1,5 H-shift is about 2.0 kcal/mol, confirming that the activated reaction is fast with a rate close to 2×10^{11} s^{-1}. According to the CASPT2 results shown in **Figure S9**, the biradical "intermediate" **A2** resulting from the H-shift is not a 'real' local minimum on the CASPT2 PES, and should decompose spontaneously into ground state enol and the degenerate S_1/S_0 singlet oxygen $O_2(^1\Delta)$, at 38.2 kcal/mol relative to HPAC S_0.

3. Atmospheric implications.

Table S3 Hydroperoxy-carbonyls discussed in this work. The notation is from the MCMv3.3.1.

compound	notation	precursor(s)
$CH_3C(=O)CH(OOH)CH_2OH$	HMVKBOOH	MVK+OH(Praske)
$CH_3C(=O)CH_2OOH$	HYPERACET	$CH_3C(=O)CH_3$ + OH,(Saunders)
		δ-ISOPO2 isomerisation(Peeters,Teng)
$O=CHCH_2OOH$	HCOCH2OOH	CH_3CHO + OH,(Saunders)
		isoprene + NO_3,(Schwantes)
		δ-ISOPO2 isomerisation(Peeters,Teng)
$O=CHC(CH_3)(OOH)CH(OOH)CH_2OOH$ & isomer	C536OOH	δ-ISOPO2 isomerisation(Peeters)
$CH_3C(=O)CH(OOH)CH_2OOH$	DIHPMEK	δ-ISOPO2 isomerisation(Peeters)
$O=CHC(CH_3)(OOH)CH_2OOH$	DIHPMPAL	δ-ISOPO2 isomerisation(Peeters)
$CH_3C(=O)CH(OOH)CH(=O)$	C4CO2OOH	δ-ISOPO2 isomerisation(Liu)
$CH_3CH(OOH)CH(=O)$	PROPALOOH	$CH_2CH_2CH(=O)$ + OH
$CH_3C(=O)CH_2CH_2OOH$	MEKAOOH	$CH_3C(=O)C_2H_5$ + OH(Saunders)
$CH_3C(=O)CH(OOH)CH_3$	MEKBOOH	$CH_3C(=O)C_2H_5$ + OH(Saunders)

E. Praske, J. D. Crounse, K. H. Bates, T. Kurtén, H. G. Kjaergaard, and P. O. Wennberg, *J. Phys. Chem. A*, 2015, **119**, 4562.

S. M. Saunders, M. E. Jenkin, R. G. Derwent, and M. J. Pilling, *Atmos. Chem. Phys.*, 2003, **3**, 161.

J. Peeters, J.-F. Müller, T. Stavrakou, and V. S. Nguyen, *J. Phys. Chem. A*, 2014, **118**, 8625.

A. P. Teng, J. D. Crounse, and P. O. Wennberg, *J. Am. Chem. Soc.*, 2017, **139**, 5367.

R. H. Schwantes, A. P. Teng, T. B. Nguyen, M. M. Coggon, J. D. Crounse, J. M. St. Clair, X. Zhang, K. A. Schilling, J. H. Seinfeld, and P. O. Wennberg, *J. Phys. Chem. A*, 2015, **119**, 10158.

Z. Liu, V. S. Nguyen, J. Harvey, J.-F. Müller, and J. Peeters, *Phys. Chem. Chem. Phys.*, 2017, **19**, 9096.

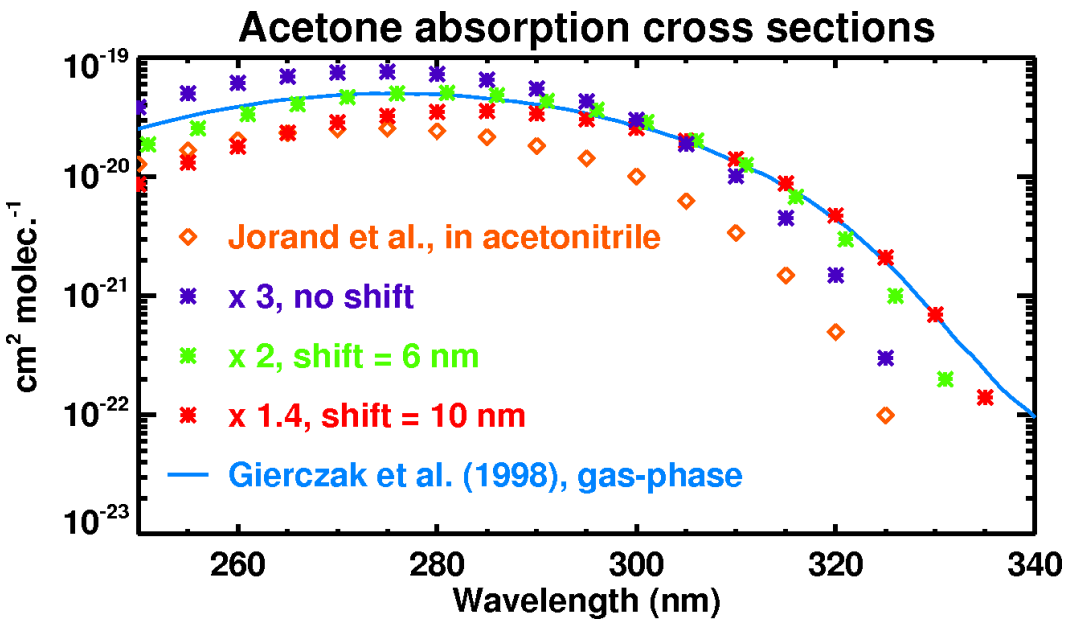


Figure S10: Absorption cross sections of acetone measured by Gierczak et al. (2012) in the gas phase (blue), and by Jorand et al. (2000) in solution in acetonitrile (diamonds). Three methods are illustrated for approximating the gas-phase cross sections from the values in acetonitrile: factor of 3 enhancement (indigo); factor of 2 and 6 nm red-shift (green); factor of 1.4 and 10 nm shift (red).

T. Gierczak, J. B. Burkholder, S. Bauerle, A. R. Ravishankara, *Chem. Phys.*, 1998, **231**, 229.

F. Jorand, L. Kerhoas, A. Heiss, J. Einhorn, and K. Sahetchian, *J. Photchem. Photobiol. A*, 2000, **134**, 119.

Absorption cross sections and calculated oscillator strengths

In principle, the absorption cross-section should be related to the calculated transition dipole moment and associated oscillator strength. Indeed, in our TDDFT calculations, 2-HPP shows a larger oscillator strength than propanal, consistent with the suggestion here that these species should have non-additive absorption cross-sections compared to simpler compounds containing separate carbonyl and hydroperoxy functional groups. However, detailed comparison is hampered by issues to do with the width of the absorption feature, and the role of vibronic coupling in the spectra of carbonyl species (see M. Nobre, A. Fernandes, F. Ferreira da Silva, R. Antunes, D. Almeida, V. Kokhan, S. V. Hoffmann, N. J. Mason, S. Eden and P. Limao-Vieira, Phys. Chem., Chem. Phys. 2008, 10, 550-560). Accordingly, we feel that the best estimate for the cross-sections instead comes from the procedure used in the main text and based on the experimental data of ref. 1.

Table S4 Ground to excited state transition electric dipole moments (Au).

	state	**X**	**Y**	**Z**	**Dip. S.**	**Osc.**
2-hpp	1	0.0267	0.0282	-0.0254	0.0021	0.0002
propanal	1	0.0000	0.0000	0.0385	0.0015	0.0001

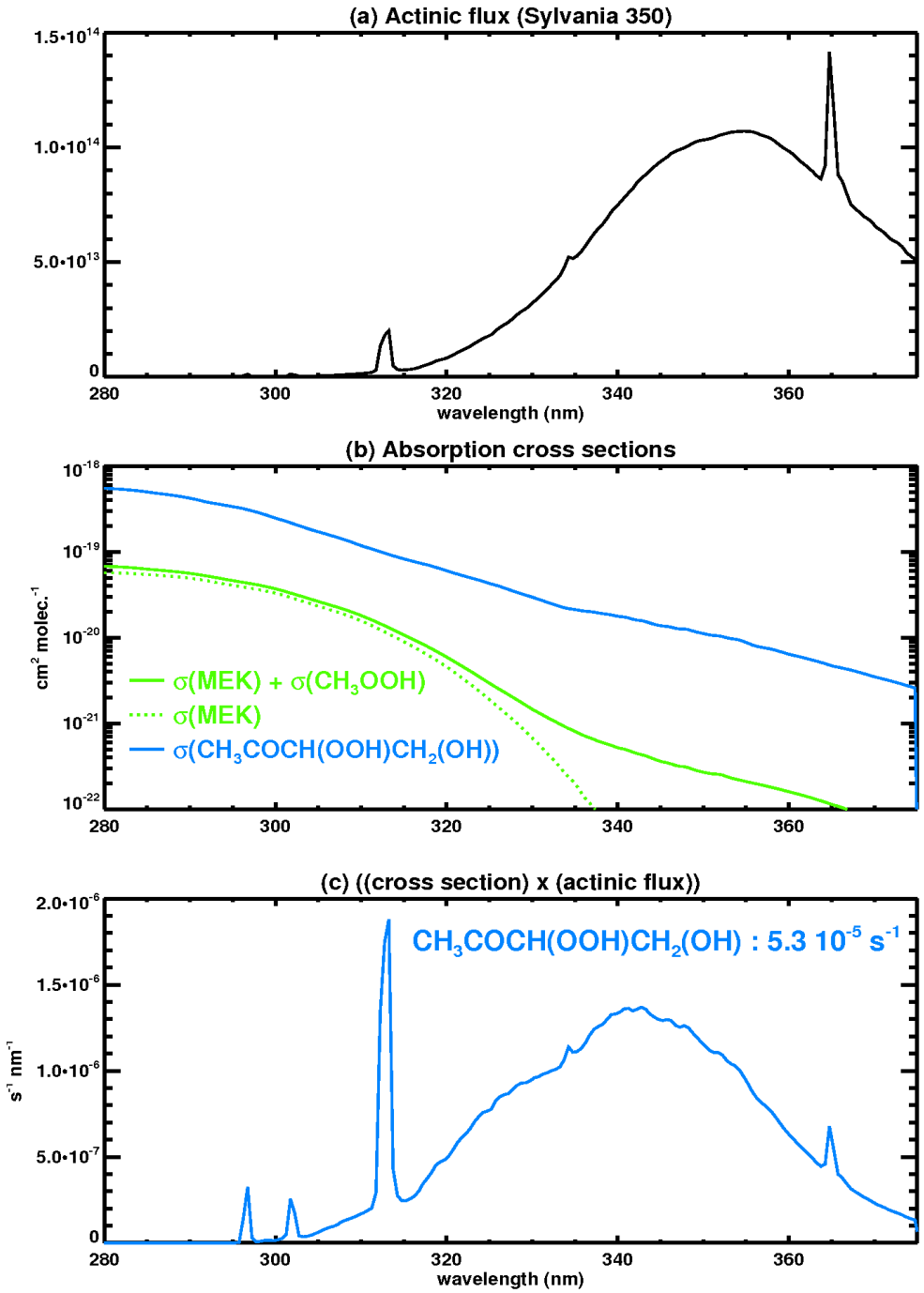


Figure S11: (a) Actinic flux of Sylvania 350 black lights (Carter et al., 2005), normalized such that the photorate $J(H_2O_2)$ matches the reported value by Praske et al. (2015). (b) Cross sections of $CH_3COCH(OOH)CH_2OH$ estimated in this work (blue), and sum of the cross sections of methylethylketone and CH_3OOH (green). (c) Product of the actinic flux and of the ketohydroperoxide absorption cross section (s^{-1} nm^{-1}), and integrated value over the whole spectrum.

W. P. L. Carter, D. R. Cocker III, D. R. Fritz, I. L. Malkina, K. Bumiller, C. G. Sauer, J. T. Pisano, C. Bufalino, and C. Song, *Atmos. Environ.*, 2005, **39**, 7768.

E. Praske, J. D. Crounse, K. H. Bates, T. Kurtén, H. G. Kjaergaard, and P. O. Wennberg, *J. Phys. Chem. A*, 2015, **119**, 4562.

List of Cartesian coordinates.

a. The geometries in Figure 1

2-HPP-S_0

Geometry with 12 atoms:
Total energy: -343.462990097

C	0.06050	1.23793	0.28113
H	0.65769	1.98415	0.84204
O	-0.89877	1.57031	-0.35865
C	0.55082	-0.19072	0.38138
H	0.53068	-0.47724	1.44169
C	1.96164	-0.30477	-0.17673
H	2.63515	0.36837	0.35440
H	2.32071	-1.32546	-0.05871
H	1.96656	-0.04825	-1.23636
O	-0.25421	-1.06514	-0.36692
O	-1.54487	-1.08285	0.22209
H	-1.96585	-0.33483	-0.22998

2-HPP-S_1

Geometry with 12 atoms:
Total energy: -343.429359917

C	-0.14537	1.25803	-0.21610
H	0.47854	2.15915	-0.17576
O	-1.38275	1.37650	0.04246
C	0.56726	-0.01860	0.32023
H	0.36891	-0.10649	1.39332
C	2.04224	0.02099	-0.01018
H	2.51195	0.86488	0.49390
H	2.51483	-0.90025	0.32767
H	2.18549	0.12140	-1.08572
O	0.03026	-1.14172	-0.32897
O	-1.27632	-1.34059	0.15801
H	-1.81405	-0.85478	-0.48905

TS1

Geometry with 12 atoms:
Total energy: -343.409058396

C	-0.19784	1.23475	-0.16684
H	0.30881	2.16863	0.09620
O	-1.46530	1.13117	-0.03686
C	0.61870	-0.01973	0.33858
H	0.44400	-0.13006	1.41335
C	2.07392	0.07135	-0.04349
H	2.51617	0.94948	0.42589
H	2.60821	-0.81419	0.29877
H	2.17373	0.16036	-1.12435
O	0.03761	-1.09347	-0.32717
O	-1.24687	-1.25969	0.12126
H	-1.62315	-0.27647	0.06280

O2-Singlet

Geometry with 2 atoms:
Total energy: -150.291292438

O	-0.00000	-0.00000	0.59564
O	0.00000	0.00000	-0.59564

O2-Triplet

Geometry with 2 atoms:
Total energy: -150.313851745

O	0.00000	0.00000	0.59607
O	0.00000	0.00000	-0.59607

4

Geometry with 10 atoms:
Total energy: -193.100927254

C	-0.58883	0.38316	0.00000
H	-0.49771	1.46317	-0.00001
O	-1.89653	0.00420	0.00000
C	0.46775	-0.41712	-0.00000
H	0.31211	-1.49367	0.00000
C	1.87975	0.08471	-0.00000
H	2.42623	-0.26278	0.87951
H	2.42623	-0.26277	-0.87951
H	1.90286	1.17515	0.00001
H	-1.94951	-0.95722	-0.00001

2-HPP-T_1

Geometry with 12 atoms:
Total energy: -343.342482097

C	-0.14144	1.24246	-0.25070
H	0.43821	2.17078	-0.17589
O	-1.39093	1.37271	0.05889
C	0.56591	-0.00178	0.31552
H	0.37666	-0.06879	1.39272
C	2.04336	0.02767	-0.01055
H	2.51496	0.88048	0.47686
H	2.51424	-0.88699	0.34651
H	2.18946	0.10643	-1.08773
O	0.04435	-1.16021	-0.29913
O	-1.28392	-1.32092	0.15287
H	-1.79645	-0.94478	-0.57919

TS2

Geometry with 12 atoms:
Total energy: -343.336237690

C	-0.20410	1.24280	-0.17469
H	0.26606	2.17160	0.16933
O	-1.47616	1.10960	-0.04210
C	0.62266	-0.01813	0.33619
H	0.44299	-0.11438	1.41286
C	2.07625	0.07968	-0.04720
H	2.50816	0.97536	0.39837
H	2.62211	-0.78971	0.31762
H	2.17436	0.14274	-1.13003
O	0.04413	-1.09671	-0.31986
O	-1.23898	-1.25778	0.12314
H	-1.61456	-0.25262	0.05658

TS3

Geometry with 12 atoms:
Total energy: -343.333223091

C	0.72942	-1.46410	-0.11373
H	0.32521	-2.09361	0.71181
O	1.79598	-0.92027	-0.09130
C	-0.76345	0.06825	0.39305
H	-0.55066	0.21447	1.44746
C	-2.02454	-0.55161	-0.08730
H	-2.24562	-1.44135	0.50162
H	-2.86453	0.14349	0.00646
H	-1.92612	-0.83797	-1.13525
O	-0.32580	1.05686	-0.41115
O	0.79272	1.69055	0.17684
H	1.51002	1.08266	-0.07930

CHO

Geometry with 3 atoms:
Total energy: -113.841133337

C	0.06207	0.58097	0.00000
H	-0.86897	1.20646	0.00000
O	0.06207	-0.58654	-0.00000

5

Geometry with 9 atoms:
Total energy: -229.483544969

C	0.44815	0.47021	-0.06783
H	0.19284	1.43570	0.35375
C	1.82277	-0.08642	-0.03080
H	2.54083	0.69776	-0.26713
H	2.07533	-0.49395	0.95575
H	1.93434	-0.89129	-0.75973
O	-0.50579	-0.49407	0.09438
O	-1.78841	0.10906	0.05456
H	-2.01532	0.02911	-0.88242

TS4

Geometry with 9 atoms:
Total energy: -229.482107439

C	-0.47458	0.41563	-0.28053
H	-0.16518	1.44869	-0.22146
C	-1.80851	-0.07588	0.14371
H	-2.57501	0.64136	-0.14752
H	-2.04029	-1.03431	-0.32535
H	-1.86365	-0.21795	1.23034
O	0.52851	-0.49894	-0.18251
O	1.72109	0.15453	0.26982
H	2.34590	-0.12094	-0.41356

OH

Geometry with 2 atoms:
Total energy: -75.727566017

O	0.00000	0.00000	0.10811
H	-0.00000	-0.00000	-0.86490

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Geometry with 7 atoms:
Total energy: -153.808598651

C	-0.23408	0.39883	-0.00000
H	-0.31814	1.50391	0.00000
C	1.16315	-0.14745	-0.00000
H	1.69660	0.22376	-0.87833
H	1.69658	0.22375	0.87835
H	1.14660	-1.23485	-0.00001
O	-1.22451	-0.27810	-0.00000

b. The geometries of 2-HPP(1) in ground S_0 state, optimized at M06-2X-D3/6-311++G(2d,p) level of theory (Figure 2)

2-HPP-1a

Geometry with 12 atoms:
Total energy: -343.462990097

C	0.06050	1.23793	0.28113
H	0.65769	1.98415	0.84204
O	-0.89877	1.57031	-0.35865
C	0.55082	-0.19072	0.38138
H	0.53068	-0.47724	1.44169
C	1.96164	-0.30477	-0.17673
H	2.63515	0.36837	0.35440
H	2.32071	-1.32546	-0.05871
H	1.96656	-0.04825	-1.23636
O	-0.25421	-1.06514	-0.36692
O	-1.54487	-1.08285	0.22209
H	-1.96585	-0.33483	-0.22998

2-HPP-1b

Geometry with 12 atoms:
Total energy: -343.461918978

C	0.94921	-0.94196	0.03685
H	1.04260	-2.03704	-0.10317
O	1.87566	-0.21241	-0.18626
C	-0.40774	-0.46276	0.50779
H	-0.56670	-0.89150	1.50504
C	-1.51405	-0.92657	-0.43254
H	-1.49994	-2.01293	-0.53313
H	-2.47960	-0.62574	-0.02945
H	-1.38695	-0.47615	-1.41544
O	-0.41049	0.92553	0.74194
O	-0.21822	1.59001	-0.49908
H	0.75041	1.60610	-0.54921

2-HPP-1c

Geometry with 12 atoms:
Total energy: -343.460558093

C	0.84467	-0.74384	0.32045
H	0.44900	-1.11402	1.28608
O	1.84934	-1.17558	-0.16753
C	0.05017	0.38614	-0.30764

H	0.01411	0.23136	-1.39074
C	0.68864	1.72169	0.03573
H	0.10769	2.53624	-0.39506
H	0.73236	1.85509	1.11746
H	1.70015	1.74714	-0.36742
O	-1.25675	0.41964	0.23332
O	-1.84769	-0.84534	-0.03943
H	-2.46339	-0.62953	-0.75243

2-HPP-1d

Geometry with 12 atoms:
Total energy: -343.460342431

C	-1.01470	-0.73131	0.18489
H	-0.68717	-1.76407	0.40769
O	-2.07907	-0.49308	-0.30923
C	-0.02127	0.34897	0.58343
H	-0.22257	0.59256	1.63384
C	-0.11988	1.58920	-0.28016
H	0.58054	2.34798	0.06789
H	0.08897	1.34538	-1.32170
H	-1.13337	1.98478	-0.22978
O	1.27877	-0.21495	0.64354
O	1.56269	-0.74615	-0.64682
H	2.20959	-0.11430	-0.98682

2-HPP-1e

Geometry with 12 atoms:
Total energy: -343.459813760

C	0.83020	-0.76116	0.31703
H	0.40599	-1.15017	1.26465
O	1.84816	-1.18903	-0.14492
C	0.05733	0.38577	-0.30567
H	0.01725	0.24052	-1.38919
C	0.71489	1.70965	0.04622
H	0.15061	2.53252	-0.39008
H	0.75352	1.84277	1.12841
H	1.73013	1.71737	-0.34807
O	-1.25110	0.43529	0.22202
O	-1.87932	-0.77077	-0.22230
H	-2.41397	-0.99245	0.55038

2-HPP-1f

Geometry with 12 atoms:
Total energy: -343.459548107

C	-0.99443	-0.74417	0.19611
H	-0.63758	-1.76612	0.43265
O	-2.07076	-0.54973	-0.28955
C	-0.02760	0.36518	0.57594
H	-0.23049	0.61734	1.62412
C	-0.15491	1.59262	-0.30253
H	-1.18275	1.95178	-0.27243
H	0.51589	2.37445	0.05043
H	0.09268	1.34425	-1.33349
O	1.28608	-0.15945	0.63509
O	1.59464	-0.58719	-0.69593
H	2.02413	-1.43255	-0.51533

2-HPP-1g

Geometry with 12 atoms:
Total energy: -343.458238709

C	-1.29108	-0.71010	0.01732
H	-1.15857	-1.79745	-0.13252
O	-2.36951	-0.19167	-0.02389
C	-0.01404	0.05910	0.31221
H	0.15767	-0.03288	1.39363
C	-0.08662	1.51191	-0.10210
H	-0.93790	1.98759	0.38351
H	0.82399	2.03380	0.18902
H	-0.22214	1.58666	-1.18181
O	1.00081	-0.67202	-0.35650
O	2.24681	-0.27522	0.19751
H	2.66253	0.16811	-0.55327

2-HPP-1h

Geometry with 12 atoms:
Total energy: -343.457758423

C	-1.28584	-0.70988	-0.01938
H	-1.13838	-1.77256	-0.28907
O	-2.37673	-0.22089	0.04317
C	-0.01674	0.06406	0.29627
H	0.14056	-0.02122	1.38082
C	-0.09425	1.51642	-0.12208
H	-0.94623	1.98899	0.36537
H	0.82034	2.03477	0.15997
H	-0.22707	1.58451	-1.20207
O	1.01067	-0.65276	-0.36872
O	2.25219	-0.13998	0.09593
H	2.64275	-0.92899	0.49310

2-HPP-1i

Geometry with 12 atoms:
Total energy: -343.455734545

C	0.52729	1.12939	0.36713
H	1.22050	1.53094	1.13653
O	-0.01476	1.84761	-0.41754
C	0.38675	-0.38310	0.38755
H	0.22108	-0.69717	1.42622
C	1.65646	-1.01278	-0.16757
H	2.52506	-0.66614	0.39337
H	1.60149	-2.09758	-0.09301
H	1.77707	-0.73129	-1.21388
O	-0.66762	-0.83018	-0.42518
O	-1.87309	-0.33917	0.15067
H	-2.32451	-1.16585	0.36457

2-HPP-1j

Geometry with 12 atoms:
Total energy: -343.455111471

C	-1.49987	0.08261	0.26357
H	-2.10835	0.89643	0.70847

O	-2.01076	-0.86578	-0.25394
C	-0.01017	0.31965	0.37521
H	0.23613	0.32804	1.44639
C	0.36095	1.65721	-0.25366
H	-0.17329	2.47293	0.23608
H	1.43027	1.82700	-0.14465
H	0.10885	1.65109	-1.31463
O	0.63601	-0.76393	-0.24966
O	2.02388	-0.62599	0.04329
H	2.20789	-1.48672	0.44018

2-HPP-1k

Geometry with 12 atoms:
Total energy: -343.454698639

C	-1.50238	0.08029	0.27521
H	-2.11249	0.86931	0.76050
O	-2.01102	-0.83577	-0.29935
C	-0.01331	0.31536	0.39557
H	0.22481	0.36931	1.46659
C	0.35613	1.62724	-0.28760
H	-0.20394	2.45666	0.14721
H	1.41800	1.82463	-0.15533
H	0.12860	1.56846	-1.35301
O	0.63278	-0.80159	-0.16751
O	2.01368	-0.66923	0.16000
H	2.41887	-0.77304	-0.71006

2-HPP-1l

Geometry with 12 atoms:
Total energy: -343.454222995

C	-1.23052	0.59135	-0.05540
H	-1.56922	1.60809	-0.34684
O	-1.94560	-0.35717	-0.17181
C	0.18363	0.54224	0.50296
H	0.13358	0.97312	1.51087
C	1.14787	1.35459	-0.35071
H	0.82373	2.39500	-0.39878
H	2.14454	1.32725	0.08902
H	1.19201	0.95922	-1.36477
O	0.60850	-0.77756	0.74480
O	0.71359	-1.43451	-0.51454
H	1.65748	-1.63786	-0.53816

c. The geometries of 2-HPP(2) and the transitions states for conformational interconversion in S_1 state, optimized at TD-M06-2X-D3/6-311++G(2d,p) level of theory (Figure S1)

2-HPP-2a

Geometry with 12 atoms:
Total energy: -343.429546875

C	-0.14537	1.25804	-0.21610
H	0.47854	2.15915	-0.17571
O	-1.38275	1.37649	0.04245
C	0.56726	-0.01860	0.32023
H	0.36892	-0.10650	1.39332
C	2.04224	0.02099	-0.01018
H	2.51196	0.86486	0.49392
H	2.51482	-0.90027	0.32764
H	2.18548	0.12143	-1.08573
O	0.03026	-1.14172	-0.32897
O	-1.27632	-1.34058	0.15801
H	-1.81405	-0.85476	-0.48904

2-HPP-2a'

Geometry with 12 atoms:
Total energy: -343.433931470

C	-0.10443	1.31674	-0.07791
H	0.34060	1.79306	-0.96123
O	-1.36721	1.40179	0.04995
C	0.55907	-0.02250	0.33033
H	0.35187	-0.17852	1.39116
C	2.03919	0.01027	0.01949
H	2.50324	0.85996	0.51783
H	2.50423	-0.91019	0.36915
H	2.19751	0.09666	-1.05593
O	0.00563	-1.09940	-0.39439
O	-1.26528	-1.38990	0.15063
H	-1.84548	-0.78797	-0.34203

2-HPP-2b

Geometry with 12 atoms:
Total energy: -343.433815967

C	-1.19384	0.16213	-0.44008
H	-1.38392	0.85240	-1.26839
O	-2.19732	-0.42356	0.07759
C	0.02545	0.45186	0.45772
H	-0.32613	0.71110	1.46083
C	0.86840	1.56164	-0.14314
H	0.31813	2.50181	-0.11177
H	1.78544	1.66286	0.43663
H	1.13186	1.33002	-1.17355
O	0.75971	-0.72960	0.70491
O	1.38583	-1.15049	-0.49321
H	0.68882	-1.68286	-0.90504

2-HPP-2b'

Geometry with 12 atoms:
Total energy: -343.432476757

C	-1.20139	0.31551	-0.42079
H	-1.01285	0.19042	-1.49425
O	-2.18146	-0.32485	0.07680
C	0.04966	0.50025	0.45025
H	-0.27260	0.81183	1.44607
C	0.97207	1.52536	-0.18443
H	0.47641	2.49372	-0.23081
H	1.87606	1.60967	0.41875
H	1.25035	1.21714	-1.19110
O	0.70703	-0.72544	0.72964

O	1.23378	-1.24228	-0.48324
H	0.68569	-2.02888	-0.60445

2-HPP-2c

Geometry with 12 atoms:
Total energy: -343.434348725

C	0.87318	-0.81550	0.32891
H	0.79454	-0.87321	1.42252
O	2.01618	-1.01473	-0.19501
C	0.02146	0.33024	-0.27971
H	-0.06744	0.13506	-1.35155
C	0.61721	1.69868	-0.00218
H	0.03137	2.47366	-0.49815
H	0.62786	1.89139	1.07085
H	1.64045	1.72520	-0.37432
O	-1.24761	0.32660	0.31525
O	-1.94034	-0.83608	-0.12339
H	-2.72361	-0.43900	-0.52628

2-HPP-2c'

Geometry with 12 atoms:
Total energy: -343.429892301

C	-0.81243	-0.86732	-0.30149
H	-0.18736	-1.77045	-0.34053
O	-2.01076	-0.99496	0.09788
C	-0.02857	0.34281	0.28774
H	0.08782	0.18720	1.36787
C	-0.72278	1.65047	-0.02298
H	-1.72284	1.63590	0.40901
H	-0.15707	2.48142	0.39848
H	-0.80838	1.77818	-1.10162
O	1.23401	0.40326	-0.31776
O	1.96572	-0.74703	0.07736
H	2.65867	-0.35820	0.62731

2-HPP-2d

Geometry with 12 atoms:
Total energy: -343.434303633

C	-1.04797	-0.75785	-0.08386
H	-0.91221	-1.79280	0.25412
O	-2.24203	-0.34553	-0.24827
C	-0.04735	0.23518	0.55683
H	-0.31668	0.38079	1.61041
C	-0.04016	1.55780	-0.18308
H	0.69904	2.22425	0.26416
H	0.18866	1.40430	-1.23592
H	-1.02678	2.01549	-0.10503
O	1.21293	-0.37494	0.65877
O	1.73514	-0.58042	-0.64906
H	2.53245	-0.03573	-0.61855

2-HPP-2d'

Geometry with 12 atoms:
Total energy: -343.428834185

C	-1.04084	-0.76891	-0.05953
H	-0.60888	-1.27189	-0.93644
O	-2.25714	-0.40749	-0.11820
C	-0.05832	0.28309	0.53604
H	-0.38076	0.48637	1.55971
C	-0.01373	1.55782	-0.28709
H	-1.00575	2.00812	-0.30229
H	0.69041	2.26417	0.15798
H	0.28104	1.34473	-1.31392
O	1.19655	-0.32056	0.71722
O	1.71853	-0.67510	-0.55430
H	2.43773	-0.03828	-0.65931

2-HPP-2e

Geometry with 12 atoms:
Total energy: -343.430520244

C	0.92557	-0.65954	0.43299
H	1.11831	-0.42046	1.48795
O	1.88761	-1.14559	-0.23691
C	0.01460	0.39450	-0.27411
H	-0.01541	0.13550	-1.33350
C	0.48983	1.81403	-0.03874
H	-0.14383	2.51367	-0.58485
H	0.44789	2.05446	1.02392
H	1.51797	1.91428	-0.38470
O	-1.27130	0.29705	0.27468
O	-1.87562	-0.89171	-0.19628
H	-1.43057	-1.56942	0.33832

2-HPP-2e'

Geometry with 12 atoms:
Total energy: -343.427225496

C	-0.75143	-0.92677	-0.22984
H	-0.13279	-1.81844	-0.05346
O	-1.99059	-1.00914	0.01916
C	-0.03298	0.35123	0.31408
H	0.09627	0.23772	1.39689
C	-0.78772	1.61215	-0.03966
H	-0.24475	2.48163	0.32941
H	-0.90467	1.68769	-1.12044
H	-1.77541	1.57866	0.41843
O	1.22364	0.45062	-0.29148
O	2.01786	-0.61959	0.19614
H	2.38677	-0.96209	-0.62888

2-HPP-2f

Geometry with 12 atoms:
Total energy: -343.431349899

C	-1.03425	-0.77170	0.16803
H	-1.11398	-1.62171	0.85834
O	-2.10891	-0.38266	-0.38494
C	0.00826	0.29629	0.61953
H	-0.14821	0.51602	1.68096
C	-0.07847	1.55602	-0.21685
H	-1.04617	2.03021	-0.05178
H	0.71740	2.23681	0.08411

H	0.02899	1.32793	-1.27458
O	1.27631	-0.30786	0.62384
O	1.70707	-0.51848	-0.70852
H	1.19296	-1.30093	-0.96433

2-HPP-2f'

Geometry with 12 atoms:

Total energy: -343.426553215

C	-1.01828	-0.70895	-0.18117
H	-0.68036	-0.96606	-1.19529
O	-2.25646	-0.49210	-0.01048
C	-0.06684	0.32750	0.49300
H	-0.44851	0.51810	1.49735
C	0.03879	1.60790	-0.31443
H	-0.95572	2.03602	-0.43892
H	0.67563	2.32396	0.20758
H	0.46277	1.40356	-1.29645
O	1.17410	-0.28117	0.73454
O	1.75631	-0.61426	-0.51554
H	1.83251	-1.57406	-0.42693

2-HPP-2g

Geometry with 12 atoms:

Total energy: -343.433725112

C	-1.27393	-0.71224	-0.14622
H	-1.22520	-1.80043	-0.01097
O	-2.41003	-0.17090	0.08145
C	-0.01820	0.04500	0.28108
H	0.13079	-0.05871	1.36362
C	-0.06608	1.50485	-0.12112
H	-0.89204	2.00505	0.38598
H	0.86380	1.99477	0.16693
H	-0.21014	1.59007	-1.19848
O	1.02235	-0.67035	-0.37345
O	2.23694	-0.27540	0.25233
H	2.68796	0.17672	-0.47221

2-HPP-2g'

Geometry with 12 atoms:

Total energy: -343.430722145

C	1.30997	-0.64294	0.23170
H	1.31673	-0.87136	1.30650
O	2.41479	-0.23331	-0.26434
C	0.03587	0.05145	-0.26094
H	-0.00955	-0.04293	-1.34953
C	-0.03506	1.50798	0.16601
H	0.82969	2.04670	-0.22139
H	-0.93890	1.97342	-0.22914
H	-0.03391	1.57863	1.25501
O	-0.99894	-0.73388	0.31237
O	-2.21130	-0.31994	-0.30008
H	-2.66509	0.11368	0.43438

2-HPP-2h

Geometry with 12 atoms:

Total energy: -343.433680152

C	-1.26098	-0.72801	-0.14277
H	-1.19328	-1.81697	-0.02638
O	-2.40398	-0.21169	0.10766
C	-0.01398	0.05353	0.26904
H	0.15656	-0.05575	1.34883
C	-0.09968	1.51511	-0.11717
H	-0.90993	1.99959	0.42932
H	0.84110	2.00626	0.12846
H	-0.28699	1.60428	-1.18693
O	1.03412	-0.61963	-0.41817
O	2.25226	-0.14827	0.14437
H	2.58124	-0.94450	0.58122

2-HPP-2h'

Geometry with 12 atoms:

Total energy: -343.430811517

C	1.30785	-0.62037	0.27195
H	1.35750	-0.72467	1.36461
O	2.39742	-0.30684	-0.31776
C	0.03555	0.06747	-0.23743
H	-0.01441	-0.06344	-1.32267
C	-0.02701	1.53648	0.14035
H	0.82145	2.06427	-0.29556
H	-0.95225	1.97560	-0.23357
H	0.00511	1.64202	1.22519
O	-1.00208	-0.68393	0.37523
O	-2.22143	-0.23114	-0.19643
H	-2.50711	-1.02001	-0.67553

2-HPP-2i

Geometry with 12 atoms:

Total energy: -343.429569641

C	-0.79631	-0.91883	0.49176
H	-0.17686	-1.75057	0.85171
O	-1.61259	-1.18102	-0.44609
C	-0.04331	0.42392	0.43571
H	0.35629	0.57253	1.44235
C	-0.93209	1.56633	-0.01270
H	-1.80749	1.62178	0.63220
H	-0.38330	2.50573	0.04096
H	-1.26088	1.40346	-1.03847
O	1.03344	0.39553	-0.48459
O	1.97190	-0.56066	-0.00817
H	2.76048	-0.01228	0.09344

2-HPP-2i'

Geometry with 12 atoms:

Total energy: -343.432590136

C	-0.75913	-0.92900	0.44490
H	-0.97574	-1.34276	1.43590
O	-1.58454	-1.18211	-0.48563
C	-0.01821	0.43540	0.42492
H	0.36598	0.57427	1.43757
C	-0.89856	1.58416	-0.03063

H	-1.78228	1.64541	0.60299
H	-0.34160	2.51827	0.03390
H	-1.21727	1.42849	-1.06036
O	1.06514	0.39571	-0.47325
O	2.05446	-0.46721	0.05096
H	1.72579	-1.33812	-0.22180

2-HPP-2j

Geometry with 12 atoms:
Total energy: -343.431310070

C	1.47837	0.19114	0.20177
H	1.68605	0.52870	1.22397
O	2.18065	-0.78569	-0.22652
C	0.03989	0.29320	-0.27090
H	-0.00900	0.00623	-1.32452
C	-0.50201	1.69122	-0.04686
H	0.02209	2.40882	-0.67694
H	-1.56310	1.70218	-0.29520
H	-0.38211	1.97530	0.99919
O	-0.68925	-0.67290	0.49106
O	-1.97896	-0.78852	-0.11351
H	-1.95095	-1.69763	-0.43876

2-HPP-2j'

Geometry with 12 atoms:
Total energy: -343.431578563

C	-1.37754	-0.48454	0.49475
H	-1.48000	-1.44373	1.01698
O	-2.13644	-0.34516	-0.52452
C	0.00160	0.14506	0.49154
H	0.37261	0.10616	1.51958
C	-0.00008	1.56162	-0.04854
H	-0.63484	2.19785	0.56787
H	1.01621	1.95220	-0.03810
H	-0.37354	1.56918	-1.07233
O	0.81836	-0.71688	-0.31224
O	2.16670	-0.27193	-0.14982
H	2.56666	-1.04283	0.27210

2-HPP-2k

Geometry with 12 atoms:
Total energy: -343.430291816

C	1.47576	0.20798	0.21100
H	1.67428	0.55039	1.23329
O	2.20953	-0.74932	-0.21074
C	0.04422	0.28537	-0.27827
H	0.01519	0.02093	-1.33793
C	-0.52912	1.66739	-0.03107
H	0.00891	2.41217	-0.61624
H	-1.57765	1.68216	-0.32824
H	-0.45284	1.92291	1.02703
O	-0.66804	-0.72442	0.44327
O	-1.92545	-0.89250	-0.21568
H	-2.54134	-0.62303	0.47736

2-HPP-2k'

Geometry with 12 atoms:
Total energy: -343.431277028

C	-1.39481	-0.46909	0.48079
H	-1.50724	-1.44221	0.97531
O	-2.12933	-0.30212	-0.55229
C	-0.00340	0.13484	0.50628
H	0.34187	0.09700	1.54247
C	0.03033	1.54781	-0.04323
H	-0.63773	2.18887	0.53140
H	1.04129	1.94638	0.02962
H	-0.28815	1.55325	-1.08624
O	0.81236	-0.76009	-0.26069
O	2.17031	-0.38355	-0.03113
H	2.43053	-0.05857	-0.90260

2-HPP-2l

Geometry with 12 atoms:
Total energy: -343.428612909

C	-1.22418	0.20503	-0.45217
H	-0.97388	-0.04785	-1.49038
O	-2.20866	-0.41335	0.06536
C	-0.00882	0.46972	0.44494
H	-0.37322	0.74414	1.43663
C	0.84797	1.57016	-0.15589
H	0.29505	2.50794	-0.16126
H	1.75042	1.69349	0.44509
H	1.13012	1.32501	-1.17887
O	0.72424	-0.71459	0.72058
O	1.26774	-1.19282	-0.50384
H	2.21518	-1.12605	-0.32922

2-HPP-2l'

Geometry with 12 atoms:
Total energy: -343.432203574

C	-0.76547	-0.92611	0.51737
H	-0.17177	-1.70071	1.01889
O	-1.48601	-1.29000	-0.46299
C	-0.07201	0.44945	0.43717
H	0.30468	0.63718	1.44565
C	-1.00486	1.54077	-0.04784
H	-1.88549	1.57889	0.59093
H	-0.49223	2.50125	-0.01669
H	-1.32091	1.33838	-1.07068
O	1.01963	0.45695	-0.46404
O	2.03296	-0.37573	0.07541
H	2.08719	-1.06946	-0.59527

2-HPP-2m

Geometry with 12 atoms:
Total energy: -343.425119318

C	-0.12960	1.25530	-0.23419
H	0.51918	2.13832	-0.27457
O	-1.35028	1.46507	0.06058
C	0.54417	-0.01233	0.31149

H	0.34245	-0.08406	1.38873
C	2.02832	-0.00063	0.01174
H	2.50317	0.83603	0.52298
H	2.48231	-0.92842	0.35692
H	2.19021	0.09572	-1.06155
O	0.03006	-1.16615	-0.31886
O	-1.34712	-1.25563	-0.01751
H	-1.35594	-1.85799	0.73957

2-HPP-2m'

Geometry with 12 atoms:
Total energy: -343.431981759

C	-0.14882	-1.28763	0.19429
H	0.16237	-1.62440	1.19080
O	-1.36121	-1.52232	-0.12215
C	0.52325	-0.01494	-0.31692
H	0.29457	0.07802	-1.38163
C	2.01576	-0.07070	-0.05546
H	2.48920	0.83945	-0.42163
H	2.20626	-0.15697	1.01480
H	2.44764	-0.93113	-0.56300
O	0.06631	1.15441	0.34901
O	-1.29320	1.35370	-0.00432
H	-1.23642	2.14834	-0.55106

2-HPP-2n

Geometry with 12 atoms:
Total energy: -343.432456925

C	-1.29246	-0.24652	0.53837
H	-1.50618	-0.89051	1.40005
O	-1.70554	-0.67574	-0.58870
C	0.02067	0.53420	0.61142
H	0.03868	1.00320	1.59760
C	0.13003	1.56739	-0.49567
H	1.07214	2.10828	-0.39747
H	0.08659	1.08771	-1.47199
H	-0.69433	2.27545	-0.42230
O	1.15937	-0.31690	0.67817
O	1.26961	-1.01858	-0.55190
H	2.06611	-0.62479	-0.93114

2-HPP-2n'

Geometry with 12 atoms:
Total energy: -343.425109892

C	-1.28972	-0.22017	0.53861
H	-2.12718	0.25341	1.06487
O	-1.57528	-0.84678	-0.53170
C	0.01951	0.59515	0.57070
H	0.01003	1.14455	1.51351
C	0.15622	1.53383	-0.61918
H	1.10554	2.06985	-0.56003
H	0.10498	0.97786	-1.55360
H	-0.65609	2.26025	-0.61161
O	1.13671	-0.25499	0.72105
O	1.22485	-1.08297	-0.42456
H	1.95641	-0.68093	-0.91231

2-HPP-2o

Geometry with 12 atoms:
Total energy: -343.433069392

C	-1.35302	0.16889	0.43479
H	-1.84936	-0.05545	1.38706
O	-1.65916	-0.57331	-0.55314
C	0.12422	0.61281	0.56385
H	0.19521	1.13557	1.51903
C	0.55234	1.50095	-0.59034
H	-0.03452	2.41810	-0.57964
H	1.60896	1.74595	-0.47589
H	0.40724	0.99740	-1.54279
O	0.97051	-0.50658	0.74942
O	1.11085	-1.18806	-0.48230
H	0.35371	-1.79389	-0.46934

2-HPP-2o'

Geometry with 12 atoms:
Total energy: -343.426710108

C	-1.29871	-0.07365	0.53317
H	-2.10077	0.55331	0.94284
O	-1.56004	-0.77424	-0.49340
C	0.09305	0.63116	0.55935
H	0.13267	1.17771	1.50331
C	0.31846	1.53995	-0.63576
H	-0.41883	2.34255	-0.63014
H	1.31761	1.97403	-0.57655
H	0.22552	0.98012	-1.56313
O	1.09208	-0.34689	0.70869
O	1.16472	-1.09851	-0.48281
H	0.59285	-1.85541	-0.27667

d. The geometries of the transitions states for conformational interconversion of 2-HPP(2) in S_1 state, optimized at TD-M06-2X-D3/6-311++G(2d,p) level of theory

TS[2a-2a']

Geometry with 12 atoms:
Total energy: -343.446082433

C	-0.15765	1.25650	-0.16674
H	0.39318	2.03166	-0.70074
O	-1.40068	1.40678	0.07330
C	0.55661	-0.00931	0.32390
H	0.35500	-0.12988	1.39200
C	2.03623	0.06153	0.01328
H	2.48132	0.91433	0.52378
H	2.52203	-0.85154	0.35377
H	2.19244	0.16390	-1.06072
O	0.05557	-1.15185	-0.34270
O	-1.24974	-1.39088	0.13922
H	-1.79626	-0.89323	-0.48932

TS[2a'-2a]

Geometry with 12 atoms:
Total energy: -343.446082433

C	-0.15765	1.25650	-0.16674
H	0.39318	2.03166	-0.70074
O	-1.40068	1.40678	0.07330
C	0.55661	-0.00931	0.32390
H	0.35500	-0.12988	1.39200
C	2.03623	0.06153	0.01328
H	2.48132	0.91433	0.52378
H	2.52203	-0.85154	0.35377
H	2.19244	0.16390	-1.06072
O	0.05557	-1.15185	-0.34270
O	-1.24974	-1.39088	0.13922
H	-1.79626	-0.89323	-0.48932

TS[2a-2e]

Geometry with 12 atoms:
Total energy: -343.432862360

C	1.01649	-0.49836	0.45603
H	1.38927	-0.10758	1.41131
O	1.82919	-1.17832	-0.24647
C	0.00597	0.43267	-0.27752
H	0.01651	0.15695	-1.33268
C	0.31653	1.89983	-0.05830
H	1.31434	2.12273	-0.43379
H	-0.41203	2.51559	-0.58628
H	0.27495	2.13954	1.00468
O	-1.27851	0.21632	0.25049
O	-1.72125	-1.06160	-0.15969
H	-1.25250	-1.64329	0.46083

TS[2a'-2i']

Geometry with 12 atoms:
Total energy: -343.433775115

C	-0.02231	1.27226	0.42178
H	0.77287	2.01254	0.57540
O	-0.94361	1.53688	-0.40580
C	0.57208	-0.20680	0.39630
H	0.54643	-0.51480	1.44711
C	1.96172	-0.26009	-0.19804
H	2.63630	0.37237	0.37778
H	2.33208	-1.28584	-0.17217
H	1.94110	0.08680	-1.23104
O	-0.22012	-1.05337	-0.36878
O	-1.50349	-1.12413	0.21185
H	-1.95992	-0.37839	-0.21545

TS[2a'-2j]

Geometry with 12 atoms:
Total energy: -343.427692449

C	1.45824	0.02101	0.15479
H	1.79660	0.40956	1.12244
O	1.85994	-1.13734	-0.18533
C	0.02821	0.39323	-0.24853
H	-0.14299	0.05570	-1.27034
C	-0.18328	1.88937	-0.10337
H	0.48708	2.43790	-0.76354
H	-1.21695	2.12236	-0.35954
H	-0.00219	2.19631	0.92723
O	-0.88126	-0.31148	0.59688
O	-1.86484	-0.94674	-0.21177
H	-1.65121	-1.87897	-0.07178

TS[2a-2l']

Geometry with 12 atoms:
Total energy: -343.437140102

C	-0.03357	1.30793	0.28987
H	0.02608	1.86265	1.23459
O	-1.07992	1.47142	-0.41311
C	0.58793	-0.13913	0.37716
H	0.56020	-0.43740	1.42911
C	1.99667	-0.13722	-0.17872
H	2.60465	0.58781	0.35996
H	2.43225	-1.13109	-0.06298
H	1.98024	0.13357	-1.23381
O	-0.14324	-1.05296	-0.38419
O	-1.39849	-1.24986	0.23698
H	-1.93633	-0.55380	-0.17414

TS[2a'-2l]

Geometry with 12 atoms:
Total energy: -343.423221857

C	-0.59931	-1.00367	0.33838
H	-0.60267	-0.96022	1.43331
O	-1.74871	-1.09593	-0.21276
C	0.51277	-0.29812	-0.39436
H	0.46454	-0.60191	-1.44226
C	1.85768	-0.64755	0.21507
H	2.06826	-1.70948	0.09247
H	2.63845	-0.07043	-0.28025
H	1.86659	-0.40191	1.27834
O	0.41056	1.15367	-0.41904
O	-0.74926	1.61354	0.25114
H	-0.36273	2.06975	1.00911

TS[2a-2m]

Geometry with 12 atoms:
Total energy: -343.425699697

C	-0.06324	1.27534	-0.23636
H	0.64005	2.11628	-0.26240
O	-1.27111	1.55113	0.04838
C	0.53635	-0.03817	0.31152
H	0.31634	-0.10879	1.38261
C	2.02096	-0.09373	0.01691
H	2.52931	0.72136	0.53072
H	2.43059	-1.04074	0.36525
H	2.19368	-0.00349	-1.05528
O	-0.03025	-1.15131	-0.33162

O	-1.39310	-1.19906	0.07262
H	-1.51869	-2.15137	0.17168

TS[2a'-2m']

Geometry with 12 atoms:

Total energy: -343.431126971

C	0.07716	1.30467	0.18924
H	-0.28310	1.64594	1.16740
O	1.28617	1.58439	-0.09658
C	-0.52422	-0.01143	-0.31583
H	-0.28721	-0.10005	-1.37848
C	-2.01756	-0.03173	-0.05431
H	-2.48971	0.81164	-0.55455
H	-2.44482	-0.96021	-0.43045
H	-2.21357	0.03646	1.01638
O	-0.00244	-1.14482	0.34879
O	1.34101	-1.28905	-0.11106
H	1.50817	-2.20703	0.13587

TS[2b-2b']

Geometry with 12 atoms:

Total energy: -343.443476478

C	-1.19886	0.20421	-0.41416
H	-1.24896	0.57025	-1.44094
O	-2.20577	-0.40283	0.07862
C	0.02774	0.46582	0.45545
H	-0.30537	0.73578	1.46150
C	0.88121	1.56079	-0.15982
H	0.33659	2.50418	-0.15365
H	1.79485	1.66752	0.42440
H	1.15083	1.30570	-1.18333
O	0.76526	-0.71998	0.71420
O	1.35417	-1.17113	-0.49246
H	0.70224	-1.81685	-0.79968

TS[2b'-2b]

Geometry with 12 atoms:

Total energy: -343.443476478

C	-1.19886	0.20421	-0.41416
H	-1.24896	0.57025	-1.44094
O	-2.20577	-0.40283	0.07862
C	0.02774	0.46582	0.45545
H	-0.30537	0.73578	1.46150
C	0.88121	1.56079	-0.15982
H	0.33659	2.50418	-0.15365
H	1.79485	1.66752	0.42440
H	1.15083	1.30570	-1.18333
O	0.76526	-0.71998	0.71420
O	1.35417	-1.17113	-0.49246
H	0.70224	-1.81685	-0.79968

TS[2b-2f']

Geometry with 12 atoms:

Total energy: -343.430125752

C	-1.07879	-0.48959	-0.35085
H	-0.93133	-0.47203	-1.43801
O	-2.27816	-0.47607	0.07263
C	-0.05665	0.36110	0.45265
H	-0.48718	0.55352	1.43624
C	0.28906	1.65332	-0.26520
H	-0.61556	2.24436	-0.40804
H	1.00079	2.22653	0.33080
H	0.73252	1.43896	-1.23646
O	1.07784	-0.41725	0.75152
O	1.69783	-0.78634	-0.46760
H	1.39898	-1.70301	-0.55653

TS[2b'-2f]

Geometry with 12 atoms:

Total energy: -343.433014083

C	-1.06217	-0.59016	-0.31444
H	-0.66807	-1.58967	-0.52733
O	-2.29298	-0.46804	-0.01381
C	-0.07586	0.33083	0.46204
H	-0.48150	0.50700	1.46224
C	0.12757	1.63877	-0.28211
H	-0.83526	2.13558	-0.39955
H	0.80188	2.28098	0.28729
H	0.54696	1.45147	-1.26867
O	1.12538	-0.33999	0.73158
O	1.74072	-0.63653	-0.52031
H	2.11374	-1.50561	-0.32655

TS[2b'-2k]

Geometry with 12 atoms:

Total energy: -343.423928285

C	1.41839	0.25892	0.34161
H	1.35187	0.42074	1.42506
O	2.29422	-0.58173	-0.04601
C	0.08972	0.32351	-0.41370
H	0.32908	0.36688	-1.47826
C	-0.68752	1.55027	0.01382
H	-0.08119	2.42956	-0.19904
H	-1.62460	1.61784	-0.53389
H	-0.91175	1.52303	1.08007
O	-0.58817	-0.93060	-0.20625
O	-1.95526	-0.73521	0.13496
H	-1.99323	-1.17395	0.99398

TS[2b'-2l]

Geometry with 12 atoms:

Total energy: -343.427958205

C	1.22847	0.19101	0.45069
H	0.97084	-0.05260	1.48943
O	2.19811	-0.44614	-0.06836
C	0.01148	0.47272	-0.44734
H	0.38009	0.73948	-1.43925
C	-0.82605	1.58809	0.15534
H	-0.26002	2.51799	0.14578
H	-1.73375	1.71132	-0.43638

```
 H   -1.10410    1.35230    1.18094
 O   -0.73720   -0.69489   -0.71795
 O   -1.30239   -1.11952    0.52488
 H   -2.00470   -1.69504    0.19869
```

TS[2b'-2m']

```
Geometry with  12 atoms:
Total energy:     -343.424416042
 C   -0.45096   -1.07559    0.33392
 H   -0.46968   -0.99337    1.42760
 O   -1.58378   -1.26815   -0.22605
 C    0.55969   -0.21255   -0.38951
 H    0.52341   -0.47897   -1.44888
 C    1.94833   -0.41905    0.18168
 H    2.63982    0.27134   -0.30164
 H    1.94680   -0.21368    1.25257
 H    2.28435   -1.44071    0.00811
 O    0.27869    1.21384   -0.32857
 O   -0.90703    1.49897    0.38280
 H   -1.57014    1.54131   -0.31973
```

TS[2b-2o]

```
Geometry with  12 atoms:
Total energy:     -343.431602065
 C    0.87814   -1.06392   -0.05046
 H    1.06723   -2.05247    0.38786
 O    1.86286   -0.28189   -0.20153
 C   -0.47819   -0.44532    0.50379
 H   -0.65935   -0.85610    1.50002
 C   -1.59702   -0.79543   -0.45813
 H   -1.66457   -1.87732   -0.56788
 H   -2.53858   -0.41393   -0.05737
 H   -1.40739   -0.35238   -1.43307
 O   -0.34649    0.91945    0.75052
 O   -0.07987    1.58576   -0.46468
 H    0.89309    1.59358   -0.47513
```

TS[2b'-2o']

```
Geometry with  12 atoms:
Total energy:     -343.438230979
 C    1.00190   -0.99362    0.11769
 H    0.97204   -1.92752   -0.45736
 O    1.89498   -0.14509   -0.19704
 C   -0.42599   -0.47068    0.53040
 H   -0.61179   -0.86224    1.53490
 C   -1.49034   -0.93541   -0.44368
 H   -1.51015   -2.02522   -0.47578
 H   -2.46340   -0.57366   -0.10738
 H   -1.29143   -0.55050   -1.44166
 O   -0.41774    0.91143    0.73811
 O   -0.26581    1.56992   -0.50462
 H    0.69997    1.64738   -0.57087
```

TS[2c-2c']

```
Geometry with  12 atoms:
Total energy:     -343.443336700
 C   -0.75986   -0.96330    0.15723
 H   -0.40331   -1.86848    0.65432
 O   -1.96630   -0.93868   -0.25786
 C    0.00795    0.34572    0.38835
 H    0.33198    0.36444    1.43393
 C   -0.80865    1.56903    0.02509
 H   -0.22644    2.46934    0.21527
 H   -1.08240    1.53729   -1.02882
 H   -1.71850    1.59343    0.62318
 O    1.16433    0.40086   -0.42515
 O    2.01177   -0.66523   -0.01978
 H    2.78367   -0.18031    0.30040
```

TS[2c'-2c]

```
Geometry with  12 atoms:
Total energy:     -343.443336700
 C   -0.75986   -0.96330    0.15723
 H   -0.40331   -1.86848    0.65432
 O   -1.96630   -0.93868   -0.25786
 C    0.00795    0.34572    0.38835
 H    0.33198    0.36444    1.43393
 C   -0.80865    1.56903    0.02509
 H   -0.22644    2.46934    0.21527
 H   -1.08240    1.53729   -1.02882
 H   -1.71850    1.59343    0.62318
 O    1.16433    0.40086   -0.42515
 O    2.01177   -0.66523   -0.01978
 H    2.78367   -0.18031    0.30040
```

TS[2c-2e]

```
Geometry with  12 atoms:
Total energy:     -343.433435510
 C    0.86713   -0.82293    0.33985
 H    0.78226   -0.87302    1.43322
 O    2.01063   -1.02852   -0.17842
 C    0.02574    0.33061   -0.27813
 H   -0.05788    0.13196   -1.34984
 C    0.63135    1.69485   -0.00339
 H    0.05727    2.47095   -0.51066
 H    0.63491    1.89503    1.06846
 H    1.65825    1.70790   -0.36594
 O   -1.24596    0.33891    0.29816
 O   -1.94320   -0.79303   -0.22566
 H   -2.79186   -0.68687    0.22213
```

TS[2c'-2e']

```
Geometry with  12 atoms:
Total energy:     -343.429433271
 C   -0.81682   -0.86421   -0.31068
 H   -0.18801   -1.76407   -0.36417
 O   -2.01083   -0.99653    0.09693
 C   -0.02883    0.34398    0.28804
 H    0.08700    0.18140    1.36620
 C   -0.72223    1.65241   -0.02075
```

H	-1.72416	1.63348	0.40673
H	-0.15966	2.48174	0.40805
H	-0.80404	1.78543	-1.09906
O	1.23144	0.40052	-0.31404
O	1.95295	-0.74846	0.11799
H	2.80772	-0.35530	0.33559

TS[2c-2f']

Geometry with 12 atoms:

Total energy: -343.422307613

C	0.72630	-0.87819	0.10637
H	0.35268	-1.20951	1.08530
O	1.98159	-1.00237	-0.08778
C	0.09542	0.41600	-0.41344
H	0.31510	0.46901	-1.48460
C	0.61692	1.65492	0.29492
H	1.69217	1.74559	0.14055
H	0.12297	2.54154	-0.10541
H	0.40918	1.58711	1.36287
O	-1.33361	0.40767	-0.27547
O	-1.83809	-0.77456	0.30560
H	-2.00302	-1.33605	-0.46457

TS[2c-2g']

Geometry with 12 atoms:

Total energy: -343.427143264

C	1.16162	-0.79283	0.21296
H	1.11377	-1.08509	1.27026
O	2.30708	-0.52209	-0.27289
C	0.00137	0.14494	-0.20974
H	-0.19963	-0.03080	-1.26730
C	0.30754	1.60702	0.06371
H	-0.52924	2.22601	-0.26588
H	0.46723	1.76375	1.13098
H	1.20711	1.90729	-0.47363
O	-1.12149	-0.27965	0.54061
O	-2.19452	-0.53660	-0.35206
H	-2.81093	0.17084	-0.12126

TS[2c'-2g]

Geometry with 12 atoms:

Total energy: -343.429821875

C	1.14907	-0.77698	0.24194
H	0.86504	-1.83581	0.28146
O	2.31865	-0.50596	-0.18570
C	0.00089	0.15258	-0.20651
H	-0.22666	-0.02918	-1.26118
C	0.34613	1.60771	0.04077
H	1.24284	1.87614	-0.51970
H	-0.48181	2.24013	-0.28225
H	0.53294	1.77141	1.10180
O	-1.12797	-0.23670	0.55775
O	-2.20032	-0.51922	-0.33225
H	-2.83183	0.17245	-0.09571

TS[2c-2i]

Geometry with 12 atoms:

Total energy: -343.436334126

C	-0.74621	-0.97957	0.00826
H	-0.21925	-1.60472	-0.72124
O	-2.01980	-0.94926	-0.02439
C	-0.00655	0.34697	0.35002
H	0.20046	0.33137	1.42643
C	-0.79297	1.57859	-0.04875
H	-0.22853	2.47460	0.20860
H	-0.98696	1.56801	-1.12087
H	-1.74668	1.58796	0.47720
O	1.20737	0.41660	-0.35230
O	2.00554	-0.68965	0.04317
H	2.71043	-0.25477	0.54079

TS[2c-2m]

Geometry with 12 atoms:

Total energy: -343.437766507

C	1.04239	-0.50722	0.45512
H	1.40290	-0.15989	1.42989
O	1.85327	-1.19890	-0.24805
C	0.03186	0.40266	-0.26527
H	0.02548	0.11631	-1.31861
C	0.35207	1.87606	-0.08155
H	-0.37857	2.49148	-0.60776
H	0.33139	2.13377	0.97780
H	1.34591	2.08319	-0.47587
O	-1.25985	0.23206	0.27727
O	-1.69606	-1.08304	-0.03704
H	-2.46387	-0.89484	-0.59259

TS[2c'-2m']

Geometry with 12 atoms:

Total energy: -343.433856725

C	1.05036	-0.48661	0.46904
H	0.62918	-0.97187	1.35779
O	1.85633	-1.17190	-0.24305
C	0.04559	0.43558	-0.26472
H	0.07122	0.18421	-1.32859
C	0.36227	1.90016	-0.02580
H	1.36778	2.11301	-0.38464
H	-0.35366	2.52892	-0.55763
H	0.31739	2.12236	1.03999
O	-1.25590	0.24299	0.24144
O	-1.64897	-1.08829	-0.06538
H	-2.39293	-0.93385	-0.66209

TS[2d-2d']

Geometry with 12 atoms:

Total energy: -343.440613613

C	-1.25962	-0.27693	0.53805
H	-1.92204	-0.32161	1.40353
O	-1.69323	-0.72458	-0.57526
C	0.02111	0.54705	0.59431

H	0.02156	1.05318	1.56122
C	0.12687	1.54201	-0.55161
H	-0.70359	2.24579	-0.50778
H	1.06432	2.09478	-0.47251
H	0.08742	1.02759	-1.51018
O	1.17719	-0.27554	0.69339
O	1.27681	-1.04218	-0.49633
H	2.03599	-0.63411	-0.93319

TS[2d'-2d]

Geometry with 12 atoms:

Total energy: -343.440613613

C	-1.25962	-0.27693	0.53805
H	-1.92204	-0.32161	1.40353
O	-1.69323	-0.72458	-0.57526
C	0.02111	0.54705	0.59431
H	0.02156	1.05318	1.56122
C	0.12687	1.54201	-0.55161
H	-0.70359	2.24579	-0.50778
H	1.06432	2.09478	-0.47251
H	0.08742	1.02759	-1.51018
O	1.17719	-0.27554	0.69339
O	1.27681	-1.04218	-0.49633
H	2.03599	-0.63411	-0.93319

TS[2d-2e']

Geometry with 12 atoms:

Total energy: -343.421446251

C	0.74160	-0.87121	0.07898
H	0.21789	-1.79538	-0.20137
O	2.01566	-0.91167	0.02641
C	0.09073	0.41217	-0.44051
H	0.31941	0.51316	-1.50923
C	0.58378	1.62984	0.31861
H	0.07529	2.51988	-0.05241
H	0.38079	1.51713	1.38407
H	1.65881	1.74714	0.17556
O	-1.34084	0.36135	-0.35701
O	-1.83038	-0.81950	0.24163
H	-1.90443	-0.56819	1.17260

TS[2d-2f]

Geometry with 12 atoms:

Total energy: -343.433285240

C	-1.03082	-0.77111	-0.09591
H	-0.84712	-1.80602	0.21812
O	-2.24100	-0.39750	-0.22285
C	-0.05316	0.24827	0.54879
H	-0.33543	0.39605	1.59820
C	-0.06938	1.56539	-0.20285
H	0.65278	2.24823	0.24563
H	0.17841	1.41080	-1.25079
H	-1.06887	1.99632	-0.13722
O	1.21626	-0.32539	0.66419
O	1.74378	-0.47790	-0.65751
H	2.58796	-0.89434	-0.44479

TS[2d'-2f']

Geometry with 12 atoms:

Total energy: -343.427954828

C	-1.03411	-0.78360	-0.04262
H	-0.58954	-1.30417	-0.90282
O	-2.25052	-0.43090	-0.11598
C	-0.05820	0.29334	0.53497
H	-0.37877	0.49852	1.55875
C	-0.03812	1.55999	-0.30047
H	-1.03873	1.99106	-0.31386
H	0.65708	2.27886	0.13722
H	0.26374	1.34294	-1.32327
O	1.19844	-0.29402	0.71318
O	1.70450	-0.61792	-0.58086
H	2.64951	-0.48284	-0.43797

TS[2d-2h]

Geometry with 12 atoms:

Total energy: -343.424069287

C	-1.28945	-0.59665	-0.30255
H	-1.21081	-1.68968	-0.36804
O	-2.43173	-0.10477	-0.03456
C	-0.07770	0.05115	0.41901
H	-0.28321	0.04006	1.49758
C	0.13121	1.47040	-0.06246
H	0.94971	1.94772	0.47416
H	0.34476	1.48652	-1.12951
H	-0.78933	2.02361	0.12524
O	0.99679	-0.85275	0.17784
O	2.14263	-0.18089	-0.31372
H	2.74295	-0.25038	0.44009

TS[2d'-2h']

Geometry with 12 atoms:

Total energy: -343.426453786

C	-1.28927	-0.62173	-0.26071
H	-1.08276	-0.89935	-1.30245
O	-2.44549	-0.16084	0.00661
C	-0.08284	0.05571	0.43604
H	-0.30720	0.06828	1.50661
C	0.14503	1.46628	-0.07151
H	-0.77570	2.02711	0.08885
H	0.95660	1.95279	0.46903
H	0.38289	1.46509	-1.13382
O	0.99578	-0.85462	0.23295
O	2.12791	-0.20109	-0.32119
H	2.76295	-0.28316	0.40188

TS[2d-2l]

Geometry with 12 atoms:

Total energy: -343.432648026

C	-1.09352	-0.51018	-0.35702
H	-0.71483	-1.49072	-0.66631

O	-2.31233	-0.41521	0.00323
C	-0.07158	0.33752	0.45097
H	-0.49230	0.52938	1.44133
C	0.23586	1.63748	-0.27099
H	0.95032	2.22363	0.31168
H	0.63824	1.43677	-1.26272
H	-0.68378	2.21032	-0.38714
O	1.07824	-0.41947	0.74516
O	1.66050	-0.83919	-0.48126
H	2.46653	-0.30740	-0.51163

TS[2d-2n']

Geometry with 12 atoms:

Total energy: -343.441723299

C	-1.10232	-0.69885	0.33504
H	-1.34981	-1.44194	1.09872
O	-2.00492	-0.43330	-0.52843
C	0.00371	0.31375	0.65320
H	-0.05871	0.58223	1.71276
C	-0.08739	1.54715	-0.22530
H	0.73282	2.22478	0.01291
H	-0.03808	1.27080	-1.27682
H	-1.03398	2.05643	-0.04479
O	1.27590	-0.30665	0.61236
O	1.54766	-0.69952	-0.72757
H	2.31470	-0.14881	-0.93120

TS[2d'-2n]

Geometry with 12 atoms:

Total energy: -343.436424391

C	-1.06992	-0.75042	0.34928
H	-0.65871	-1.76298	0.26652
O	-2.06020	-0.46018	-0.40128
C	-0.00497	0.33770	0.63530
H	-0.10034	0.63418	1.68502
C	-0.14482	1.54063	-0.27743
H	-1.12138	2.00145	-0.12685
H	0.63200	2.26815	-0.03906
H	-0.06470	1.24176	-1.32082
O	1.28409	-0.23316	0.62468
O	1.56638	-0.68572	-0.69482
H	2.30927	-0.11756	-0.93642

TS[2e-2a]

Geometry with 12 atoms:

Total energy: -343.432862360

C	1.01649	-0.49836	0.45603
H	1.38927	-0.10758	1.41131
O	1.82919	-1.17832	-0.24647
C	0.00597	0.43267	-0.27752
H	0.01651	0.15695	-1.33268
C	0.31653	1.89983	-0.05830
H	1.31434	2.12273	-0.43379
H	-0.41203	2.51559	-0.58628
H	0.27495	2.13954	1.00468
O	-1.27851	0.21632	0.25049
O	-1.72125	-1.06160	-0.15969
H	-1.25250	-1.64329	0.46083

TS[2e-2c]

Geometry with 12 atoms:

Total energy: -343.433435510

C	0.86713	-0.82293	0.33985
H	0.78226	-0.87302	1.43322
O	2.01063	-1.02852	-0.17842
C	0.02574	0.33061	-0.27813
H	-0.05788	0.13196	-1.34984
C	0.63135	1.69485	-0.00339
H	0.05727	2.47095	-0.51066
H	0.63491	1.89503	1.06846
H	1.65825	1.70790	-0.36594
O	-1.24596	0.33891	0.29816
O	-1.94320	-0.79303	-0.22566
H	-2.79186	-0.68687	0.22213

TS[2e'-2c']

Geometry with 12 atoms:

Total energy: -343.429433271

C	-0.81682	-0.86421	-0.31068
H	-0.18801	-1.76407	-0.36417
O	-2.01083	-0.99653	0.09693
C	-0.02883	0.34398	0.28804
H	0.08700	0.18140	1.36620
C	-0.72223	1.65241	-0.02075
H	-1.72416	1.63348	0.40673
H	-0.15966	2.48174	0.40805
H	-0.80404	1.78543	-1.09906
O	1.23144	0.40052	-0.31404
O	1.95295	-0.74846	0.11799
H	2.80772	-0.35530	0.33559

TS[2e'-2d]

Geometry with 12 atoms:

Total energy: -343.421446251

C	0.74160	-0.87121	0.07898
H	0.21789	-1.79538	-0.20137
O	2.01566	-0.91167	0.02641
C	0.09073	0.41217	-0.44051
H	0.31941	0.51316	-1.50923
C	0.58378	1.62984	0.31861
H	0.07529	2.51988	-0.05241
H	0.38079	1.51713	1.38407
H	1.65881	1.74714	0.17556
O	-1.34084	0.36135	-0.35701
O	-1.83038	-0.81950	0.24163
H	-1.90443	-0.56819	1.17260

TS[2e-2h']

Geometry with 12 atoms:

Total energy: -343.425447014

C	1.17190	-0.76674	0.26204
H	1.18183	-0.92693	1.34888
O	2.28845	-0.56146	-0.31176
C	0.00675	0.15157	-0.19812
H	-0.17078	-0.04391	-1.25634
C	0.28447	1.62108	0.05409
H	-0.56371	2.21317	-0.29364
H	0.42570	1.79737	1.12077
H	1.18433	1.92810	-0.47897
O	-1.11735	-0.28360	0.54456
O	-2.22871	-0.36531	-0.33073
H	-2.37521	-1.32027	-0.36531

TS[2e'-2h]

Geometry with 12 atoms:
Total energy: -343.429505998

C	1.13238	-0.80530	0.21724
H	0.84655	-1.86387	0.20883
O	2.31184	-0.52374	-0.17319
C	0.00035	0.15579	-0.21260
H	-0.24129	-0.00502	-1.26764
C	0.37658	1.59952	0.05007
H	-0.45190	2.24450	-0.24301
H	0.58681	1.74241	1.10961
H	1.26565	1.86136	-0.52555
O	-1.12990	-0.21663	0.55739
O	-2.24729	-0.31690	-0.31746
H	-2.53882	-1.22131	-0.14450

TS[2e'-2i']

Geometry with 12 atoms:
Total energy: -343.433213975

C	-0.69847	-0.99063	0.07766
H	-0.33017	-1.83339	0.67457
O	-1.93563	-0.98369	-0.21008
C	-0.00132	0.36835	0.38284
H	0.26204	0.37783	1.44473
C	-0.84674	1.56025	-0.00876
H	-0.30012	2.47724	0.20616
H	-1.08159	1.52396	-1.07191
H	-1.77710	1.55214	0.55711
O	1.18452	0.46337	-0.36700
O	2.06580	-0.54546	0.08951
H	1.98859	-1.19941	-0.62055

TS[2e'-2i]

Geometry with 12 atoms:
Total energy: -343.444274667

C	-0.77987	-0.90509	0.45000
H	-0.63171	-1.61472	1.26512
O	-1.62052	-1.18038	-0.46574
C	-0.02755	0.43074	0.43169
H	0.35286	0.56729	1.44625
C	-0.89451	1.58972	-0.02581
H	-0.32412	2.51588	0.03032
H	-1.21922	1.43486	-1.05411
H	-1.77379	1.66531	0.61175
O	1.07257	0.41233	-0.46172
O	2.04660	-0.47667	0.04834
H	1.81837	-1.30309	-0.40172

TS[2f-2b']

Geometry with 12 atoms:
Total energy: -343.433014083

C	-1.06217	-0.59016	-0.31444
H	-0.66807	-1.58967	-0.52733
O	-2.29298	-0.46804	-0.01381
C	-0.07586	0.33083	0.46204
H	-0.48150	0.50700	1.46224
C	0.12757	1.63877	-0.28211
H	-0.83526	2.13558	-0.39955
H	0.80188	2.28098	0.28729
H	0.54696	1.45147	-1.26867
O	1.12538	-0.33999	0.73158
O	1.74072	-0.63653	-0.52031
H	2.11374	-1.50561	-0.32655

TS[2f'-2b]

Geometry with 12 atoms:
Total energy: -343.430125752

C	-1.07879	-0.48959	-0.35085
H	-0.93133	-0.47203	-1.43801
O	-2.27816	-0.47607	0.07263
C	-0.05665	0.36110	0.45265
H	-0.48718	0.55352	1.43624
C	0.28906	1.65332	-0.26520
H	-0.61556	2.24436	-0.40804
H	1.00079	2.22653	0.33080
H	0.73252	1.43896	-1.23646
O	1.07784	-0.41725	0.75152
O	1.69783	-0.78634	-0.46760
H	1.39898	-1.70301	-0.55653

TS[2f'-2c]

Geometry with 12 atoms:
Total energy: -343.422307613

C	0.72630	-0.87819	0.10637
H	0.35268	-1.20951	1.08530
O	1.98159	-1.00237	-0.08778
C	0.09542	0.41600	-0.41344
H	0.31510	0.46901	-1.48460
C	0.61692	1.65492	0.29492
H	1.69217	1.74559	0.14055
H	0.12297	2.54154	-0.10541
H	0.40918	1.58711	1.36287
O	-1.33361	0.40767	-0.27547
O	-1.83809	-0.77456	0.30560
H	-2.00302	-1.33605	-0.46457

TS[2f-2d]

Geometry with 12 atoms:
Total energy: -343.433285240

C	-1.03082	-0.77111	-0.09591
H	-0.84712	-1.80602	0.21812
O	-2.24100	-0.39750	-0.22285
C	-0.05316	0.24827	0.54879
H	-0.33543	0.39605	1.59820
C	-0.06938	1.56539	-0.20285
H	0.65278	2.24823	0.24563
H	0.17841	1.41080	-1.25079
H	-1.06887	1.99632	-0.13722
O	1.21626	-0.32539	0.66419
O	1.74378	-0.47790	-0.65751
H	2.58796	-0.89434	-0.44479

TS[2f'-2d']
Geometry with 12 atoms:
Total energy: -343.427954828

C	-1.03411	-0.78360	-0.04262
H	-0.58954	-1.30417	-0.90282
O	-2.25052	-0.43090	-0.11598
C	-0.05820	0.29334	0.53497
H	-0.37877	0.49852	1.55875
C	-0.03812	1.55999	-0.30047
H	-1.03873	1.99106	-0.31386
H	0.65708	2.27886	0.13722
H	0.26374	1.34294	-1.32327
O	1.19844	-0.29402	0.71318
O	1.70450	-0.61792	-0.58086
H	2.64951	-0.48284	-0.43797

TS[2f-2f']
Geometry with 12 atoms:
Total energy: -343.433014097

C	-1.06217	-0.59016	-0.31444
H	-0.66807	-1.58967	-0.52733
O	-2.29298	-0.46804	-0.01381
C	-0.07586	0.33083	0.46204
H	-0.48150	0.50700	1.46224
C	0.12757	1.63877	-0.28211
H	-0.83526	2.13558	-0.39955
H	0.80188	2.28098	0.28729
H	0.54696	1.45147	-1.26867
O	1.12538	-0.33999	0.73158
O	1.74072	-0.63653	-0.52031
H	2.11374	-1.50561	-0.32655

TS[2f'-2f]
Geometry with 12 atoms:
Total energy: -343.433014097

C	-1.06217	-0.59016	-0.31444
H	-0.66807	-1.58967	-0.52733
O	-2.29298	-0.46804	-0.01381
C	-0.07586	0.33083	0.46204
H	-0.48150	0.50700	1.46224
C	0.12757	1.63877	-0.28211
H	-0.83526	2.13558	-0.39955
H	0.80188	2.28098	0.28729
H	0.54696	1.45147	-1.26867
O	1.12538	-0.33999	0.73158
O	1.74072	-0.63653	-0.52031
H	2.11374	-1.50561	-0.32655

TS[2f-2g]
Geometry with 12 atoms:
Total energy: -343.422439263

C	-1.28153	-0.63116	-0.27678
H	-1.23210	-1.72738	-0.23186
O	-2.41393	-0.08774	-0.08303
C	-0.07524	0.04700	0.43351
H	-0.27202	0.04045	1.51249
C	0.11129	1.46467	-0.05894
H	-0.80779	2.01359	0.14749
H	0.94191	1.94415	0.45462
H	0.29130	1.48260	-1.13340
O	1.00377	-0.84756	0.18403
O	2.18976	-0.14501	-0.13544
H	2.31474	-0.39394	-1.06057

TS[2f'-2g']
Geometry with 12 atoms:
Total energy: -343.425767005

C	1.28859	-0.60875	0.28045
H	1.09330	-0.85213	1.33252
O	2.44865	-0.17434	-0.01163
C	0.08815	0.06999	-0.42784
H	0.33207	0.09920	-1.49266
C	-0.16302	1.47174	0.09206
H	0.75386	2.04418	-0.04878
H	-0.97432	1.95112	-0.45416
H	-0.41211	1.45971	1.15242
O	-0.98494	-0.85259	-0.25817
O	-2.17532	-0.18075	0.13073
H	-2.38237	-0.63849	0.95513

TS[2f-2o']
Geometry with 12 atoms:
Total energy: -343.434115407

C	-1.06275	-0.69361	0.37694
H	-1.34523	-1.29561	1.24877
O	-1.97493	-0.47108	-0.48017
C	0.03645	0.37491	0.63801
H	-0.02891	0.68661	1.68409
C	-0.08372	1.55985	-0.29939
H	-1.03912	2.05835	-0.13671
H	0.72924	2.25636	-0.09683
H	-0.02456	1.23666	-1.33608
O	1.30023	-0.24794	0.60036
O	1.58498	-0.64523	-0.72785
H	1.08653	-1.47528	-0.79546

TS[2g-2c']

Geometry with 12 atoms:
Total energy: -343.429821875

C	1.14907	-0.77698	0.24194
H	0.86504	-1.83581	0.28146
O	2.31865	-0.50596	-0.18570
C	0.00089	0.15258	-0.20651
H	-0.22666	-0.02918	-1.26118
C	0.34613	1.60771	0.04077
H	1.24284	1.87614	-0.51970
H	-0.48181	2.24013	-0.28225
H	0.53294	1.77141	1.10180
O	-1.12797	-0.23670	0.55775
O	-2.20032	-0.51922	-0.33225
H	-2.83183	0.17245	-0.09571

TS[2g'-2c]

Geometry with 12 atoms:
Total energy: -343.427143264

C	1.16162	-0.79283	0.21296
H	1.11377	-1.08509	1.27026
O	2.30708	-0.52209	-0.27289
C	0.00137	0.14494	-0.20974
H	-0.19963	-0.03080	-1.26730
C	0.30754	1.60702	0.06371
H	-0.52924	2.22601	-0.26588
H	0.46723	1.76375	1.13098
H	1.20711	1.90729	-0.47363
O	-1.12149	-0.27965	0.54061
O	-2.19452	-0.53660	-0.35206
H	-2.81093	0.17084	-0.12126

TS[2g-2f]

Geometry with 12 atoms:
Total energy: -343.422439263

C	-1.28153	-0.63116	-0.27678
H	-1.23210	-1.72738	-0.23186
O	-2.41393	-0.08774	-0.08303
C	-0.07524	0.04700	0.43351
H	-0.27202	0.04045	1.51249
C	0.11129	1.46467	-0.05894
H	-0.80779	2.01359	0.14749
H	0.94191	1.94415	0.45462
H	0.29130	1.48260	-1.13340
O	1.00377	-0.84756	0.18403
O	2.18976	-0.14501	-0.13544
H	2.31474	-0.39394	-1.06057

TS[2g'-2f']

Geometry with 12 atoms:
Total energy: -343.425767005

C	1.28859	-0.60875	0.28045
H	1.09330	-0.85213	1.33252
O	2.44865	-0.17434	-0.01163
C	0.08815	0.06999	-0.42784
H	0.33207	0.09920	-1.49266
C	-0.16302	1.47174	0.09206
H	0.75386	2.04418	-0.04878
H	-0.97432	1.95112	-0.45416
H	-0.41211	1.45971	1.15242
O	-0.98494	-0.85259	-0.25817
O	-2.17532	-0.18075	0.13073
H	-2.38237	-0.63849	0.95513

TS[2g-2g']

Geometry with 12 atoms:
Total energy: -343.442014418

C	-1.27562	-0.74152	0.11250
H	-1.38515	-1.74862	0.52604
O	-2.36259	-0.14028	-0.20389
C	0.00099	0.02675	0.38069
H	0.28092	-0.06880	1.43600
C	-0.09701	1.48406	-0.02416
H	-0.86157	1.98974	0.56641
H	0.85859	1.97475	0.15501
H	-0.35566	1.56438	-1.08025
O	0.98871	-0.68026	-0.37638
O	2.25775	-0.24442	0.11167
H	2.62167	0.19247	-0.66861

TS[2g'-2g]

Geometry with 12 atoms:
Total energy: -343.442014418

C	-1.27562	-0.74152	0.11250
H	-1.38515	-1.74862	0.52604
O	-2.36259	-0.14028	-0.20389
C	0.00099	0.02675	0.38069
H	0.28092	-0.06880	1.43600
C	-0.09701	1.48406	-0.02416
H	-0.86157	1.98974	0.56641
H	0.85859	1.97475	0.15501
H	-0.35566	1.56438	-1.08025
O	0.98871	-0.68026	-0.37638
O	2.25775	-0.24442	0.11167
H	2.62167	0.19247	-0.66861

TS[2g-2h]

Geometry with 12 atoms:
Total energy: -343.433016996

C	-1.25478	-0.74545	-0.10985
H	-1.19382	-1.82388	0.08335
O	-2.40396	-0.21479	0.07477
C	-0.01346	0.05681	0.27427
H	0.17486	-0.03652	1.35214
C	-0.11958	1.51242	-0.13256
H	-0.92412	1.99772	0.42171
H	0.82111	2.01492	0.08890
H	-0.32710	1.58578	-1.19986
O	1.03330	-0.61423	-0.40594

O	2.23265	-0.16670	0.24132
H	2.88002	-0.71492	-0.21854

TS[2g-2k]

Geometry with 12 atoms:
Total energy: -343.429766763

C	1.37508	-0.35181	0.40631
H	1.27397	-1.21246	1.07926
O	2.41530	-0.32237	-0.33596
C	0.05656	0.12906	-0.21787
H	0.09982	-0.01172	-1.30263
C	-0.22656	1.57806	0.13349
H	0.59207	2.20400	-0.22174
H	-1.14983	1.90867	-0.34410
H	-0.30494	1.68993	1.21550
O	-0.90889	-0.76674	0.32039
O	-2.14217	-0.48859	-0.32752
H	-2.65551	-0.08869	0.38684

TS[2g'-2k']

Geometry with 12 atoms:
Total energy: -343.433120880

C	-1.27088	-0.77233	0.03231
H	-1.13520	-1.55507	-0.72499
O	-2.39737	-0.16815	0.03925
C	-0.00796	0.04906	0.33201
H	0.19200	0.00947	1.40760
C	-0.10032	1.48477	-0.15012
H	-0.91071	2.00239	0.36359
H	0.83385	2.00357	0.06640
H	-0.29539	1.50852	-1.22279
O	1.01450	-0.67929	-0.33502
O	2.25026	-0.24565	0.21605
H	2.65134	0.20686	-0.53722

TS[2h-2d]

Geometry with 12 atoms:
Total energy: -343.424069287

C	-1.28945	-0.59665	-0.30255
H	-1.21081	-1.68968	-0.36804
O	-2.43173	-0.10477	-0.03456
C	-0.07770	0.05115	0.41901
H	-0.28321	0.04006	1.49758
C	0.13121	1.47040	-0.06246
H	0.94971	1.94772	0.47416
H	0.34476	1.48652	-1.12951
H	-0.78933	2.02361	0.12524
O	0.99679	-0.85275	0.17784
O	2.14263	-0.18089	-0.31372
H	2.74295	-0.25038	0.44009

TS[2h'-2d']

Geometry with 12 atoms:
Total energy: -343.426453786

C	-1.28927	-0.62173	-0.26071
H	-1.08276	-0.89935	-1.30245
O	-2.44549	-0.16084	0.00661
C	-0.08284	0.05571	0.43604
H	-0.30720	0.06828	1.50661
C	0.14503	1.46628	-0.07151
H	-0.77570	2.02711	0.08885
H	0.95660	1.95279	0.46903
H	0.38289	1.46509	-1.13382
O	0.99578	-0.85462	0.23295
O	2.12791	-0.20109	-0.32119
H	2.76295	-0.28316	0.40188

TS[2h-2e']

Geometry with 12 atoms:
Total energy: -343.429505998

C	1.13238	-0.80530	0.21724
H	0.84655	-1.86387	0.20883
O	2.31184	-0.52374	-0.17319
C	0.00035	0.15579	-0.21260
H	-0.24129	-0.00502	-1.26764
C	0.37658	1.59952	0.05007
H	-0.45190	2.24450	-0.24301
H	0.58681	1.74241	1.10961
H	1.26565	1.86136	-0.52555
O	-1.12990	-0.21663	0.55739
O	-2.24729	-0.31690	-0.31746
H	-2.53882	-1.22131	-0.14450

TS[2h'-2e]

Geometry with 12 atoms:
Total energy: -343.425447014

C	1.17190	-0.76674	0.26204
H	1.18183	-0.92693	1.34888
O	2.28845	-0.56146	-0.31176
C	0.00675	0.15157	-0.19812
H	-0.17078	-0.04391	-1.25634
C	0.28447	1.62108	0.05409
H	-0.56371	2.21317	-0.29364
H	0.42570	1.79737	1.12077
H	1.18433	1.92810	-0.47897
O	-1.11735	-0.28360	0.54456
O	-2.22871	-0.36531	-0.33073
H	-2.37521	-1.32027	-0.36531

TS[2h-2g]

Geometry with 12 atoms:
Total energy: -343.433016996

C	-1.25478	-0.74545	-0.10985
H	-1.19382	-1.82388	0.08335
O	-2.40396	-0.21479	0.07477
C	-0.01346	0.05681	0.27427
H	0.17486	-0.03652	1.35214
C	-0.11958	1.51242	-0.13256
H	-0.92412	1.99772	0.42171
H	0.82111	2.01492	0.08890

H	-0.32710	1.58578	-1.19986
O	1.03330	-0.61423	-0.40594
O	2.23265	-0.16670	0.24132
H	2.88002	-0.71492	-0.21854

TS[2h-2h']

Geometry with 12 atoms:

Total energy: -343.439834123

C	-1.25513	-0.76457	0.08063
H	-1.32081	-1.78286	0.47739
O	-2.37450	-0.18069	-0.13710
C	0.00363	0.03681	0.35365
H	0.29028	-0.05901	1.40835
C	-0.13142	1.49371	-0.03853
H	-0.88622	1.98315	0.57800
H	0.82609	1.99085	0.10789
H	-0.41928	1.57193	-1.08656
O	1.00598	-0.62587	-0.42215
O	2.26181	-0.11715	0.02612
H	2.66117	-0.91024	0.40543

TS[2h'-2h]

Geometry with 12 atoms:

Total energy: -343.439834123

C	-1.25513	-0.76457	0.08063
H	-1.32081	-1.78286	0.47739
O	-2.37450	-0.18069	-0.13710
C	0.00363	0.03681	0.35365
H	0.29028	-0.05901	1.40835
C	-0.13142	1.49371	-0.03853
H	-0.88622	1.98315	0.57800
H	0.82609	1.99085	0.10789
H	-0.41928	1.57193	-1.08656
O	1.00598	-0.62587	-0.42215
O	2.26181	-0.11715	0.02612
H	2.66117	-0.91024	0.40543

TS[2h-2j]

Geometry with 12 atoms:

Total energy: -343.430954066

C	1.35895	-0.42139	0.38542
H	1.24673	-1.33285	0.98557
O	2.40376	-0.33349	-0.34512
C	0.04938	0.12154	-0.20957
H	0.05898	-0.02940	-1.29567
C	-0.15379	1.58400	0.13536
H	0.67191	2.17031	-0.26859
H	-1.09058	1.93905	-0.29439
H	-0.17868	1.70627	1.21781
O	-0.94560	-0.71421	0.36748
O	-2.18790	-0.33303	-0.20665
H	-2.39767	-1.11247	-0.73762

TS[2h'-2j']

Geometry with 12 atoms:

Total energy: -343.433566514

C	-1.25598	-0.78943	0.10636
H	-1.09820	-1.67542	-0.52111
O	-2.38258	-0.19745	-0.01532
C	0.00135	0.05900	0.34586
H	0.25616	0.02123	1.41114
C	-0.14039	1.49304	-0.12331
H	-0.91885	2.00140	0.44657
H	0.80678	2.01044	0.02473
H	-0.40425	1.51465	-1.18031
O	1.01090	-0.63679	-0.37797
O	2.26004	-0.11380	0.05570
H	2.62162	-0.86366	0.54619

TS[2i'-2a']

Geometry with 12 atoms:

Total energy: -343.433775115

C	-0.02231	1.27226	0.42178
H	0.77287	2.01254	0.57540
O	-0.94361	1.53688	-0.40580
C	0.57208	-0.20680	0.39630
H	0.54643	-0.51480	1.44711
C	1.96172	-0.26009	-0.19804
H	2.63630	0.37237	0.37778
H	2.33208	-1.28584	-0.17217
H	1.94110	0.08680	-1.23104
O	-0.22012	-1.05337	-0.36878
O	-1.50349	-1.12413	0.21185
H	-1.95992	-0.37839	-0.21545

TS[2i-2c]

Geometry with 12 atoms:

Total energy: -343.436334126

C	-0.74621	-0.97957	0.00826
H	-0.21925	-1.60472	-0.72124
O	-2.01980	-0.94926	-0.02439
C	-0.00655	0.34697	0.35002
H	0.20046	0.33137	1.42643
C	-0.79297	1.57859	-0.04875
H	-0.22853	2.47460	0.20860
H	-0.98696	1.56801	-1.12087
H	-1.74668	1.58796	0.47720
O	1.20737	0.41660	-0.35230
O	2.00554	-0.68965	0.04317
H	2.71043	-0.25477	0.54079

TS[2i-2e']

Geometry with 12 atoms:

Total energy: -343.444274667

C	-0.77987	-0.90509	0.45000
H	-0.63171	-1.61472	1.26512
O	-1.62052	-1.18038	-0.46574
C	-0.02755	0.43074	0.43169
H	0.35286	0.56729	1.44625
C	-0.89451	1.58972	-0.02581

H	-0.32412	2.51588	0.03032
H	-1.21922	1.43486	-1.05411
H	-1.77379	1.66531	0.61175
O	1.07257	0.41233	-0.46172
O	2.04660	-0.47667	0.04834
H	1.81837	-1.30309	-0.40172

TS[2i'-2e']

Geometry with 12 atoms:

Total energy: -343.433213975

C	-0.69847	-0.99063	0.07766
H	-0.33017	-1.83339	0.67457
O	-1.93563	-0.98369	-0.21008
C	-0.00132	0.36835	0.38284
H	0.26204	0.37783	1.44473
C	-0.84674	1.56025	-0.00876
H	-0.30012	2.47724	0.20616
H	-1.08159	1.52396	-1.07191
H	-1.77710	1.55214	0.55711
O	1.18452	0.46337	-0.36700
O	2.06580	-0.54546	0.08951
H	1.98859	-1.19941	-0.62055

TS[2i-2k']

Geometry with 12 atoms:

Total energy: -343.426641887

C	-1.21084	-0.66247	0.51210
H	-1.01964	-1.64463	0.96341
O	-2.06368	-0.65380	-0.43584
C	0.01568	0.24297	0.40526
H	0.50335	0.21517	1.37859
C	-0.35309	1.65515	-0.01264
H	-1.07688	2.08132	0.68126
H	0.54300	2.27633	-0.02088
H	-0.78592	1.64793	-1.01275
O	0.93401	-0.30779	-0.54950
O	2.17590	-0.54628	0.10293
H	2.75587	0.07295	-0.35863

TS[2i-2l']

Geometry with 12 atoms:

Total energy: -343.428735132

C	-0.79063	-0.92985	0.48532
H	-0.15750	-1.75103	0.84647
O	-1.59339	-1.19717	-0.46078
C	-0.05042	0.42575	0.43684
H	0.34164	0.57420	1.44629
C	-0.95139	1.55723	-0.01421
H	-1.83181	1.59661	0.62491
H	-0.41604	2.50371	0.04832
H	-1.27162	1.39385	-1.04261
O	1.03057	0.41211	-0.46958
O	1.97687	-0.51730	0.05773
H	2.77761	-0.21719	-0.39007

TS[2i'-2l']

Geometry with 12 atoms:

Total energy: -343.444274677

C	-0.77987	-0.90509	0.45000
H	-0.63171	-1.61472	1.26512
O	-1.62052	-1.18038	-0.46574
C	-0.02755	0.43074	0.43169
H	0.35286	0.56730	1.44625
C	-0.89451	1.58972	-0.02581
H	-1.77380	1.66531	0.61176
H	-0.32412	2.51588	0.03032
H	-1.21922	1.43486	-1.05411
O	1.07257	0.41233	-0.46172
O	2.04660	-0.47667	0.04834
H	1.81837	-1.30309	-0.40172

TS[2i'-2n']

Geometry with 12 atoms:

Total energy: -343.421446259

C	0.74160	-0.87121	0.07898
H	0.21789	-1.79538	-0.20137
O	2.01566	-0.91167	0.02641
C	0.09073	0.41217	-0.44051
H	0.31941	0.51316	-1.50923
C	0.58378	1.62984	0.31861
H	1.65881	1.74714	0.17556
H	0.07529	2.51988	-0.05241
H	0.38079	1.51713	1.38407
O	-1.34084	0.36135	-0.35701
O	-1.83038	-0.81950	0.24163
H	-1.90443	-0.56819	1.17260

TS[2i-2o]

Geometry with 12 atoms:

Total energy: -343.423550459

C	0.59041	0.95985	0.60165
H	0.07953	1.55078	1.37041
O	0.87799	1.60086	-0.46535
C	0.28999	-0.51787	0.53590
H	0.33049	-0.87587	1.56759
C	1.26899	-1.27123	-0.34558
H	2.28520	-1.15846	0.03181
H	1.00588	-2.32863	-0.35304
H	1.21978	-0.89225	-1.36603
O	-1.04751	-0.85224	0.06391
O	-1.75096	0.29181	-0.38336
H	-2.45343	0.35648	0.27582

TS[2j-2a']

Geometry with 12 atoms:

Total energy: -343.427692449

C	1.45824	0.02101	0.15479
H	1.79660	0.40956	1.12244
O	1.85994	-1.13734	-0.18533
C	0.02821	0.39323	-0.24853

H	-0.14299	0.05570	-1.27034
C	-0.18328	1.88937	-0.10337
H	0.48708	2.43790	-0.76354
H	-1.21695	2.12236	-0.35954
H	-0.00219	2.19631	0.92723
O	-0.88126	-0.31148	0.59688
O	-1.86484	-0.94674	-0.21177
H	-1.65121	-1.87897	-0.07178

TS[2j-2h]

Geometry with 12 atoms:

Total energy: -343.430954066

C	1.35895	-0.42139	0.38542
H	1.24673	-1.33285	0.98557
O	2.40376	-0.33349	-0.34512
C	0.04938	0.12154	-0.20957
H	0.05898	-0.02940	-1.29567
C	-0.15379	1.58400	0.13536
H	0.67191	2.17031	-0.26859
H	-1.09058	1.93905	-0.29439
H	-0.17868	1.70627	1.21781
O	-0.94560	-0.71421	0.36748
O	-2.18790	-0.33303	-0.20665
H	-2.39767	-1.11247	-0.73762

TS[2j'-2h']

Geometry with 12 atoms:

Total energy: -343.433566514

C	-1.25598	-0.78943	0.10636
H	-1.09820	-1.67542	-0.52111
O	-2.38258	-0.19745	-0.01532
C	0.00135	0.05900	0.34586
H	0.25616	0.02123	1.41114
C	-0.14039	1.49304	-0.12331
H	-0.91885	2.00140	0.44657
H	0.80678	2.01044	0.02473
H	-0.40425	1.51465	-1.18031
O	1.01090	-0.63679	-0.37797
O	2.26004	-0.11380	0.05570
H	2.62162	-0.86366	0.54619

TS[2j-2j']

Geometry with 12 atoms:

Total energy: -343.428931256

C	-1.52048	0.20092	0.26694
H	-2.10453	0.56600	1.11860
O	-1.99296	-0.83462	-0.31959
C	0.00402	0.37260	0.39285
H	0.27503	0.37847	1.45510
C	0.46501	1.65061	-0.28380
H	-0.02515	2.51037	0.17379
H	1.54472	1.75538	-0.17350
H	0.20502	1.61745	-1.34139
O	0.56649	-0.78141	-0.21268
O	1.96605	-0.71716	0.02546
H	2.09707	-1.50692	0.56591

TS[2j'-2j]

Geometry with 12 atoms:

Total energy: -343.428931256

C	-1.52048	0.20092	0.26694
H	-2.10453	0.56600	1.11860
O	-1.99296	-0.83462	-0.31959
C	0.00402	0.37260	0.39285
H	0.27503	0.37847	1.45510
C	0.46501	1.65061	-0.28380
H	-0.02515	2.51037	0.17379
H	1.54472	1.75538	-0.17350
H	0.20502	1.61745	-1.34139
O	0.56649	-0.78141	-0.21268
O	1.96605	-0.71716	0.02546
H	2.09707	-1.50692	0.56591

TS[2j-2k]

Geometry with 12 atoms:

Total energy: -343.429625090

C	1.48022	0.17751	0.21141
H	1.69106	0.50401	1.23622
O	2.18539	-0.79151	-0.23041
C	0.04550	0.29305	-0.26594
H	-0.00049	0.02308	-1.32445
C	-0.48926	1.69158	-0.02129
H	0.03894	2.41443	-0.64183
H	-1.55002	1.71157	-0.26965
H	-0.36638	1.96218	1.02819
O	-0.68958	-0.68425	0.46403
O	-1.94600	-0.80390	-0.23031
H	-2.43031	-1.35078	0.40003

TS[2j'-2k']

Geometry with 12 atoms:

Total energy: -343.430348504

C	-1.38513	-0.46545	0.50118
H	-1.48955	-1.40820	1.05236
O	-2.13073	-0.36283	-0.53255
C	-0.00306	0.15929	0.48881
H	0.36231	0.14512	1.51943
C	0.00263	1.56250	-0.08753
H	-0.63506	2.21439	0.50916
H	1.01943	1.95153	-0.07978
H	-0.36483	1.54654	-1.11347
O	0.81370	-0.72710	-0.27570
O	2.16466	-0.29373	-0.03061
H	2.63998	-0.91827	-0.59167

TS[2j-2l]

Geometry with 12 atoms:

Total energy: -343.422717286

C	1.42196	0.25446	0.33866
H	1.34099	0.38838	1.42522

O	2.29955	-0.58178	-0.05527
C	0.09146	0.30902	-0.41469
H	0.32899	0.32476	-1.48103
C	-0.67434	1.55129	-0.01080
H	-0.05828	2.42056	-0.23598
H	-1.60884	1.62419	-0.56318
H	-0.90499	1.53833	1.05361
O	-0.59719	-0.93415	-0.17374
O	-1.91349	-0.72201	0.31972
H	-2.44330	-1.08127	-0.40329

TS[2j'-2l']

Geometry with 12 atoms:

Total energy: -343.427933918

C	-1.20558	-0.65454	0.52798
H	-1.03433	-1.60256	1.05306
O	-2.04176	-0.70098	-0.43287
C	0.01338	0.25963	0.40340
H	0.50560	0.25258	1.37507
C	-0.36566	1.66268	-0.03380
H	-1.07776	2.10084	0.66468
H	0.53334	2.27775	-0.07018
H	-0.81389	1.63555	-1.02659
O	0.93084	-0.29611	-0.54864
O	2.21497	-0.37216	0.06054
H	2.40180	-1.31676	-0.01374

TS[2j'-2n]

Geometry with 12 atoms:

Total energy: -343.421593190

C	-1.48436	-0.33326	0.40712
H	-1.77471	-1.17808	1.04203
O	-1.89508	-0.34973	-0.79445
C	-0.06813	0.21070	0.66148
H	-0.02039	0.34185	1.74640
C	0.17475	1.52201	-0.05688
H	-0.60572	2.22112	0.24091
H	1.14484	1.93307	0.21550
H	0.14314	1.38839	-1.13599
O	0.85929	-0.83484	0.33378
O	1.87535	-0.39135	-0.56034
H	2.66284	-0.49565	-0.01107

TS[2k-2b']

Geometry with 12 atoms:

Total energy: -343.423928285

C	1.41839	0.25892	0.34161
H	1.35187	0.42074	1.42506
O	2.29422	-0.58173	-0.04601
C	0.08972	0.32351	-0.41370
H	0.32908	0.36688	-1.47826
C	-0.68752	1.55027	0.01382
H	-0.08119	2.42956	-0.19904
H	-1.62460	1.61784	-0.53389
H	-0.91175	1.52303	1.08007
O	-0.58817	-0.93060	-0.20625
O	-1.95526	-0.73521	0.13496
H	-1.99323	-1.17395	0.99398

TS[2k-2g]

Geometry with 12 atoms:

Total energy: -343.429766763

C	1.37508	-0.35181	0.40631
H	1.27397	-1.21246	1.07926
O	2.41530	-0.32237	-0.33596
C	0.05656	0.12906	-0.21787
H	0.09982	-0.01172	-1.30263
C	-0.22656	1.57806	0.13349
H	0.59207	2.20400	-0.22174
H	-1.14983	1.90867	-0.34410
H	-0.30494	1.68993	1.21550
O	-0.90889	-0.76674	0.32039
O	-2.14217	-0.48859	-0.32752
H	-2.65551	-0.08869	0.38684

TS[2k'-2g']

Geometry with 12 atoms:

Total energy: -343.433120880

C	-1.27088	-0.77233	0.03231
H	-1.13520	-1.55507	-0.72499
O	-2.39737	-0.16815	0.03925
C	-0.00796	0.04906	0.33201
H	0.19200	0.00947	1.40760
C	-0.10032	1.48477	-0.15012
H	-0.91071	2.00239	0.36359
H	0.83385	2.00357	0.06640
H	-0.29539	1.50852	-1.22279
O	1.01450	-0.67929	-0.33502
O	2.25026	-0.24565	0.21605
H	2.65134	0.20686	-0.53722

TS[2k'-2i]

Geometry with 12 atoms:

Total energy: -343.426641887

C	-1.21084	-0.66247	0.51210
H	-1.01964	-1.64463	0.96341
O	-2.06368	-0.65380	-0.43584
C	0.01568	0.24297	0.40526
H	0.50335	0.21517	1.37859
C	-0.35309	1.65515	-0.01264
H	-1.07688	2.08132	0.68126
H	0.54300	2.27633	-0.02088
H	-0.78592	1.64793	-1.01275
O	0.93401	-0.30779	-0.54950
O	2.17590	-0.54628	0.10293
H	2.75587	0.07295	-0.35863

TS[2k-2j]

Geometry with 12 atoms:

Total energy: -343.429625090

C	1.48022	0.17751	0.21141
H	1.69106	0.50401	1.23622
O	2.18539	-0.79151	-0.23041
C	0.04550	0.29305	-0.26594
H	-0.00049	0.02308	-1.32445
C	-0.48926	1.69158	-0.02129
H	0.03894	2.41443	-0.64183
H	-1.55002	1.71157	-0.26965
H	-0.36638	1.96218	1.02819
O	-0.68958	-0.68425	0.46403
O	-1.94600	-0.80390	-0.23031
H	-2.43031	-1.35078	0.40003

TS[2k'-2j']

Geometry with 12 atoms:
Total energy: -343.430348504

C	-1.38513	-0.46545	0.50118
H	-1.48955	-1.40820	1.05236
O	-2.13073	-0.36283	-0.53255
C	-0.00306	0.15929	0.48881
H	0.36231	0.14512	1.51943
C	0.00263	1.56250	-0.08753
H	-0.63506	2.21439	0.50916
H	1.01943	1.95153	-0.07978
H	-0.36483	1.54654	-1.11347
O	0.81370	-0.72710	-0.27570
O	2.16466	-0.29373	-0.03061
H	2.63998	-0.91827	-0.59167

TS[2k-2k']

Geometry with 12 atoms:
Total energy: -343.442014871

C	-1.27562	-0.74152	0.11251
H	-1.38515	-1.74862	0.52603
O	-2.36258	-0.14028	-0.20389
C	0.00099	0.02675	0.38069
H	0.28092	-0.06880	1.43600
C	-0.09701	1.48406	-0.02416
H	-0.86157	1.98974	0.56641
H	0.85859	1.97475	0.15501
H	-0.35566	1.56438	-1.08025
O	0.98871	-0.68026	-0.37638
O	2.25775	-0.24442	0.11167
H	2.62167	0.19247	-0.66862

TS[2k'-2k]

Geometry with 12 atoms:
Total energy: -343.442014871

C	-1.27562	-0.74152	0.11251
H	-1.38515	-1.74862	0.52603
O	-2.36258	-0.14028	-0.20389
C	0.00099	0.02675	0.38069
H	0.28092	-0.06880	1.43600
C	-0.09701	1.48406	-0.02416
H	-0.86157	1.98974	0.56641
H	0.85859	1.97475	0.15501
H	-0.35566	1.56438	-1.08025
O	0.98871	-0.68026	-0.37638
O	2.25775	-0.24442	0.11167
H	2.62167	0.19247	-0.66862

TS[2k-2m']

Geometry with 12 atoms:
Total energy: -343.425099030

C	1.45520	0.01385	0.15439
H	1.80033	0.40865	1.11716
O	1.86099	-1.14844	-0.16959
C	0.03012	0.39085	-0.24975
H	-0.14153	0.04717	-1.26911
C	-0.16443	1.89117	-0.11196
H	0.52620	2.42796	-0.76076
H	-1.18789	2.14724	-0.38733
H	0.00537	2.19948	0.92038
O	-0.90073	-0.29083	0.59337
O	-1.74981	-1.09938	-0.21500
H	-2.61141	-0.69654	-0.04670

TS[2k'-2o]

Geometry with 12 atoms:
Total energy: -343.423432261

C	-1.48739	-0.31038	0.41095
H	-1.78380	-1.12769	1.07855
O	-1.87898	-0.37320	-0.79500
C	-0.06869	0.23884	0.65572
H	-0.02432	0.40608	1.73527
C	0.18863	1.52432	-0.10208
H	-0.58386	2.24077	0.17492
H	1.16478	1.92784	0.15729
H	0.14893	1.36505	-1.17817
O	0.83951	-0.83044	0.35898
O	1.96984	-0.38149	-0.38123
H	1.84004	-0.84763	-1.21728

TS[2l-2a']

Geometry with 12 atoms:
Total energy: -343.423221857

C	-0.59931	-1.00367	0.33838
H	-0.60267	-0.96022	1.43331
O	-1.74871	-1.09593	-0.21276
C	0.51277	-0.29812	-0.39436
H	0.46454	-0.60191	-1.44226
C	1.85768	-0.64755	0.21507
H	2.06826	-1.70948	0.09247
H	2.63845	-0.07043	-0.28025
H	1.86659	-0.40191	1.27834
O	0.41056	1.15367	-0.41904
O	-0.74926	1.61354	0.25114
H	-0.36273	2.06975	1.00911

TS[2l'-2a]

Geometry with 12 atoms:
Total energy: -343.437140102

C	-0.03357	1.30793	0.28987
H	0.02608	1.86265	1.23459
O	-1.07992	1.47142	-0.41311
C	0.58793	-0.13913	0.37716
H	0.56020	-0.43740	1.42911
C	1.99667	-0.13722	-0.17872
H	2.60465	0.58781	0.35996
H	2.43225	-1.13109	-0.06298
H	1.98024	0.13357	-1.23381
O	-0.14324	-1.05296	-0.38419
O	-1.39849	-1.24986	0.23698
H	-1.93633	-0.55380	-0.17414

TS[2l-2b']
Geometry with 12 atoms:
Total energy: -343.427958205

C	1.22847	0.19101	0.45069
H	0.97084	-0.05260	1.48943
O	2.19811	-0.44614	-0.06836
C	0.01148	0.47272	-0.44734
H	0.38009	0.73948	-1.43925
C	-0.82605	1.58809	0.15534
H	-0.26002	2.51799	0.14578
H	-1.73375	1.71132	-0.43638
H	-1.10410	1.35230	1.18094
O	-0.73720	-0.69489	-0.71795
O	-1.30239	-1.11952	0.52488
H	-2.00470	-1.69504	0.19869

TS[2l-2d]
Geometry with 12 atoms:
Total energy: -343.432648026

C	-1.09352	-0.51018	-0.35702
H	-0.71483	-1.49072	-0.66631
O	-2.31233	-0.41521	0.00323
C	-0.07158	0.33752	0.45097
H	-0.49230	0.52938	1.44133
C	0.23586	1.63748	-0.27099
H	0.95032	2.22363	0.31168
H	0.63824	1.43677	-1.26272
H	-0.68378	2.21032	-0.38714
O	1.07824	-0.41947	0.74516
O	1.66050	-0.83919	-0.48126
H	2.46653	-0.30740	-0.51163

TS[2l'-2i']
Geometry with 12 atoms:
Total energy: -343.444274677

C	-0.77987	-0.90509	0.45000
H	-0.63171	-1.61472	1.26512
O	-1.62052	-1.18038	-0.46574
C	-0.02755	0.43074	0.43169
H	0.35286	0.56730	1.44625
C	-0.89451	1.58972	-0.02581
H	-1.77380	1.66531	0.61176
H	-0.32412	2.51588	0.03032
H	-1.21922	1.43486	-1.05411
O	1.07257	0.41233	-0.46172
O	2.04660	-0.47667	0.04834
H	1.81837	-1.30309	-0.40172

TS[2l'-2i]
Geometry with 12 atoms:
Total energy: -343.428735132

C	-0.79063	-0.92985	0.48532
H	-0.15750	-1.75103	0.84647
O	-1.59339	-1.19717	-0.46078
C	-0.05042	0.42575	0.43684
H	0.34164	0.57420	1.44629
C	-0.95139	1.55723	-0.01421
H	-1.83181	1.59661	0.62491
H	-0.41604	2.50371	0.04832
H	-1.27162	1.39385	-1.04261
O	1.03057	0.41211	-0.46958
O	1.97687	-0.51730	0.05773
H	2.77761	-0.21719	-0.39007

TS[2l-2j]
Geometry with 12 atoms:
Total energy: -343.422717286

C	1.42196	0.25446	0.33866
H	1.34099	0.38838	1.42522
O	2.29955	-0.58178	-0.05527
C	0.09146	0.30902	-0.41469
H	0.32899	0.32476	-1.48103
C	-0.67434	1.55129	-0.01080
H	-0.05828	2.42056	-0.23598
H	-1.60884	1.62419	-0.56318
H	-0.90499	1.53833	1.05361
O	-0.59719	-0.93415	-0.17374
O	-1.91349	-0.72201	0.31972
H	-2.44330	-1.08127	-0.40329

TS[2l'-2j']
Geometry with 12 atoms:
Total energy: -343.427933918

C	-1.20558	-0.65454	0.52798
H	-1.03433	-1.60256	1.05306
O	-2.04176	-0.70098	-0.43287
C	0.01338	0.25963	0.40340
H	0.50560	0.25258	1.37507
C	-0.36566	1.66268	-0.03380
H	-1.07776	2.10084	0.66468
H	0.53334	2.27775	-0.07018
H	-0.81389	1.63555	-1.02659
O	0.93084	-0.29611	-0.54864
O	2.21497	-0.37216	0.06054
H	2.40180	-1.31676	-0.01374

TS[2l-2n']

Geometry with 12 atoms:
Total energy: -343.431386317

C	1.20911	-0.74212	0.10670
H	1.42210	-1.67033	-0.43580
O	1.91734	0.26641	-0.22595
C	-0.27238	-0.55440	0.52778
H	-0.37300	-0.97506	1.53324
C	-1.22335	-1.24794	-0.43202
H	-0.99919	-2.31463	-0.46566
H	-2.25088	-1.12022	-0.08528
H	-1.12102	-0.83693	-1.43477
O	-0.58972	0.79442	0.74995
O	-0.52083	1.48121	-0.49557
H	-1.41261	1.84760	-0.55389

TS[2l'-2n]

Geometry with 12 atoms:
Total energy: -343.423943337

C	0.57478	0.96649	0.62228
H	-0.00282	1.51726	1.37554
O	0.80530	1.61254	-0.45550
C	0.31376	-0.52309	0.54319
H	0.40757	-0.89884	1.56397
C	1.27293	-1.23324	-0.39421
H	2.30181	-1.09476	-0.06231
H	1.04269	-2.29822	-0.40563
H	1.17455	-0.84268	-1.40757
O	-1.04110	-0.86861	0.13828
O	-1.79075	0.26605	-0.24372
H	-1.68023	0.27636	-1.20403

TS[2m-2a]

Geometry with 12 atoms:
Total energy: -343.425699697

C	-0.06324	1.27534	-0.23636
H	0.64005	2.11628	-0.26240
O	-1.27111	1.55113	0.04838
C	0.53635	-0.03817	0.31152
H	0.31634	-0.10879	1.38261
C	2.02096	-0.09373	0.01691
H	2.52931	0.72136	0.53072
H	2.43059	-1.04074	0.36525
H	2.19368	-0.00349	-1.05528
O	-0.03025	-1.15131	-0.33162
O	-1.39310	-1.19906	0.07262
H	-1.51869	-2.15137	0.17168

TS[2m'-2a']

Geometry with 12 atoms:
Total energy: -343.431126971

C	0.07716	1.30467	0.18924
H	-0.28310	1.64594	1.16740
O	1.28617	1.58439	-0.09658
C	-0.52422	-0.01143	-0.31583
H	-0.28721	-0.10005	-1.37848
C	-2.01756	-0.03173	-0.05431
H	-2.48971	0.81164	-0.55455
H	-2.44482	-0.96021	-0.43045
H	-2.21357	0.03646	1.01638
O	-0.00244	-1.14482	0.34879
O	1.34101	-1.28905	-0.11106
H	1.50817	-2.20703	0.13587

TS[2m'-2b']

Geometry with 12 atoms:
Total energy: -343.424416042

C	-0.45096	-1.07559	0.33392
H	-0.46968	-0.99337	1.42760
O	-1.58378	-1.26815	-0.22605
C	0.55969	-0.21255	-0.38951
H	0.52341	-0.47897	-1.44888
C	1.94833	-0.41905	0.18168
H	2.63982	0.27134	-0.30164
H	1.94680	-0.21368	1.25257
H	2.28435	-1.44071	0.00811
O	0.27869	1.21384	-0.32857
O	-0.90703	1.49897	0.38280
H	-1.57014	1.54131	-0.31973

TS[2m-2c]

Geometry with 12 atoms:
Total energy: -343.437766507

C	1.04239	-0.50722	0.45512
H	1.40290	-0.15989	1.42989
O	1.85327	-1.19890	-0.24805
C	0.03186	0.40266	-0.26527
H	0.02548	0.11631	-1.31861
C	0.35207	1.87606	-0.08155
H	-0.37857	2.49148	-0.60776
H	0.33139	2.13377	0.97780
H	1.34591	2.08319	-0.47587
O	-1.25985	0.23206	0.27727
O	-1.69606	-1.08304	-0.03704
H	-2.46387	-0.89484	-0.59259

TS[2m'-2c']

Geometry with 12 atoms:
Total energy: -343.433856725

C	1.05036	-0.48661	0.46904
H	0.62918	-0.97187	1.35779
O	1.85633	-1.17190	-0.24305
C	0.04559	0.43558	-0.26472
H	0.07122	0.18421	-1.32859
C	0.36227	1.90016	-0.02580
H	1.36778	2.11301	-0.38464
H	-0.35366	2.52892	-0.55763
H	0.31739	2.12236	1.03999
O	-1.25590	0.24299	0.24144

O	-1.64897	-1.08829	-0.06538
H	-2.39293	-0.93385	-0.66209

TS[2m'-2k]

Geometry with 12 atoms:
Total energy: -343.425099030

C	1.45520	0.01385	0.15439
H	1.80033	0.40865	1.11716
O	1.86099	-1.14844	-0.16959
C	0.03012	0.39085	-0.24975
H	-0.14153	0.04717	-1.26911
C	-0.16443	1.89117	-0.11196
H	0.52620	2.42796	-0.76076
H	-1.18789	2.14724	-0.38733
H	0.00537	2.19948	0.92038
O	-0.90073	-0.29083	0.59337
O	-1.74981	-1.09938	-0.21500
H	-2.61141	-0.69654	-0.04670

TS[2m-2m']

Geometry with 12 atoms:
Total energy: -343.440790254

C	-0.16582	1.24307	-0.23417
H	0.39135	1.97286	-0.82370
O	-1.35972	1.52911	0.11464
C	0.52271	0.00410	0.31123
H	0.29891	-0.07726	1.38049
C	2.01419	0.06085	0.04623
H	2.45058	0.91239	0.56591
H	2.48753	-0.85395	0.39990
H	2.19951	0.15934	-1.02360
O	0.07020	-1.18474	-0.32394
O	-1.30595	-1.33560	-0.02609
H	-1.29060	-2.03171	0.64449

TS[2m'-2m]

Geometry with 12 atoms:
Total energy: -343.440790254

C	-0.16582	1.24307	-0.23417
H	0.39135	1.97286	-0.82370
O	-1.35972	1.52911	0.11464
C	0.52271	0.00410	0.31123
H	0.29891	-0.07726	1.38049
C	2.01419	0.06085	0.04623
H	2.45058	0.91239	0.56591
H	2.48753	-0.85395	0.39990
H	2.19951	0.15934	-1.02360
O	0.07020	-1.18474	-0.32394
O	-1.30595	-1.33560	-0.02609
H	-1.29060	-2.03171	0.64449

TS[2n-2d']

Geometry with 12 atoms:
Total energy: -343.436424391

C	-1.06992	-0.75042	0.34928
H	-0.65871	-1.76298	0.26652
O	-2.06020	-0.46018	-0.40128
C	-0.00497	0.33770	0.63530
H	-0.10034	0.63418	1.68502
C	-0.14482	1.54063	-0.27743
H	-1.12138	2.00145	-0.12685
H	0.63200	2.26815	-0.03906
H	-0.06470	1.24176	-1.32082
O	1.28409	-0.23316	0.62468
O	1.56638	-0.68572	-0.69482
H	2.30927	-0.11756	-0.93642

TS[2n'-2d]

Geometry with 12 atoms:
Total energy: -343.441723299

C	-1.10232	-0.69885	0.33504
H	-1.34981	-1.44194	1.09872
O	-2.00492	-0.43330	-0.52843
C	0.00371	0.31375	0.65320
H	-0.05871	0.58223	1.71276
C	-0.08739	1.54715	-0.22530
H	0.73282	2.22478	0.01291
H	-0.03808	1.27080	-1.27682
H	-1.03398	2.05643	-0.04479
O	1.27590	-0.30665	0.61236
O	1.54766	-0.69952	-0.72757
H	2.31470	-0.14881	-0.93120

TS[2n'-2i']

Geometry with 12 atoms:
Total energy: -343.421446259

C	0.74160	-0.87121	0.07898
H	0.21789	-1.79538	-0.20137
O	2.01566	-0.91167	0.02641
C	0.09073	0.41217	-0.44051
H	0.31941	0.51316	-1.50923
C	0.58378	1.62984	0.31861
H	1.65881	1.74714	0.17556
H	0.07529	2.51988	-0.05241
H	0.38079	1.51713	1.38407
O	-1.34084	0.36135	-0.35701
O	-1.83038	-0.81950	0.24163
H	-1.90443	-0.56819	1.17260

TS[2n-2j']

Geometry with 12 atoms:
Total energy: -343.421593190

C	-1.48436	-0.33326	0.40712
H	-1.77471	-1.17808	1.04203
O	-1.89508	-0.34973	-0.79445
C	-0.06813	0.21070	0.66148
H	-0.02039	0.34185	1.74640
C	0.17475	1.52201	-0.05688
H	-0.60572	2.22112	0.24091
H	1.14484	1.93307	0.21550

H	0.14314	1.38839	-1.13599
O	0.85929	-0.83484	0.33378
O	1.87535	-0.39135	-0.56034
H	2.66284	-0.49565	-0.01107

TS[2n-2l']

Geometry with 12 atoms:

Total energy: -343.423943337

C	0.57478	0.96649	0.62228
H	-0.00282	1.51726	1.37554
O	0.80530	1.61254	-0.45550
C	0.31376	-0.52309	0.54319
H	0.40757	-0.89884	1.56397
C	1.27293	-1.23324	-0.39421
H	2.30181	-1.09476	-0.06231
H	1.04269	-2.29822	-0.40563
H	1.17455	-0.84268	-1.40757
O	-1.04110	-0.86861	0.13828
O	-1.79075	0.26605	-0.24372
H	-1.68023	0.27636	-1.20403

TS[2n'-2l]

Geometry with 12 atoms:

Total energy: -343.431386317

C	1.20911	-0.74212	0.10670
H	1.42210	-1.67033	-0.43580
O	1.91734	0.26641	-0.22595
C	-0.27238	-0.55440	0.52778
H	-0.37300	-0.97506	1.53324
C	-1.22335	-1.24794	-0.43202
H	-0.99919	-2.31463	-0.46566
H	-2.25088	-1.12022	-0.08528
H	-1.12102	-0.83693	-1.43477
O	-0.58972	0.79442	0.74995
O	-0.52083	1.48121	-0.49557
H	-1.41261	1.84760	-0.55389

TS[2n-2n']

Geometry with 12 atoms:

Total energy: -343.440613566

C	-1.25962	-0.27694	0.53805
H	-1.92204	-0.32162	1.40353
O	-1.69323	-0.72458	-0.57526
C	0.02111	0.54705	0.59431
H	0.02156	1.05318	1.56122
C	0.12687	1.54201	-0.55161
H	1.06431	2.09478	-0.47251
H	0.08742	1.02759	-1.51017
H	-0.70360	2.24579	-0.50777
O	1.17719	-0.27554	0.69339
O	1.27682	-1.04218	-0.49633
H	2.03599	-0.63411	-0.93319

TS[2n'-2n]

Geometry with 12 atoms:

Total energy: -343.440613566

C	-1.25962	-0.27694	0.53805
H	-1.92204	-0.32162	1.40353
O	-1.69323	-0.72458	-0.57526
C	0.02111	0.54705	0.59431
H	0.02156	1.05318	1.56122
C	0.12687	1.54201	-0.55161
H	1.06431	2.09478	-0.47251
H	0.08742	1.02759	-1.51017
H	-0.70360	2.24579	-0.50777
O	1.17719	-0.27554	0.69339
O	1.27682	-1.04218	-0.49633
H	2.03599	-0.63411	-0.93319

TS[2n-2o]

Geometry with 12 atoms:

Total energy: -343.431580101

C	-1.28992	-0.27332	0.54376
H	-1.49631	-0.89282	1.42454
O	-1.68595	-0.73916	-0.57325
C	0.00702	0.54436	0.60391
H	0.01236	1.02281	1.58536
C	0.08228	1.56880	-0.51532
H	-0.75809	2.25717	-0.43631
H	1.01532	2.12604	-0.43115
H	0.04695	1.07830	-1.48551
O	1.16341	-0.26931	0.67536
O	1.29586	-0.91412	-0.59399
H	2.19698	-1.24987	-0.51599

TS[2n'-2o']

Geometry with 12 atoms:

Total energy: -343.424471053

C	-1.29341	-0.25209	0.54079
H	-2.13811	0.22126	1.05596
O	-1.55937	-0.89648	-0.52156
C	0.00221	0.59951	0.56361
H	-0.02632	1.14944	1.50559
C	0.11135	1.53444	-0.63098
H	-0.72261	2.23610	-0.62318
H	1.04599	2.09474	-0.57289
H	0.08458	0.97042	-1.56012
O	1.13240	-0.22009	0.72303
O	1.25453	-0.99814	-0.46373
H	2.21512	-1.04537	-0.54776

TS[2o-2b]

Geometry with 12 atoms:

Total energy: -343.431602065

C	0.87814	-1.06392	-0.05046
H	1.06723	-2.05247	0.38786
O	1.86286	-0.28189	-0.20153
C	-0.47819	-0.44532	0.50379
H	-0.65935	-0.85610	1.50002
C	-1.59702	-0.79543	-0.45813

H	-1.66457	-1.87732	-0.56788
H	-2.53858	-0.41393	-0.05737
H	-1.40739	-0.35238	-1.43307
O	-0.34649	0.91945	0.75052
O	-0.07987	1.58576	-0.46468
H	0.89309	1.59358	-0.47513

TS[2o'-2b']

Geometry with 12 atoms:
Total energy: -343.438230979

C	1.00190	-0.99362	0.11769
H	0.97204	-1.92752	-0.45736
O	1.89498	-0.14509	-0.19704
C	-0.42599	-0.47068	0.53040
H	-0.61179	-0.86224	1.53490
C	-1.49034	-0.93541	-0.44368
H	-1.51015	-2.02522	-0.47578
H	-2.46340	-0.57366	-0.10738
H	-1.29143	-0.55050	-1.44166
O	-0.41774	0.91143	0.73811
O	-0.26581	1.56992	-0.50462
H	0.69997	1.64738	-0.57087

TS[2o'-2f]

Geometry with 12 atoms:
Total energy: -343.434115407

C	-1.06275	-0.69361	0.37694
H	-1.34523	-1.29561	1.24877
O	-1.97493	-0.47108	-0.48017
C	0.03645	0.37491	0.63801
H	-0.02891	0.68661	1.68409
C	-0.08372	1.55985	-0.29939
H	-1.03912	2.05835	-0.13671
H	0.72924	2.25636	-0.09683
H	-0.02456	1.23666	-1.33608
O	1.30023	-0.24794	0.60036
O	1.58498	-0.64523	-0.72785
H	1.08653	-1.47528	-0.79546

TS[2o-2i]

Geometry with 12 atoms:
Total energy: -343.423550459

C	0.59041	0.95985	0.60165
H	0.07953	1.55078	1.37041
O	0.87799	1.60086	-0.46535
C	0.28999	-0.51787	0.53590
H	0.33049	-0.87587	1.56759
C	1.26899	-1.27123	-0.34558
H	2.28520	-1.15846	0.03181
H	1.00588	-2.32863	-0.35304
H	1.21978	-0.89225	-1.36603
O	-1.04751	-0.85224	0.06391
O	-1.75096	0.29181	-0.38336
H	-2.45343	0.35648	0.27582

TS[2o-2k']

Geometry with 12 atoms:
Total energy: -343.423432261

C	-1.48739	-0.31038	0.41095
H	-1.78380	-1.12769	1.07855
O	-1.87898	-0.37320	-0.79500
C	-0.06869	0.23884	0.65572
H	-0.02432	0.40608	1.73527
C	0.18863	1.52432	-0.10208
H	-0.58386	2.24077	0.17492
H	1.16478	1.92784	0.15729
H	0.14893	1.36505	-1.17817
O	0.83951	-0.83044	0.35898
O	1.96984	-0.38149	-0.38123
H	1.84004	-0.84763	-1.21728

TS[2o-2n]

Geometry with 12 atoms:
Total energy: -343.431580101

C	-1.28992	-0.27332	0.54376
H	-1.49631	-0.89282	1.42454
O	-1.68595	-0.73916	-0.57325
C	0.00702	0.54436	0.60391
H	0.01236	1.02281	1.58536
C	0.08228	1.56880	-0.51532
H	-0.75809	2.25717	-0.43631
H	1.01532	2.12604	-0.43115
H	0.04695	1.07830	-1.48551
O	1.16341	-0.26931	0.67536
O	1.29586	-0.91412	-0.59399
H	2.19698	-1.24987	-0.51599

TS[2o'-2n']

Geometry with 12 atoms:
Total energy: -343.424471053

C	-1.29341	-0.25209	0.54079
H	-2.13811	0.22126	1.05596
O	-1.55937	-0.89648	-0.52156
C	0.00221	0.59951	0.56361
H	-0.02632	1.14944	1.50559
C	0.11135	1.53444	-0.63098
H	-0.72261	2.23610	-0.62318
H	1.04599	2.09474	-0.57289
H	0.08458	0.97042	-1.56012
O	1.13240	-0.22009	0.72303
O	1.25453	-0.99814	-0.46373
H	2.21512	-1.04537	-0.54776

TS[2o-2o']

Geometry with 12 atoms:
Total energy: -343.445033432

C	-1.28451	-0.07389	0.52375
H	-1.94892	-0.04248	1.38762
O	-1.66757	-0.66963	-0.53717
C	0.09082	0.60059	0.57050

H	0.13875	1.12571	1.52594
C	0.32173	1.54389	-0.59885
H	-0.41694	2.34419	-0.57636
H	1.32134	1.97265	-0.52121
H	0.23692	1.01049	-1.54268
O	1.12400	-0.36451	0.69286
O	1.20235	-1.08895	-0.51946
H	0.63033	-1.84934	-0.33550

TS[2o'-2o]

Geometry with 12 atoms:
Total energy: -343.445033432

C	-1.28451	-0.07389	0.52375
H	-1.94892	-0.04248	1.38762
O	-1.66757	-0.66963	-0.53717
C	0.09082	0.60059	0.57050
H	0.13875	1.12571	1.52594
C	0.32173	1.54389	-0.59885
H	-0.41694	2.34419	-0.57636
H	1.32134	1.97265	-0.52121
H	0.23692	1.01049	-1.54268
O	1.12400	-0.36451	0.69286
O	1.20235	-1.08895	-0.51946
H	0.63033	-1.84934	-0.33550

d. The geometries of the transitions states for 1,5 H-shift of 2-HPP(2a), 2-HPP(2a'), 2-HPP(2o), and 2-HPP(2o') in S_1 state, optimized at TD-M06-2X-D3/6-311++G(2d,p) level of theory

TS[H,2a']

Geometry with 12 atoms:
Total energy: -343.417130317

C	-0.19464	1.25196	0.17921
H	0.38344	2.13041	-0.10638
O	-1.41240	1.12209	-0.21228
C	0.63858	-0.06077	0.36915
H	0.57983	-0.28832	1.44025
C	2.05691	0.04970	-0.12921
H	2.54716	0.88654	0.36783
H	2.61178	-0.86112	0.09418
H	2.06540	0.22335	-1.20487
O	-0.00150	-1.08836	-0.32255
O	-1.28064	-1.20158	0.14668
H	-1.63643	-0.19348	-0.00068

TS[H,2a]

Geometry with 12 atoms:
Total energy: -343.409225650

C	-0.19784	1.23475	-0.16683
H	0.30881	2.16863	0.09620
O	-1.46530	1.13117	-0.03686
C	0.61870	-0.01973	0.33858
H	0.44400	-0.13006	1.41335
C	2.07392	0.07135	-0.04349
H	2.51617	0.94947	0.42589
H	2.60821	-0.81420	0.29877
H	2.17373	0.16037	-1.12435
O	0.03761	-1.09347	-0.32717
O	-1.24687	-1.25969	0.12126
H	-1.62315	-0.27648	0.06280

TS[H,2o']

Geometry with 12 atoms:
Total energy: -343.404506684

C	0.89494	-0.93585	0.48666
H	0.90394	-2.02475	0.60339
O	1.60288	-0.38748	-0.42896
C	-0.58352	-0.37360	0.56840
H	-1.01806	-0.70126	1.51243
C	-1.41427	-0.77442	-0.63793
H	-1.61833	-1.84333	-0.58428
H	-2.36134	-0.23246	-0.63063
H	-0.88804	-0.56415	-1.56588
O	-0.40737	0.99945	0.71095
O	0.13733	1.51635	-0.43543
H	0.93631	0.84260	-0.61024

TS[H,2o]

Geometry with 12 atoms:
Total energy: -343.415759333

C	0.60509	-1.18115	0.08744
H	0.67107	-2.14978	0.58465
O	1.68292	-0.56459	-0.24486
C	-0.62573	-0.30708	0.52426
H	-0.98075	-0.60582	1.51164
C	-1.72748	-0.42869	-0.52386
H	-2.01815	-1.47358	-0.61895
H	-2.59099	0.15931	-0.20789
H	-1.36839	-0.07419	-1.48723
O	-0.18186	1.00117	0.70686
O	0.44479	1.43241	-0.43444
H	1.20919	0.69363	-0.52981