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Table 3. Energies (a.u.) of Reactants, Complexes, Transition Structure (TS-2) and Products for the Reaction: HOOOH + HOH → 2 HOH + $^1O_2$

	6-31++G	6-31++G*	ZPE
HOOOH	-225.452 93[a]	-225.541 48[b]	21.4
HOH	-75.993 26	-76.017 89	14.4
HOOOH + HOH	-301.446 18 (0.0)[d]	-301.559 37 (0.0)	
(HOOOH)(HOH)	-301.466 03 (-12.4)	-301.571 86 (-7.8)	38.1
TS-2	-301.410 14 (+22.6)	-301.489 63 (+43.8)	35.2
$^1O_2$	-149.468 35	-149.536 99	
(HOH)(HOH)($^1O_2$)	-301.471 84 (-16.1)	-301.583 96 (-15.4)	
2 HOH + $^1O_2$	-301.454 86 (-5.4)	-301.572 77 (-8.4)	

[a]R (H-O) = 0.958 Å, R (O-O) = 1.428 Å, ∠H-O-O = 104.8°, ∠O-O-O = 106.8°, ∠H-O-O-O-H = 85.7°.

[b]R (H-O) = 0.952 Å, R (O-O) = 1.371 Å, ∠H-O-O= 103.6°, ∠O-O-O = 107.5 °, ∠H-O-O-O-H = 81.7°.

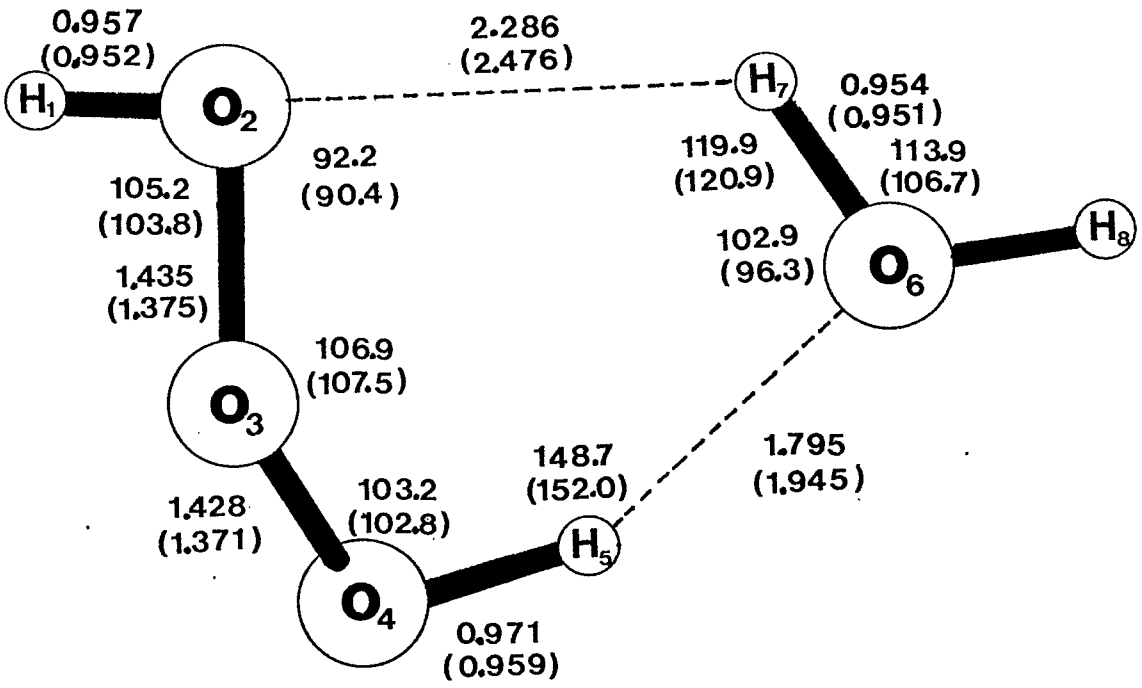
[c]Zero-point energy 6-31++G*//6-31++G*in kcal/mol. [d]Relative energies (kcal/mol) are given in parentheses.

Table 4. Energies (a.u.) of Reactants, Complexes, Transition Structure (TS-3), and Products for the Reaction: HOOOH + 2 HOH → 3 HOH + $^1O_2$.

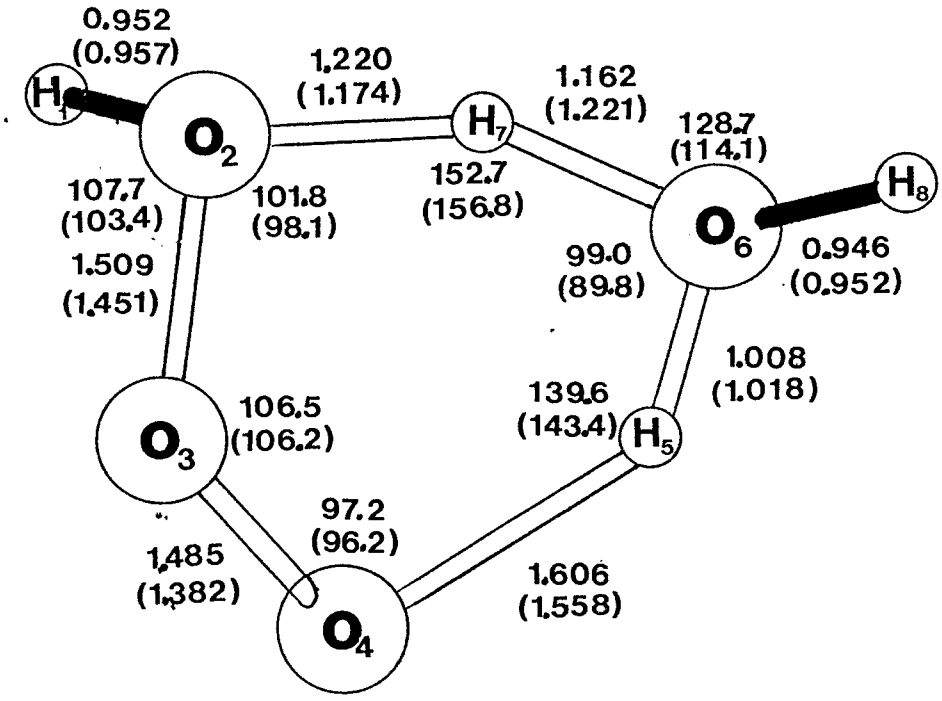
	6-31++G	MP4/6-31++G*//6-31++G
HOOOH	-225.452 93	-226.132 76
HOH	-75.993 26	-76.218 75
HOOOH + 2 HOH	-377.439 45 (0.0)[a]	-378.570 26 (0.0)
$(HOH)_2$	-151.999 26	-152.442 46
HOOOH + $(HOH)_2$	-377.452 19 (-8.0)	-378.575 22 (-3.1)
(HOOOH)-2(HOH)	-377.484 26 (-28.1)	-378.604 98 (-21.8)
TS-3	-377.430 90 (+5.4)	-378.548 42 (+13.7)
$^1O_2$	-149.468 35	-149.920 02
$(HOH)_3$ + $^1O_2$	-377.486 25 (-29.4)	-378.605 64 (-22.2)
3 HOH + $^1O_2$	-377.448 13 (-5.4)	-378.576 29 (-3.8)

[a] Relative energies (kcal/mol) are given in parentheses.

J-2472-3



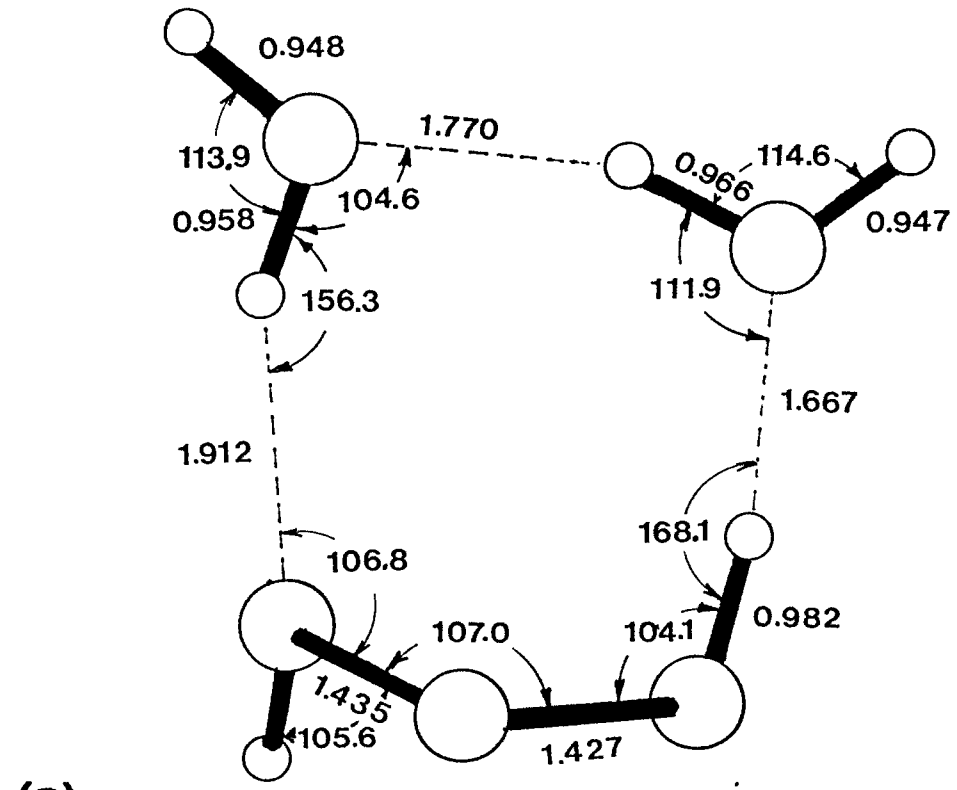
(a)



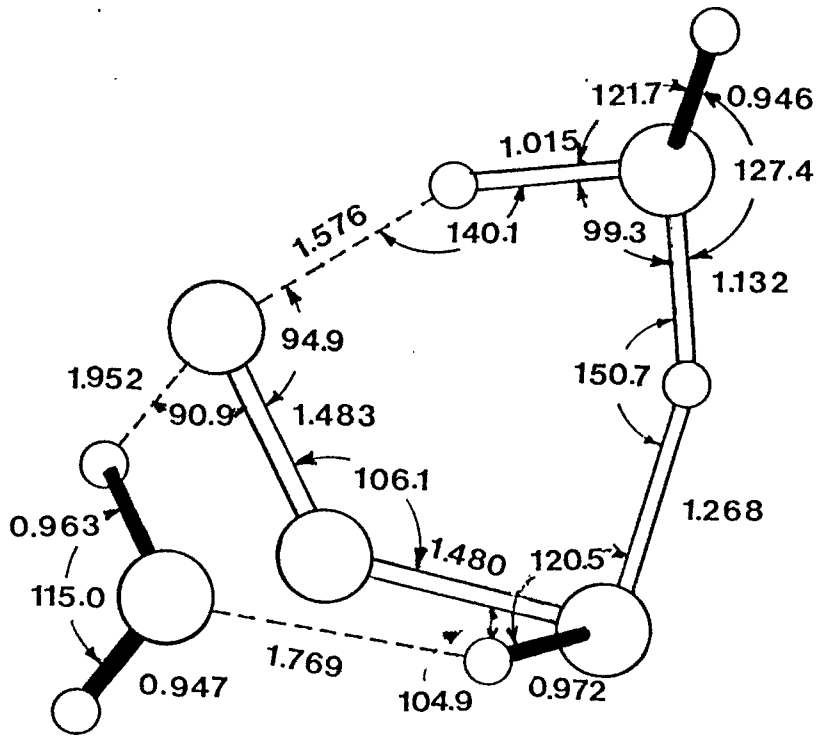
(b) TS-2

Figure 2. Optimized 6-31++G and 6-31++G* (in brackets) structures (in angstroms and degrees) of: (a) the complex HOOOH-HOH and (b) the transition state, TS-2, for HOOOH + HOH → 2 HOH + $^1O_2$

J-2472-4



(a)



(b)

TS—3

Figure 3. Optimized 6-31++G structures (in angstroms and degrees) of: (a) the complex HOOOH-2HOH and (b) the transition state, TS-3, for HOOOH + 2 HOH → 3 HOH + $^1O_2$