Table S3: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP\LANL2DZ for structures described in Figures 5 and 9. Italicized relative free energy values are in kcal mol^{-1} while values in parentheses are in kJ mol^{-1}.

Structure	Electronic energy (Hartrees)	ZPE (kcal mol^{-1})	$H_{298}^{o} - H_{0}^{o}$ (kcal mol^{-1})	Entropy (cal mol^{-1} K^{-1})	Relative free energy at 298 K (kcal mol^{-1})
1A	-1639.2886242	312.6	19.6	196.8	*0.0* (0.0)
TS$_{(1A\rightarrow 1D)}$	-1639.2696380	312.8	19.8	200.6	*11.1* (46.4)
1D	-1639.2817215	311.3	20.0	202.8	*3.1* (13.0)
TS$_{(1D\rightarrow 1F)}$	-1639.2355338	312.4	19.9	201.9	*31.9* (133.5)
1F	-1639.250696	312.3	20.2	203.2	*22.1* (92.5)
TS$_{(1F\rightarrow 1G)}$	-1639.2404708	311.4	19.9	200.6	*28.1* (117.6)
1G	-1639.259443	314.5	19.2	199.2	*18.1* (75.7)
TS$_{(1G\rightarrow 3B)}$	-1639.253522	310.8	20.2	197.7	*19.3* (80.8)
3B	-1639.2720841	313.2	20.0	201.0	*10.1* (42.3)
TS$_{(3B\rightarrow 4A)}$ + HOC_2O_2OH	-1639.0980300	307.6	20.3	248.1	*99.8* (417.6)
4A + HOC_2O_2OH	-1639.2268208	309.6	20.9	250.6	*21.4* (89.5)