Supporting information for
Theoretical Analysis of the OH-Initiated Atmospheric Oxidation Reactions of Imidazole

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S1 RRKM-ME uncertainty analysis

In order to assess the uncertainty of calculated product yields due to the uncertainty in RRKM-ME model parameters and the calculated PES, we employed the automated procedure present in KinBot[1]. Here the approach was adapted for the MESMER code[2]. Briefly, the procedure is as follows. The RRKM-ME calculation was repeated 100 times, applying to each new calculation a random variation in model parameters within a pre-defined uncertainty range. Zero-point corrected energies were varied by applying an additive uniformly distributed shift in the± 0.25 and ± 0.5 ranges for wells and transition states, respectively. For other values, a multiplicative random factor f was picked from a log-normally distributed uncertainty range $1/a \leq f \leq a$. For vibrational wavenumbers, Lennard-Jones ε/k_B and σ parameters, we selected a variation range of $1/1.2 \leq f \leq 1.2$, while for the transition states' imaginary wavenumbers the range was $1/1.1 \leq f \leq 1.1$. For vibrational modes of the same species, a single random factor was selected and modified by the function given in Equation S1, which dampens or amplifies the factor when it is applied to wavenumbers larger or smaller than 100 cm^{-1} respectively. For variation in the $\langle \Delta E \rangle_{\mathrm{down}}$ parameter, we selected a single random factor to be applied to all modelled wells in a calculation, from a variation range of $1/1.2 \leq f \leq 1.2$.

Additionally, we included variations in rate coefficients of reactions modelled with ILT and bimolecular sinks respectively, applying random multiplicative factors. We selected a variation range of $1/1.2 \leq f \leq 1.2$ for the imidazole + OH reaction, a range of $1/3 \leq f \leq 3$ for O_2 addition to alkyl radicals and dissociation of post-reactive complexes, and a range of $1/1.2 \leq f \leq 1.2$ for $RO_2 + NO$ reactions. For the initial O_2 addition reactions (producing first-generation RO_2), we employed an additional random factor. First, a single factor was picked from an external variation range of $1/3 \leq f \leq 3$ and applied to all reactions. Next, a second random factor was picked for each individual reaction from an internal variation range of $1/1.2 \leq f \leq 1.2$. For the sake of limiting computational costs, the grain size was increased to 100 cm^{-1} in the RRKM-ME calculations for the uncertainty analysis. Once the results from this analysis were obtained, standard deviations ($\pm\sigma$) were calculated from the logit-transformed distribution of branching ratios, to ensure that uncertainty ranges are kept within 0 and 1.

$$\begin{cases} f_{v,i} = \left(\left(\dfrac{100\,\mathrm{cm}^{-1}}{\nu_i} \right) (f-1) \right) + 1, & \text{for } f > 1 \\ f_{v,i} = \left(\left(\left(\dfrac{100\,\mathrm{cm}^{-1}}{\nu_i} \right) (1-f) \right) + 1 \right)^{-1}, & \text{for } f < 1 \end{cases} \tag{S1}$$

S2 M12a cyclization and 1,5 H-shift

From the three consecutive reaction steps involved in the H-shift leading from M12a to M19a, the first bond torsion (via TS17a) has the highest associated energy barrier, and would therefore be the rate-determining step of the channel. Also, the calculated ZPE-corrected energy is lower for the transition state of the H-shift (TS19a) than for its connected reactant (M18a). For this reason, this step was not included explicitly in the ME treatment, assuming that species M17a is directly connected to M19a through the torsional transition state TS18a.

Species M12a may also react by cyclization (via TS16a), where the carbonyl O attacks the radical center, forming a 6-membered ring. Alongside ring closure, a new radical center develops at a N-imino substituted carbon, which grants the transition state TS16a considerable resonance stabilization. Due to this effect, the barrier to this reaction is relatively low, with a value of 7.05 kcal mol^{-1}. An analogous reaction (via TS16s) is possible for species M12s, but it is endothermic and has a much higher barrier (17.30 kcal mol^{-1}). In this case, formation of a 6-membered ring leads to a net loss of resonance stabilization and requires an intramolecular H-bond to be broken.

Cyclization constitutes a minor channel for M12a, with a yield of 0.4 % at 298 K, and it is negligible for M12s. The H-shift channel initiated via the torsional transition state TS17a is also minor for M12a, but with a slightly higher yield (1.9% at 298 K), despite involving a reaction energy barrier ~ 2.6 kcal mol^{-1} higher than cyclization. The entropic penalty to cyclization, as seen from the smaller ratio between transition state and reactant partition functions (Q_{TS}/Q_R) in Table 3, cannot explain this observation, and neither can tunnelling, having a minimal impact on the rate coefficients of these reactions. Thus, excess vibrational energy carried over from the preceding reactions (4a-$RO_2 + NO \longrightarrow$ 4a-$RO + NO_2$ and 4a-RO C−C bond scission) may be affecting product yields, favoring the H-shift over cyclization.

M12a cyclization (via TS16a) is exothermic, but mildly so ($\Delta E = -11.4$ kcal mol^{-1}), meaning that back-reaction may be significant for vibrationally hot molecules. The 1,5 H-shift (via TS17a through TS19a) is ~ 13.7 kcal mol^{-1} more exothermic, and should be much less affected by back-reactions. Over the short time-scales in which these radicals exist, this effect can diminish the yields from cyclization. Results from a RRKM-ME time-evolution calculated with the thermalized alkoxyl radical 4a-RO as the starting reactant, in which case the excess energy from the 4a-$RO_2 + NO \longrightarrow$ 4a-$RO + NO_2$ reaction is ignored, show that the yield of these channels are both reduced, and cyclization (0.4%) surpasses the H-shift (0.3%) in importance. If the excess energy from 4a-RO C−C bond scission is also ignored, assigning the thermalized M12a species as starting reactant, both channels become negligible (yield $\sim 0.0\%$).

S3 Endocyclization pathways

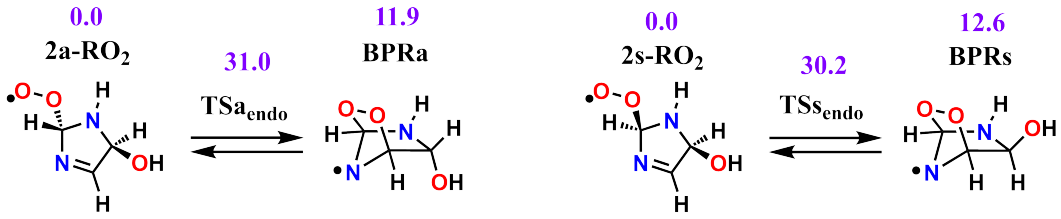

Figure S1 2-RO_2 endocyclization. Relative zero-point-corrected energies given in kcal mol^{-1}, calculated at the ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97X-D/aug-cc-pVTZ level of theory.

S4 Numerical values for product yields and standard deviations

S4.1 First-generation RO_2

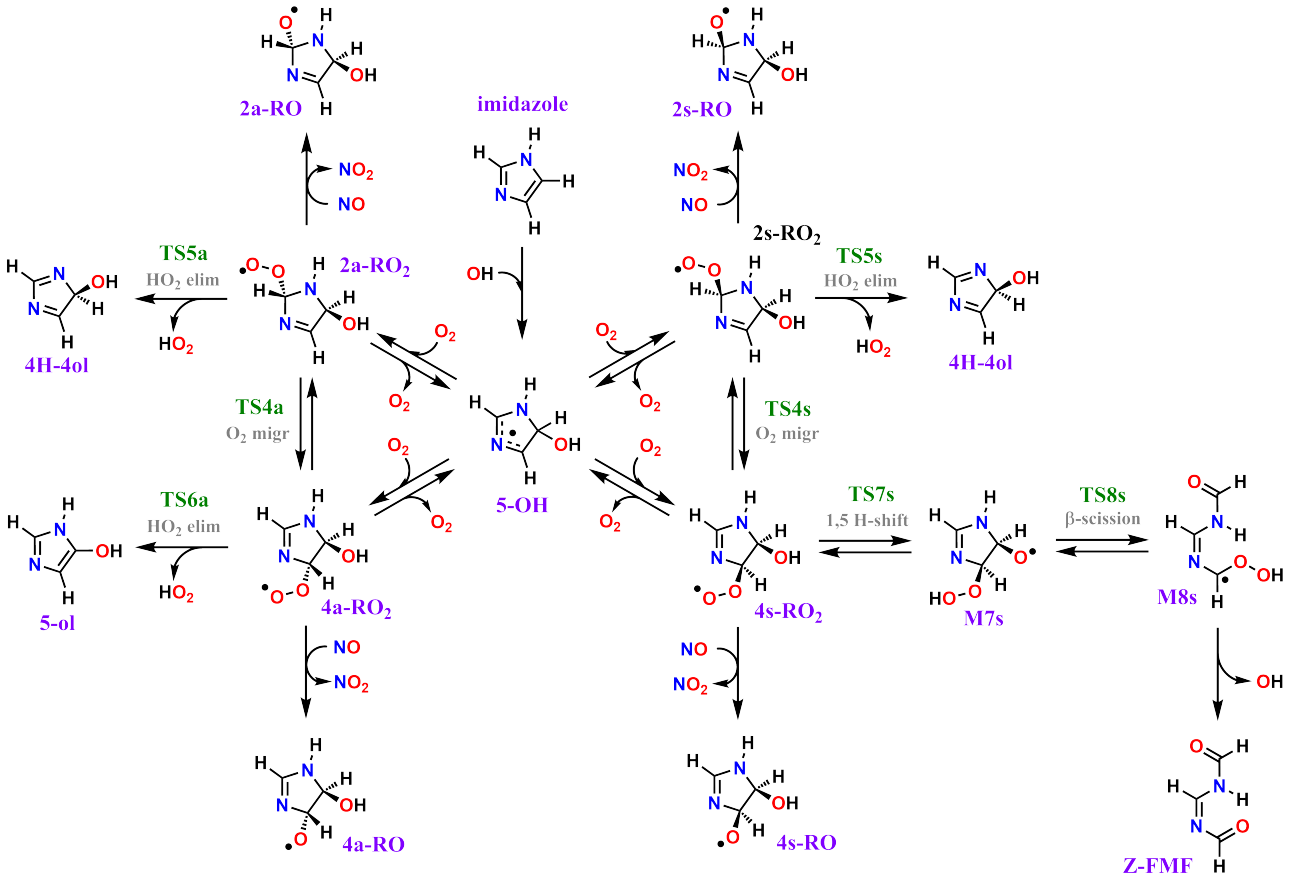

Figure S2 Reaction mechanism for first-generation RO_2.

Table S1 Product yields obtained from RRKM-ME calculations for reaction of first-generation RO_2 radicals at 1 atm and 10 ppt NO. Standard deviations ($\pm\sigma$) calculated with the logit-transformed distribution of yields obtained with uncertainty analysis.

Temperature (K)	Product yields (%) ($\pm\sigma$); [NO] = 10 ppt					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
250.00	$0.0(^{+0.1}_{-0.0})$	$0.2(^{+0.1}_{-0.1})$	$0.7(^{+0.7}_{-0.5})$	$31.2(^{+10.5}_{-7.5})$	$67.7(^{+7.5}_{-10.7})$	$0.2(^{+0.1}_{-0.0})$
262.50	$0.0(^{+0.1}_{-0.0})$	$1.2(^{+0.9}_{-0.5})$	$3.1(^{+2.3}_{-1.3})$	$25.2(^{+8.7}_{-6.6})$	$70.3(^{+6.7}_{-10.3})$	$0.2(^{+0.1}_{-0.1})$
275.00	$0.0(^{+0.1}_{-0.0})$	$6.3(^{+4.4}_{-2.5})$	$13.3(^{+6.9}_{-5.6})$	$20.5(^{+8.1}_{-6.7})$	$59.6(^{+8.0}_{-12.6})$	$0.2(^{+0.1}_{-0.1})$
287.50	$0.1(^{+0.1}_{-0.0})$	$20.4(^{+9.7}_{-6.6})$	$34.0(^{+10.6}_{-13.2})$	$11.6(^{+3.9}_{-3.3})$	$33.8(^{+9.7}_{-11.1})$	$0.1(^{+0.0}_{-0.0})$
298.00	$0.1(^{+0.1}_{-0.0})$	$33.7(^{+15.6}_{-9.4})$	$47.0(^{+11.3}_{-16.6})$	$4.9(^{+2.2}_{-2.3})$	$14.2(^{+5.0}_{-5.9})$	$0.1(^{+0.0}_{-0.0})$
312.50	$0.2(^{+0.1}_{-0.1})$	$45.0(^{+17.4}_{-11.3})$	$50.1(^{+11.2}_{-18.1})$	$1.2(^{+0.4}_{-0.5})$	$3.4(^{+1.8}_{-1.4})$	$0.0(^{+0.1}_{-0.0})$
325.00	$0.3(^{+0.2}_{-0.1})$	$50.9(^{+16.1}_{-12.5})$	$47.4(^{+12.2}_{-16.7})$	$0.3(^{+0.2}_{-0.1})$	$1.0(^{+0.6}_{-0.4})$	$0.0(^{+0.1}_{-0.0})$
337.50	$0.4(^{+0.3}_{-0.2})$	$55.4(^{+17.8}_{-9.3})$	$43.8(^{+9.1}_{-18.0})$	$0.1(^{+0.0}_{-0.0})$	$0.3(^{+0.1}_{-0.1})$	$0.0(^{+0.1}_{-0.0})$
350.00	$0.5(^{+0.3}_{-0.2})$	$59.2(^{+14.0}_{-13.1})$	$40.2(^{+13.0}_{-14.2})$	$0.0(^{+0.1}_{-0.0})$	$0.1(^{+0.0}_{-0.0})$	$0.0(^{+0.1}_{-0.0})$

Table S2 Product yields obtained from RRKM-ME calculations for reaction of first-generation RO_2 radicals at 1 atm, with 100 ppt NO and 1 ppb NO. Standard deviations ($\pm\sigma$) calculated with the logit-transformed distribution of yields obtained with uncertainty analysis.

Temperature (K)	Product yields (%) ($\pm\sigma$); [NO] = 100 ppt					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
250.00	$0.0(^{+0.1}_{-0.0})$	$0.1(^{+0.1}_{-0.0})$	$0.1(^{+0.1}_{-0.0})$	$43.1(^{+4.0}_{-5.1})$	$56.5(^{+5.0}_{-3.9})$	$0.2(^{+0.1}_{-0.1})$
262.50	$0.0(^{+0.1}_{-0.0})$	$0.2(^{+0.1}_{-0.0})$	$0.4(^{+0.3}_{-0.2})$	$32.9(^{+8.9}_{-7.2})$	$66.3(^{+7.0}_{-8.9})$	$0.2(^{+0.1}_{-0.1})$
275.00	$0.0(^{+0.1}_{-0.0})$	$0.8(^{+0.6}_{-0.3})$	$1.7(^{+1.4}_{-0.8})$	$26.3(^{+7.3}_{-8.0})$	$70.9(^{+7.9}_{-8.2})$	$0.2(^{+0.1}_{-0.1})$
287.50	$0.0(^{+0.1}_{-0.0})$	$4.0(^{+3.3}_{-1.1})$	$6.7(^{+4.5}_{-3.6})$	$23.0(^{+7.1}_{-7.9})$	$65.9(^{+9.2}_{-11.6})$	$0.3(^{+0.1}_{-0.1})$
298.00	$0.0(^{+0.1}_{-0.0})$	$12.4(^{+6.4}_{-4.7})$	$17.3(^{+9.2}_{-7.2})$	$18.1(^{+4.4}_{-6.6})$	$51.9(^{+9.9}_{-11.4})$	$0.3(^{+0.1}_{-0.1})$
312.50	$0.1(^{+0.1}_{-0.0})$	$31.8(^{+11.1}_{-10.0})$	$35.5(^{+11.9}_{-12.8})$	$8.4(^{+3.3}_{-3.0})$	$24.0(^{+7.7}_{-8.3})$	$0.1(^{+0.0}_{-0.0})$
325.00	$0.2(^{+0.1}_{-0.1})$	$45.5(^{+14.1}_{-12.5})$	$42.4(^{+12.9}_{-15.0})$	$3.0(^{+1.1}_{-1.2})$	$8.7(^{+4.1}_{-3.8})$	$0.1(^{+0.0}_{-0.0})$
337.50	$0.4(^{+0.2}_{-0.2})$	$53.5(^{+16.9}_{-10.7})$	$42.3(^{+10.4}_{-17.1})$	$1.0(^{+0.5}_{-0.4})$	$2.8(^{+1.2}_{-1.1})$	$0.0(^{+0.1}_{-0.0})$
350.00	$0.5(^{+0.4}_{-0.2})$	$58.5(^{+15.1}_{-11.2})$	$39.7(^{+10.9}_{-15.1})$	$0.3(^{+0.1}_{-0.1})$	$0.9(^{+0.3}_{-0.4})$	$0.0(^{+0.1}_{-0.0})$
Temperature (K)	Product yields (%) ($\pm\sigma$); [NO] = 1 ppb					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
250.00	$0.0(^{+0.1}_{-0.0})$	$0.0(^{+0.1}_{-0.0})$	$0.0(^{+0.1}_{-0.0})$	$47.1(^{+2.6}_{-3.2})$	$52.5(^{+3.1}_{-2.7})$	$0.3(^{+0.2}_{-0.1})$
262.50	$0.0(^{+0.1}_{-0.0})$	$0.1(^{+0.1}_{-0.0})$	$0.1(^{+0.1}_{-0.0})$	$43.8(^{+4.3}_{-5.3})$	$55.7(^{+5.2}_{-4.3})$	$0.3(^{+0.2}_{-0.1})$
275.00	$0.0(^{+0.1}_{-0.0})$	$0.1(^{+0.1}_{-0.0})$	$0.2(^{+0.2}_{-0.1})$	$35.0(^{+7.7}_{-6.1})$	$64.3(^{+6.0}_{-7.7})$	$0.3(^{+0.1}_{-0.1})$
287.50	$0.0(^{+0.1}_{-0.0})$	$0.5(^{+0.4}_{-0.2})$	$0.8(^{+0.6}_{-0.4})$	$27.9(^{+8.5}_{-7.9})$	$70.4(^{+7.8}_{-8.9})$	$0.3(^{+0.1}_{-0.1})$
298.00	$0.0(^{+0.1}_{-0.0})$	$1.8(^{+1.1}_{-0.6})$	$2.4(^{+1.8}_{-1.0})$	$25.3(^{+9.8}_{-6.0})$	$70.1(^{+6.0}_{-11.1})$	$0.4(^{+0.1}_{-0.1})$
312.50	$0.0(^{+0.1}_{-0.0})$	$8.2(^{+4.6}_{-2.9})$	$9.1(^{+5.7}_{-3.5})$	$21.4(^{+7.4}_{-6.8})$	$60.9(^{+8.1}_{-12.7})$	$0.4(^{+0.1}_{-0.1})$
325.00	$0.1(^{+0.0}_{-0.0})$	$22.1(^{+8.8}_{-7.0})$	$20.6(^{+9.6}_{-7.4})$	$14.8(^{+4.1}_{-5.4})$	$42.1(^{+8.6}_{-11.3})$	$0.3(^{+0.1}_{-0.1})$
337.50	$0.3(^{+0.2}_{-0.1})$	$39.9(^{+15.1}_{-10.5})$	$31.5(^{+10.2}_{-13.1})$	$7.3(^{+2.7}_{-2.9})$	$20.8(^{+5.8}_{-7.4})$	$0.2(^{+0.1}_{-0.1})$
350.00	$0.4(^{+0.2}_{-0.2})$	$52.5(^{+12.4}_{-13.0})$	$35.7(^{+12.8}_{-12.7})$	$2.9(^{+1.3}_{-1.2})$	$8.4(^{+3.2}_{-3.1})$	$0.1(^{+0.0}_{-0.0})$

S4.2 Alkoxyl radical products

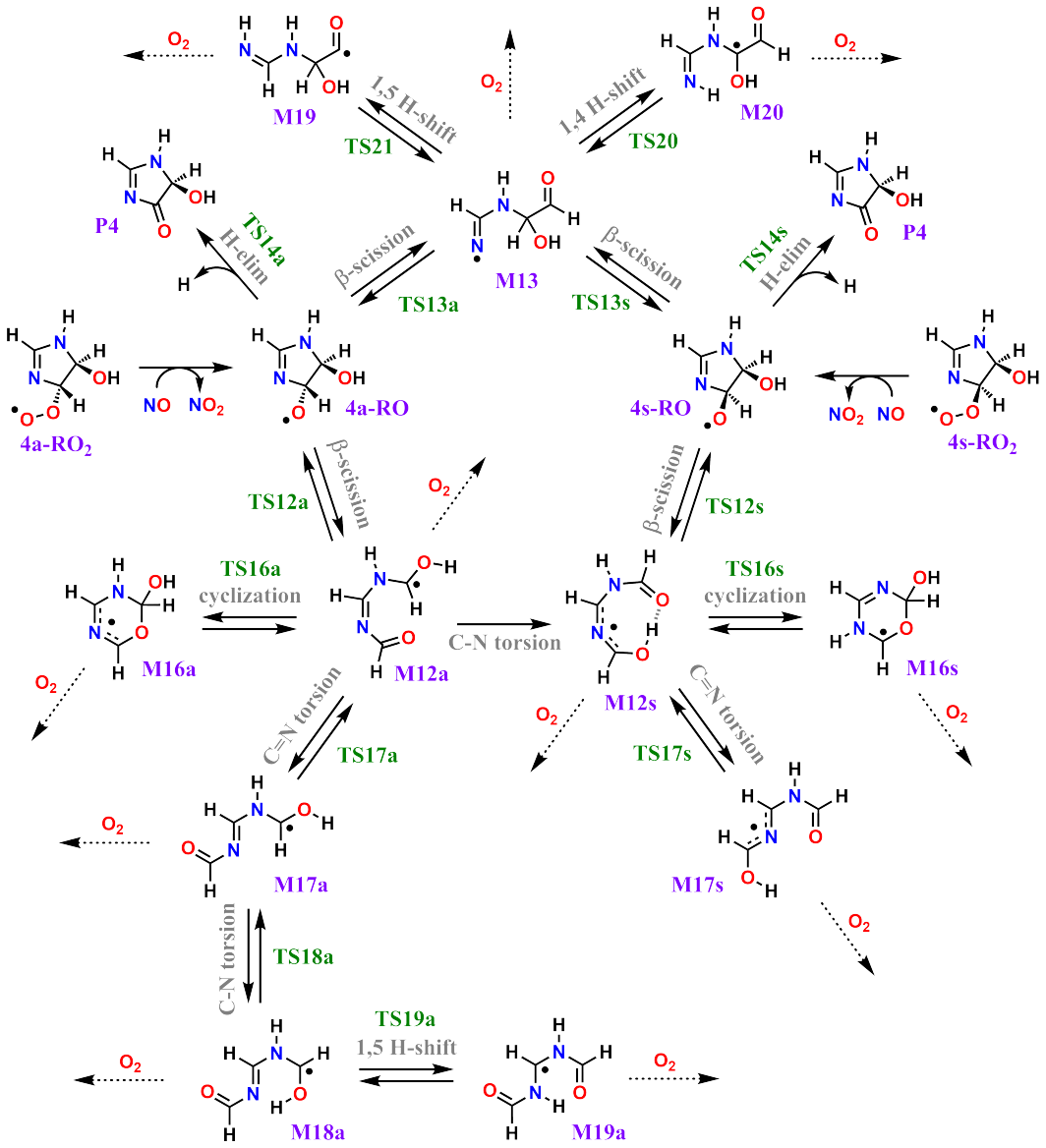

Figure S3 Reaction mechanism for alkoxyl radical products.

Table S3 Product yields obtained from RRKM-ME calculations for reaction of alkoxyl radical 4a-RO at 1 atm. Standard deviations ($\pm\sigma$) calculated with the logit-transformed distribution of yields obtained with uncertainty analysis.

Temperature (K)	Product yields (%) ($\pm\sigma$)		
	M12s-OO + M17s-OO	M19a-OO	M16a-OO
250.00	$98.2(^{+0.8}_{-1.5})$	$1.5(^{+1.4}_{-0.6})$	$0.5(^{+0.3}_{-0.2})$
275.00	$98.0(^{+0.9}_{-1.8})$	$1.7(^{+1.6}_{-0.7})$	$0.4(^{+0.3}_{-0.2})$
298.15	$97.8(^{+1.0}_{-1.4})$	$1.9(^{+1.3}_{-0.8})$	$0.4(^{+0.3}_{-0.1})$
325.00	$97.5(^{+1.1}_{-1.7})$	$2.2(^{+1.7}_{-1.0})$	$0.4(^{+0.1}_{-0.1})$
350.00	$97.1(^{+1.0}_{-2.1})$	$2.6(^{+2.0}_{-0.8})$	$0.3(^{+0.2}_{-0.1})$

Table S4 Product yields obtained from RRKM-ME calculations for reaction of alkoxyl radical 4s-RO at 1 atm. Standard deviations ($\pm\sigma$) calculated with the logit-transformed distribution of yields obtained with uncertainty analysis.

Temperature (K)	Product yields (%) ($\pm\sigma$)			
	M12s-OO + M17s-OO	M13-OO	M20-OO	M21-OO
250.00	$96.3(^{+1.6}_{-3.3})$	$3.1(^{+2.2}_{-1.6})$	$0.2(^{+0.4}_{-0.1})$	$0.6(^{+1.1}_{-0.4})$
275.00	$96.0(^{+1.7}_{-2.5})$	$2.5(^{+1.7}_{-1.6})$	$0.4(^{+0.6}_{-0.3})$	$1.4(^{+1.6}_{-1.0})$
298.15	$95.8(^{+1.6}_{-3.3})$	$1.5(^{+1.5}_{-0.8})$	$0.5(^{+1.1}_{-0.3})$	$2.4(^{+1.8}_{-1.4})$
325.00	$95.7(^{+2.1}_{-2.5})$	$0.6(^{+0.6}_{-0.4})$	$0.6(^{+0.7}_{-0.4})$	$3.3(^{+1.9}_{-1.9})$
350.00	$95.6(^{+1.7}_{-3.3})$	$0.2(^{+0.2}_{-0.1})$	$0.5(^{+0.7}_{-0.3})$	$3.7(^{+2.8}_{-1.6})$

S4.3 Second-generation RO_2

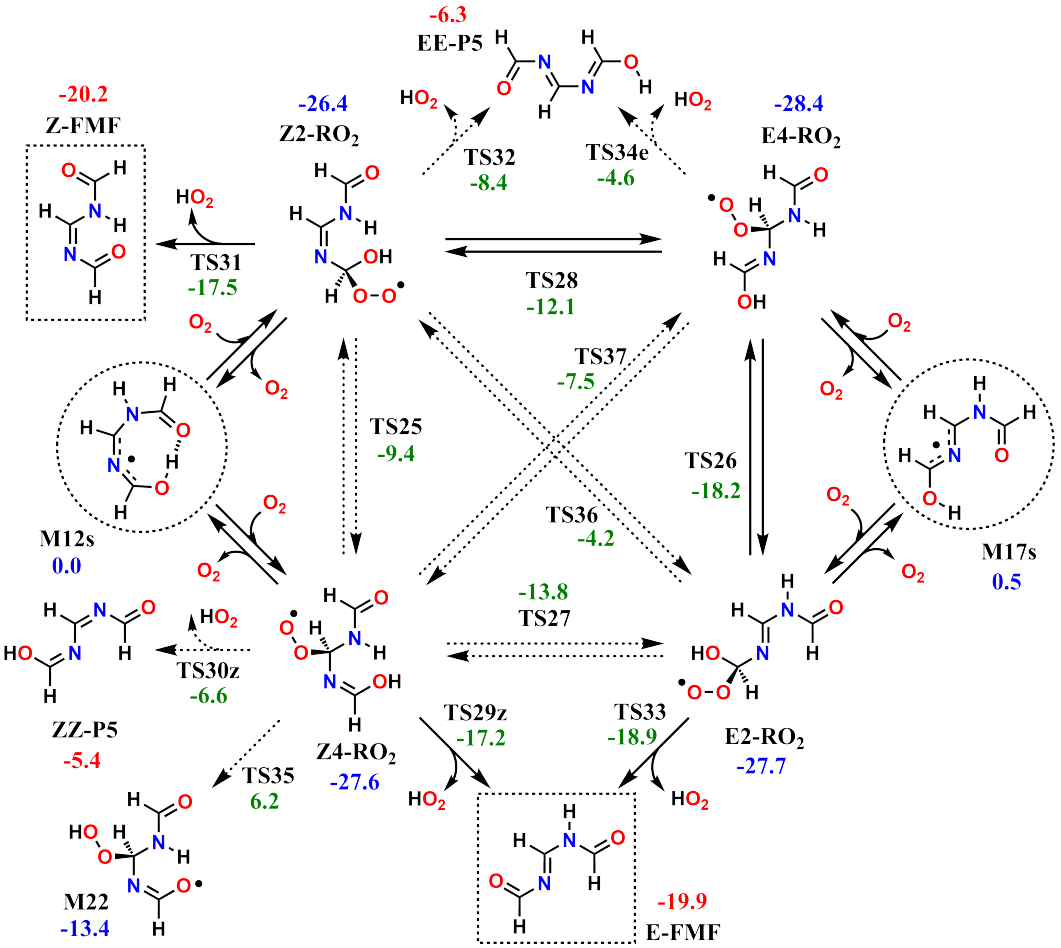

Figure S4 Reaction mechanism for second-generation RO_2. Relative zero-point-corrected energies given in kcal mol^{-1}, calculated at the ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97X-D/aug-cc-pVTZ level of theory.[3–7]

Table S5 Product yields obtained from RRKM-ME calculations for reaction of second-generation RO_2 radicals at 1 atm, derived from 4a-RO and from 4s-RO. Standard deviations ($\pm\sigma$) calculated with the logit-transformed distribution of yields obtained with uncertainty analysis.

Temperature (K)	Product yields (%) ($\pm\sigma$)			
	from 4a-RO		From 4s-RO	
	E-FMF	Z-FMF	E-FMF	Z-FMF
250.00	$91.5(^{+3.2}_{-6.6})$	$8.5(^{+6.1}_{-3.3})$	$91.2(^{+2.5}_{-7.5})$	$8.5(^{+5.9}_{-2.8})$
275.00	$91.4(^{+3.4}_{-7.0})$	$8.6(^{+6.0}_{-3.4})$	$91.4(^{+3.7}_{-6.9})$	$8.6(^{+5.8}_{-3.5})$
298.15	$91.2(^{+3.4}_{-7.0})$	$8.8(^{+6.4}_{-3.3})$	$91.2(^{+4.3}_{-7.4})$	$8.8(^{+5.4}_{-4.2})$
325.00	$91.0(^{+2.5}_{-7.0})$	$9.0(^{+6.7}_{-2.8})$	$91.0(^{+3.4}_{-8.5})$	$9.0(^{+7.5}_{-2.9})$
350.00	$90.7(^{+4.1}_{-6.8})$	$9.3(^{+5.8}_{-4.1})$	$90.7(^{+4.3}_{-7.8})$	$9.3(^{+6.1}_{-4.3})$

S5 Barriers and rate coefficients for second-generation RO_2

Table S6 Reaction barrier heights ($\Delta^{\ddagger}E_{v=0}$) calculated as the difference in zero-point corrected energy between TS and reactant, calculated at ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97X-D/aug-cc-pVTZ level of theory, for unimolecular reaction steps available to second-generation RO_2 intermediates. Thermal rate coefficients estimated with lowest-conformer TST (k_{LC-TST}) and multi-conformer TST (k_{MC-TST}), ratio between MC-TST and LC-TST rate coefficients (k_{MC}/k_{LC}),ratio of lowest-conformer partition functions (Q_{TS}/Q_R) and Eckart tunnelling factors (κ).

Reaction step	$\Delta^{\ddagger}E_{v=0}$ (kcal mol^{-1})	k_{LC-TST} (s^{-1})	k_{MC-TST} (s^{-1})	k_{MC}/k_{LC}	Q_{TS}/Q_R	κ
E2-RO_2 $\longrightarrow$ E4-RO_2	9.49	1.78×10^{5}	5.15×10^{4}	0.29	0.24	1.05
E2-RO_2 $\longrightarrow$ Z4-RO_2	13.96	9.74×10^{1}	4.65×10^{1}	0.48	0.25	1.06
E2-RO_2 $\longrightarrow$ Z2-RO_2	23.47	4.90×10^{-5}	6.02×10^{-5}	1.23	1.19	1.05
E2-RO_2 $\longrightarrow$ E-FMF $+HO_2$	8.83	4.30×10^{6}	2.21×10^{6}	0.51	0.84	2.43
E4-RO_2 $\longrightarrow$ E2-RO_2	10.15	5.83×10^{4}	1.69×10^{4}	0.29	0.21	1.05
E4-RO_2 $\longrightarrow$ Z2-RO_2	16.34	1.92×10^{0}	1.26×10^{0}	0.66	0.28	1.06
E4-RO_2 $\longrightarrow$ Z4-RO_2	20.94	8.70×10^{-4}	1.95×10^{-3}	2.24	0.29	1.06
E4-RO_2 $\longrightarrow$ EE-P5 $+HO_2$	23.76	6.39×10^{-5}	6.22×10^{-5}	0.97	1.14	2.36
Z2-RO_2 $\longrightarrow$ Z4-RO_2	16.99	1.09×10^{0}	6.38×10^{-1}	0.59	0.46	1.07
Z2-RO_2 $\longrightarrow$ E4-RO_2	14.38	5.27×10^{1}	3.47×10^{1}	0.66	0.61	1.06
Z2-RO_2 $\longrightarrow$ E2-RO_2	22.16	4.42×10^{-4}	5.44×10^{-4}	1.23	2.26	1.05
Z2-RO_2 $\longrightarrow$ Z-FMF $+HO_2$	8.93	6.42×10^{6}	1.02×10^{7}	1.59	1.48	2.45
Z2-RO_2 $\longrightarrow$ EE-P5 $+HO_2$	17.99	1.65×10^{0}	1.05×10^{0}	0.64	1.43	2.87
Z4-RO_2 $\longrightarrow$ Z2-RO_2	18.16	1.49×10^{-1}	8.73×10^{-2}	0.59	0.79	1.07
Z4-RO_2 $\longrightarrow$ E2-RO_2	13.83	1.21×10^{2}	5.75×10^{1}	0.48	0.82	1.06
Z4-RO_2 $\longrightarrow$ E4-RO_2	20.15	3.28×10^{-3}	7.33×10^{-3}	2.23	1.11	1.06
Z4-RO_2 $\longrightarrow$ E-FMF $+HO_2$	10.37	5.82×10^{5}	3.14×10^{5}	0.54	1.75	2.12
Z4-RO_2 $\longrightarrow$ ZZ-P5 $+HO_2$	20.97	1.11×10^{-2}	5.03×10^{-2}	0.45	2.82	1.49
Z4-RO_2 $\longrightarrow$ M22	21.41	9.07×10^{-4}	4.42×10^{-4}	0.49	0.61	1.18

S6 Pressure dependence of product yields

Additional RRKM-ME calculations at different pressures (0.1, 0.5, 5 and 10 atm) were performed for the first-generation RO_2 reactions, whose results are shown in Table S7. We note here that the only parameter changed in these ME runs was the pressure, and the excess reactant concentrations ($[O_2]$ and [NO]) were kept at the values they would have at 1 atm and 298 K. This was done in order to observe the effect that pressure change *alone* (change of collision frequency) would have on the kinetics of the reaction. The results show a very weak pressure dependence of product yields, possibly indicating that the kinetics of this part of the oxidation mechanism is close to the high-pressure limit. The largest change in yields at the investigated pressure range (0.1-10 atm) was $\sim 0.5\%$. Naturally, as the pressure decreases, a slight increase in the yield of unimolecular channels is observed, as vibrationally hot molecules may react prior to significant collisional quenching.

Table S7 Product yields obtained from RRKM-ME calculations for reaction of first-generation RO_2 radicals at a range of pressures (0.1, 0.5, 1, 5, and 10 atm). The different NO concentrations used correspond to mixing ratios at 1 atm, 298 K (10 ppt, 100 ppt, and 1 ppb).

Pressure (atm)	Product yields (%); [NO] = 10 ppt					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
0.1	0.131	33.838	46.792	4.926	14.254	0.070
0.5	0.118	33.695	46.903	4.942	14.281	0.070
1	0.116	33.671	46.923	4.945	14.285	0.070
5	0.114	33.647	46.943	4.948	14.286	0.070
10	0.114	33.643	46.947	4.949	14.286	0.070
Pressure (atm)	Product yields (%); [NO] = 100 ppt					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
0.1	0.059	12.572	17.179	18.038	51.893	0.256
0.5	0.046	12.367	17.183	18.094	52.051	0.256
1	0.044	12.333	17.184	18.103	52.077	0.257
5	0.042	12.300	17.185	18.112	52.102	0.257
10	0.042	12.293	17.185	18.113	52.107	0.257
Pressure (atm)	Product yields (%); [NO] = 1 ppb					
	5-ol	4H-4ol	Z-FMF	4s-RO	4a-RO	2-RO
0.1	0.023	2.027	2.491	25.514	69.576	0.358
0.5	0.010	1.780	2.427	25.384	70.031	0.357
1	0.008	1.738	2.415	25.346	70.125	0.357
5	0.006	1.696	2.401	25.286	70.244	0.356
10	0.006	1.688	2.398	25.267	70.275	0.356

S7 Time evolution profiles for first-generation RO_2

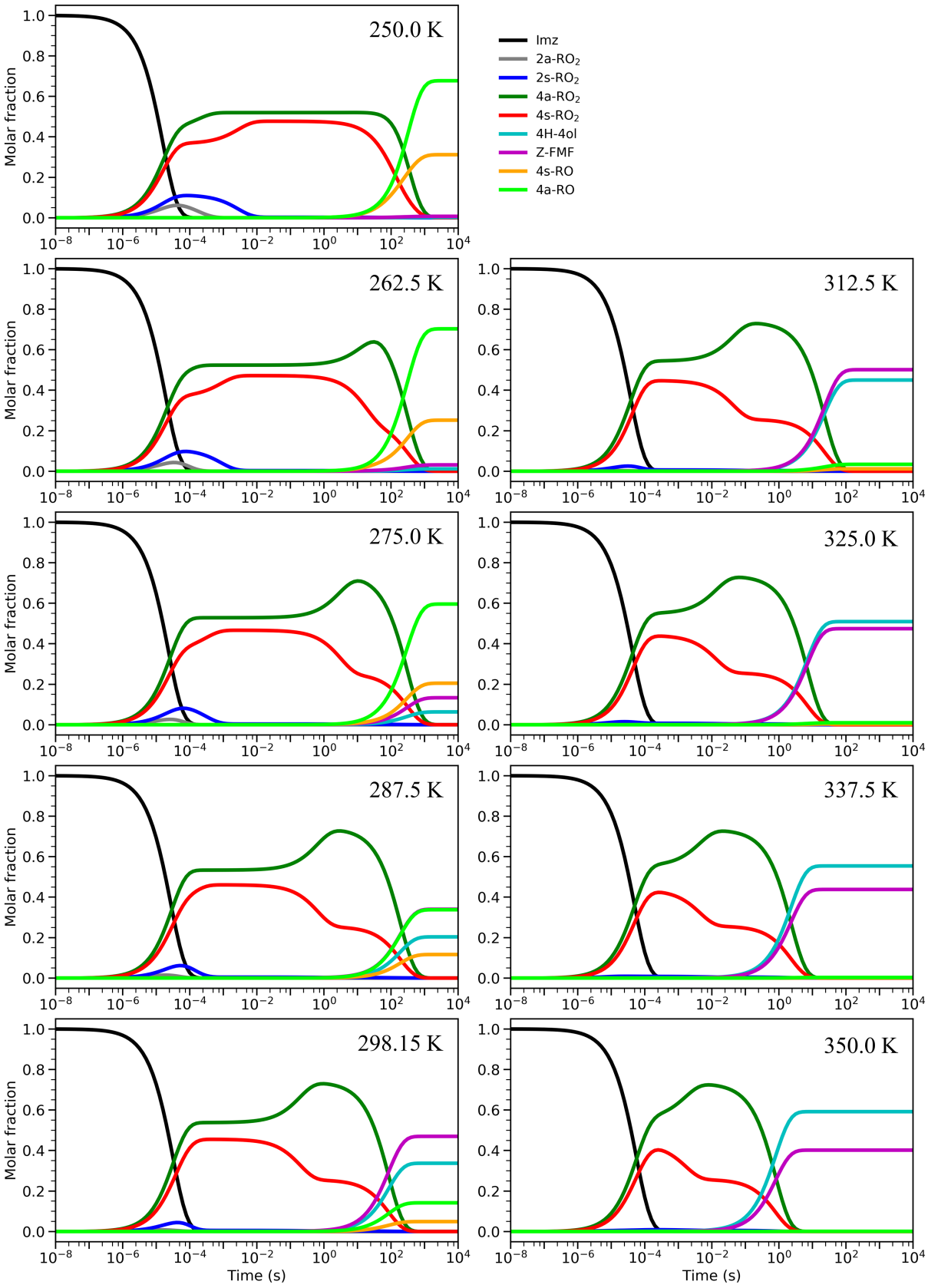

Figure S5 Time evolution of species distributions from RRKM-ME calculation for the first-generation RO_2 radicals, at 298 K, 1 atm and 10 ppt NO, with imidazole + OH as starting reactants.

S8 Vertical excitation energies for first-generation RO_2

Test time dependent DFT (TDDFT) single-point calculations (Table S8) indicate that, for all four first-generation RO_2, the first electronic excited state is higher in energy than the entrance level (5-OH $+O_2$) by at at least 6 kcal mol^{-1}. Except for isomer 2a-RO_2, excitation energies obtained with single-point calculations done at the RI-CC2/def2-TZVP[8,9] level using Turbomole v'7.8[10,11] agree with TDDFT results within $\sim$ 2 kcal mol^{-1}. Moreover, %T2 diagnostics from CC2 calculations indicate a small contribution of double excitations ($< 4\%$). This suggests that RO_2 isomers 2s-RO_2, 4a-RO_2, and 4s-RO_2 are unlikely to be formed in their electronic excited states directly from 5-OH $+O_2$ association. On the other hand, RI-CC2 calculation for isomer 2a-RO_2 yielded a (unphysical) negative first-excitation energy, indicating that the TDDFT results are not reliable for this species. We argue, however, that even if formation of electronically-excited 2a-RO_2 is indeed possible, excited-state reaction channels are unlikely to be competitive with relaxation to the ground-state via internal conversion.[12]

Table S8 Vertical excitation energy for transition from the electronic ground-state to the first excited state, for the first-generation RO_2, estimated with single-point Time Dependent Density Functional Theory (TDDFT) calculations at the ωB97XD/aug-cc-pVTZ level of theory, and with single-point RI-CC2/def2-TZVP calculations with frozen core orbitals and UHF reference. Diagnostics for double excitation contributions (%T2) obtained from CC2 calculations. Energies are given in kcal mol^{-1}

Species	$E(D_0 \rightarrow D_1)$		%T2
	TDDFT	CC2	
2a-RO_2	26.9	—	—
2s-RO_2	28.4	30.7	3.98
4a-RO_2	26.7	28.6	3.66
4s-RO_2	27.3	29.4	3.75

S9 Multiconfigurational character diagnostics

In addition to the T1 diagnostics, which are provided with CCSD(T)-F12a calculations in Molpro[13–15], we calculate the percentage of the triples (T) contribution to the total atomization energy as a diagnostic for multiconfigurational character. Values of %TAE[(T)] were calculated as follows[16,17]:

$$\%TAE[(T)] = 100 \times \frac{TAE_{CCSD(T)} - TAE_{CCSD}}{TAE_{CCSD(T)}} \tag{S2}$$

Where $TAE_{CCSD(T)}$ and TAE_{CCSD} are calculated as shown for imidazole ($C_3N_2H_4$):

$$TAE_{CCSD(T)}(C_3N_2H_4) = [(3 \times E_{CCSD(T)}C) + (2 \times E_{CCSD(T)}N) + (4 \times E_{CCSD(T)}H)] - E_{CCSD(T)}(C_3N_2H_4) \tag{S3}$$

$$TAE_{CCSD}(C_3N_2H_4) = [(3 \times E_{CCSD}C) + (2 \times E_{CCSD}N) + (4 \times E_{CCSD}H)] - E_{CCSD}(C_3N_2H_4) \tag{S4}$$

The calculated %TAE[(T)] values indicate that, apart from O_2, NO_2, and NO, all of the species investigated in this work display mild multiconfigurational character. %TAE[(T)] values in the range of 2-5% indicate the presence of mild static (non-dynamical) correlation, values in the 5-10% range indicate moderate static correlation, and values larger than 10% indicate severe static correlation.

Table S9 Percentage triples (T) contribution to the total atomization energy $\%TAE[(T)]$ and T1 diagnostics from ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12 calculations.

Species	$\%TAE[(T)]$	T1 diagnostic	Species	$\%TAE[(T)]$	T1 diagnostic
imidazole	2.16	0.013	4a-ROONO	3.08	0.017
OH	1.23	0.007	4s-ROONO	3.10	0.017
5-OH	2.13	0.019	4a-RO	2.17	0.020
O_2	6.50	0.008	4s-RO	2.14	0.019
HO_2	3.72	0.034	TS12a	0.05	0.028
NO	5.34	0.020	TS12s	2.34	0.031
NO_2	7.44	0.024	TS13a	2.50	0.025
2a-RO_2	2.48	0.023	TS13s	2.51	0.027
2s-RO_2	2.51	0.024	TS14a	2.49	0.018
4a-RO_2	2.48	0.024	TS14s	2.48	0.018
4s-RO_2	2.51	0.024	TS15a	2.30	0.020
TS4a	3.19	0.031	TS16a	2.59	0.024
TS4s	3.28	0.040	TS16s	2.55	0.026
TS5a	2.93	0.029	TS17a	2.34	0.021
TS5s	2.95	0.029	TS17s	2.35	0.018
TS6a	3.13	0.032	TS18a	2.23	0.018
TS7s	2.95	0.037	TS19a	2.49	0.021
TS8s	2.70	0.020	TS20	2.49	0.024
M7s	2.86	0.019	TS21	2.50	0.025
M8s	2.62	0.019	M12a	2.31	0.021
PC5a	2.54	0.023	M12s	2.38	0.019
PC5s	2.58	0.024	M13	2.13	0.016
PC6a	2.53	0.023	M16a	2.25	0.015
4H-4ol	2.29	0.015	M16s	2.22	0.018
5-ol	2.28	0.013	M17a	2.23	0.020
Z-FMF	2.41	0.017	M17s	2.29	0.019
E-FMF	2.37	0.017	M18a	2.40	0.026
TSa endo	2.97	0.037	M19a	2.25	0.020
TSs endo	3.20	0.031	M20	2.29	0.016
BPRa	2.50	0.016	M21	2.28	0.017
BPRs	2.53	0.018	P5	2.37	0.016
TS direct H-abs	0.07	0.048	TS FMF N-inversion	2.43	0.017

Table S10 Percentage triples (T) contribution to the total atomization energy $\%TAE[(T)]$ and T1 diagnostics from ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12 calculations.

Species	$\%TAE[(T)]$	T1 diagnostic	Species	$\%TAE[(T)]$	T1 diagnostic
E2-RO_2	2.57	0.023	TS34z	2.99	0.027
E4-RO_2	2.57	0.023	TS35	0.07	0.037
Z2-RO_2	2.62	0.024	TS36	2.67	0.024
Z4-RO_2	2.64	0.025	TS37	2.69	0.024
TS25	3.18	0.027	PC29e	2.64	0.024
TS26	3.06	0.025	PC29z	2.60	0.024
TS27	3.10	0.027	PC30e	2.72	0.024
TS28	3.12	0.027	PC30z	2.73	0.024
TS29e	2.94	0.025	PC31	2.61	0.024
TS29z	2.91	0.024	PC32	2.66	0.024
TS30e	3.05	0.027	PC33	2.58	0.024
TS30z	3.00	0.022	PC34e	2.66	0.024
TS31	2.94	0.024	PC34z	2.64	0.023
TS32	2.88	0.026	M22	2.60	0.019
TS33	2.91	0.024	EE-P5	2.42	0.017
TS34e	2.96	0.027	ZZ-P5	2.50	0.018

S10 ROCCSD(T)-F12a/cc-pVTZ-F12 and UCCSD(T)-F12a/cc-pVDZ-F12 single-point energies

Table S11 Zero-point corrected energies for first-generation RO_2 and most important transition states calculated at the ROHF-ROCCSD(T)-F12a/cc-pV*n*Z-F12 (n = D or T) level, and at the ROHF-UCCSD(T)-F12a/cc-pVDZ-F12 level, relative to the entrance channel (5-OH + O_2), given in kcal mol^{-1}.

Species	$E_{RO,VDZ}$	$E_{RO,VTZ}$	$E_{U,VDZ}$	$E_{RO,VDZ}-E_{RO,VTZ}$	$E_{RO,VDZ}-E_{U,VDZ}$
5-OH + O_2	0.00	0.00	0.00	0.00	0.00
2a-RO_2	−16.74	−17.09	−16.34	0.35	−0.40
2s-RO_2	−17.92	−18.29	−17.55	0.37	−0.37
4a-RO_2	−20.74	−21.19	−20.35	0.45	−0.39
4s-RO_2	−20.40	−20.88	−20.09	0.48	−0.31
TS4a	−6.70	−6.97	−6.08	0.27	−0.62
TS4s	−6.02	−6.19	−5.77	0.17	−0.25
TS5a	0.83	0.83	1.51	0.00	−0.68
TS5s	1.25	0.99	1.68	0.26	−0.43
TS6a	3.56	3.13	4.02	0.43	−0.46
TS7s	0.08	−0.19	−2.12	0.27	+2.20

S11 Electronic energies, zero-point vibrational energies and partition functions

Table S12 Electronic energies ($E_{e,DFT}$), zero-point vibrational energies (E_{zpv}) and total molecular partition functions ($Q_{tot}(v=0)$) calculated at the ωB97XD/aug-cc-pVTZ level of theory, under the Harmonic-Oscillator-Rigid-Rotor approximation, at 1 atm and 298 K. Single-point electronic energies ($E_{e,CC}$) calculated at the ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97XD/aug-cc-pVTZ level of theory. Energy values given in Hartrees (Eh).

Species	$E_{e,DFT}$ (Eh)	$E_{e,CC}$ (Eh)	E_{zpv} (Eh)	$Q_{tot}(v=0)$
imidazole	−226.223232548	−225.909573732973	0.072020	0.115658×10^{13}
OH	−75.7407450132	−75.662876938771	0.008608	0.604563×10^{08}
O_2	−150.334299668	−150.175421936388	0.003882	0.150051×10^{10}
HO_2	−150.921000002	−150.761615558093	0.014547	0.153865×10^{11}
NO	−129.897115420	−129.757653213855	0.004610	0.154202×10^{10}
NO_2	−205.088487163	−204.867212142322	0.009049	0.536679×10^{11}
5-OH	−302.009885037	−301.615111502248	0.085350	0.344644×10^{14}
2a-RO_2	−452.368386456	−451.823730526359	0.095747	0.621312×10^{15}
2s-RO_2	−452.370845889	−451.825952717879	0.096091	0.373118×10^{15}
4a-RO_2	−452.377296150	−451.830135808682	0.095790	0.795759×10^{15}
4s-RO_2	−452.377508888	−451.830346775931	0.096537	0.488441×10^{15}
TS4a	−452.347489533	−451.805636689923	0.093659	0.380877×10^{15}
TS4s	−452.348297654	−451.803692857243	0.092790	0.724947×10^{15}
TS5a	−452.334513625	−451.789135158380	0.089551	0.114173×10^{16}
TS5s	−452.334557947	−451.789139655172	0.089823	0.895742×10^{15}
TS6a	−452.334865790	−451.785358677512	0.089726	0.825654×10^{15}
TS7s	−452.344319753	−451.791379592525	0.090203	0.189395×10^{15}
TS8s	−452.349406190	−451.800630359954	0.092456	0.106208×10^{16}
PC5a	−452.353125363	−451.810229347024	0.092407	0.456404×10^{17}
PC5s	−452.361416900	−451.817776551819	0.093334	0.466762×10^{16}
PC6a	−452.393146268	−451.842819427856	0.093499	0.318203×10^{17}
M7s	−452.351258488	−451.803187846204	0.093536	0.103330×10^{16}
M8s	−452.372682172	−451.821408603242	0.091292	0.231958×10^{17}
4H-4ol	−301.414627674	−301.031665629080	0.075237	0.969329×10^{13}
5-ol	−301.449592827	−301.059273568953	0.076222	0.828035×10^{13}
Z-FMF	−376.688321974	−376.222362532819	0.079091	0.232849×10^{15}
E-FMF	−376.688049803	−376.221293929702	0.078588	0.314788×10^{15}
TSa endo	−452.320250408	−451.772408911549	0.093809	0.129351×10^{15}
TSs endo	−452.319409182	−451.775381038013	0.093684	0.123243×10^{15}
BPRa	−452.346580652	−451.805565003876	0.096517	0.133966×10^{15}
BPRs	−452.347525638	−451.806584638995	0.096856	0.102670×10^{15}
TS FMF N-inversion	−376.668195372	−376.197014271671	0.077608	0.306067×10^{15}
TS direct H-abs	−452.326806925	−451.774108431936	0.088631	0.341259×10^{16}

Table S13 Electronic energies ($E_{e,DFT}$), zero-point vibrational energies (E_{zpv}) and total molecular partition functions ($Q_{tot}(v=0)$) calculated at the ωB97XD/aug-cc-pVTZ level of theory, under the Harmonic-Oscillator-Rigid-Rotor approximation, at 1 atm and 298 K. Single-point electronic energies ($E_{e,CC}$) calculated at the ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97XD/aug-cc-pVTZ level of theory. Energy values given in Hartrees (Eh).

Species	$E_{e,DFT}$ (Eh)	$E_{e,CC}$ (Eh)	E_{zpv} (Eh)	$Q_{tot}(v=0)$
4a-ROONO	−582.309869202	−581.630508181587	0.104068	0.176546×10^{17}
4s-ROONO	−582.309660324	−581.630942272112	0.104618	0.117275×10^{17}
4a-RO	−377.208002981	−376.736932413013	0.089940	0.214019×10^{15}
4s-RO	−377.207865120	−376.737984500920	0.090036	0.142245×10^{15}
TS12a	−377.203040668	−376.729464082689	0.088578	0.184008×10^{15}
TS12s	−377.202441750	−376.728350746805	0.088410	0.152445×10^{15}
TS13a	−377.189129205	−376.719635234914	0.087886	0.157020×10^{15}
TS13s	−377.194283971	−376.724660566323	0.088458	0.995138×10^{14}
TS14a	−377.170587462	−376.704004342929	0.082543	0.132117×10^{15}
TS14s	−377.171685735	−376.705594337650	0.082150	0.208349×10^{15}
TS15a	−377.219036757	−376.744836923211	0.087305	0.639515×10^{15}
TS16a	−377.212996415	−376.740819865154	0.088810	0.104282×10^{15}
TS16s	−377.220509506	−376.748526131318	0.089475	0.750997×10^{14}
TS17a	−377.213160441	−376.735459333007	0.087611	0.864943×10^{15}
TS17s	−377.233217246	−376.755119226473	0.087593	0.436610×10^{15}
TS18a	−377.221313169	−376.747579583709	0.086731	0.273204×10^{16}
TS19a	−377.244261834	−376.769046804001	0.085790	0.203250×10^{15}
TS20	−377.183935435	−376.714061393842	0.084086	0.275396×10^{15}
TS21	−377.186226954	−376.715849544618	0.083475	0.542227×10^{15}
M12a	−377.226880983	−376.752074460066	0.088841	0.735335×10^{15}
M12s	−377.253059629	−376.776427311038	0.089813	0.594836×10^{15}
M13	−377.213713056	−376.746040086351	0.087816	0.106335×10^{16}
M16a	−377.244483090	−376.774592992347	0.091163	0.840861×10^{14}
M16s	−377.228476298	−376.758325227930	0.091336	0.103363×10^{15}
M17a	−377.233342825	−376.759180261072	0.088566	0.176654×10^{16}
M17s	−377.249727877	−376.773958088501	0.088204	0.210359×10^{16}
M18a	−377.245036268	−376.768759973816	0.088957	0.401353×10^{15}
M19a	−377.271567034	−376.794695502791	0.089504	0.845576×10^{15}
M20	−377.247844505	−376.773489403080	0.090177	0.572888×10^{15}
M21	−377.217283181	−376.749489319278	0.088777	0.229191×10^{16}
P5	−376.684096138	−376.218863008304	0.080590	0.618520×10^{14}

Table S14 Electronic energies ($E_{e,DFT}$), zero-point vibrational energies (E_{zpv}) and total molecular partition functions ($Q_{tot}(v=0)$) calculated at the ωB97XD/aug-cc-pVTZ level of theory, under the Harmonic-Oscillator-Rigid-Rotor approximation, at 1 atm and 298 K. Single-point electronic energies ($E_{e,CC}$) calculated at the ROHF-ROCCSD(T)-F12a/cc-pVDZ-F12//ωB97XD/aug-cc-pVTZ level of theory. Energy values given in Hartrees (Eh).

Species	$E_{e,DFT}$ (Eh)	$E_{e,CC}$ (Eh)	E_{zpv} (Eh)	$Q_{tot}(v=0)$
E2-RO_2	−527.625759726	−527.000779361207	0.098437	0.301463×10^{17}
E4-RO_2	−527.627061510	−527.002170163868	0.098777	0.349290×10^{17}
Z2-RO_2	−527.623772267	−526.999269767715	0.099005	0.158249×10^{17}
Z4-RO_2	−527.626326014	−527.001391876376	0.099276	0.127063×10^{17}
TS25	−527.592727659	−526.970258733304	0.097063	0.732149×10^{16}
TS26	−527.609169450	−526.984814046279	0.097591	0.736032×10^{16}
TS27	−527.600554018	−526.977259787046	0.097165	0.763224×10^{16}
TS28	−527.597848257	−526.974692297824	0.097336	0.961118×10^{16}
TS29e	−527.598313169	−526.969221851031	0.093449	0.171434×10^{17}
TS29z	−527.608023646	−526.978882926670	0.093260	0.162136×10^{17}
TS30e	−527.582875329	−526.958493290871	0.093207	0.143605×10^{17}
TS30z	−527.589268732	−526.961798908208	0.093075	0.261475×10^{17}
TS31	−527.604743481	−526.979947930682	0.093914	0.234325×10^{17}
TS32	−527.593048646	−526.964109722016	0.092516	0.226368×10^{17}
TS33	−527.607317493	−526.981714878582	0.093444	0.254571×10^{17}
TS34e	−527.584988467	−526.957851720314	0.092327	0.398007×10^{17}
TS34z	−527.583461835	−526.957309536309	0.092287	0.603376×10^{17}
TS35	−527.594320693	−526.963354326633	0.095336	0.568073×10^{16}
TS36	−527.590935465	−526.961497524727	0.096550	0.358348×10^{17}
TS37	−527.594077648	−526.964277383705	0.096847	0.715411×10^{17}
PC29e	−527.618698464	−526.992587986847	0.096173	0.510286×10^{18}
PC29z	−527.628656450	−527.001282631543	0.096119	0.589012×10^{18}
PC30e	−527.597498337	−526.973654189782	0.095572	0.841129×10^{18}
PC30z	−527.602206243	−526.976472272938	0.095935	0.189480×10^{18}
PC31	−527.623347869	−526.997944097581	0.096183	0.155801×10^{19}
PC32	−527.603951947	−526.978578979483	0.095783	0.439384×10^{18}
PC33	−527.624661682	−526.998299431262	0.095784	0.173996×10^{19}
PC34e	−527.603951943	−526.978578482214	0.095788	0.436733×10^{18}
PC34z	−527.599119255	−526.975529318668	0.095204	0.226133×10^{19}
M22	−527.598492294	−526.976026780244	0.096521	0.122082×10^{18}
EE-P5	−376.664094946	−376.199558479277	0.078473	0.317189×10^{15}
ZZ-P5	−376.664706774	−376.198731679595	0.079028	0.126421×10^{15}

S12 Cartesian coordinates, vibrational wavenumbers and rotational constants

Cartesian coordinates correspond to the structures of lowest-free energy conformers, optimized at the ωB97XD/aug-cc-pVTZ level of theory.[3–5]

imidazole							
Cartesian Coordinates (Å)							
N	0.73933	0.81175	-0.00006				
C	0.99086	-0.52109	0.00005				
N	-0.11185	-1.21990	-0.00000				
C	-1.12695	-0.29772	-0.00004				
C	-0.62292	0.96780	0.00006				
H	1.99188	-0.91951	0.00006				
H	-2.16068	-0.59773	-0.00007				
H	-1.09161	1.93477	0.00010				
H	1.42208	1.54560	-0.00009				
Vibrational wavenumbers (cm^{-1})							
552.6	653.8	688.9	758.9	850.9	904.2	913.0	952.5
1088.8	1110.0	1159.6	1185.6	1296.7	1393.2	1460.9	1528.8
1584.1	3261.9	3264.4	3295.3	3708.8			
Rotational Constants (GHz):				9.8462	9.5198	4.8401	

OH						
Cartesian Coordinates (Å)						
H	0.00000	0.00000	-0.86236			
O	0.00000	0.00000	0.10780			
Vibrational wavenumbers (cm^{-1})						
3778.6						
Rotational Constants (GHz):				0.0000	566.3471	566.3471

O_2						
Cartesian Coordinates (Å)						
O	0.00000	0.00000	0.59800			
O	0.00000	0.00000	-0.59800			
Vibrational wavenumbers (cm^{-1})						
1704.0						
Rotational Constants (GHz):				0.0000	44.1780	44.1780

HO_2							
Cartesian Coordinates (Å)							
O	0.05500	0.70984	0.00000				
O	0.05500	-0.60202	0.00000				
H	-0.87996	-0.86254	0.00000				
Vibrational wavenumbers (cm^{-1})							
1237.2	1463.4	3685.0					
Rotational Constants (GHz):				629.1948	34.5325	32.7359	

NO							
Cartesian Coordinates (Å)							
N	0.00000	0.00000	-0.60826				
O	0.00000	0.00000	0.53223				
Vibrational wavenumbers (cm^{-1})							
2023.6							
Rotational Constants (GHz):				0.0000	52.0379	52.0379	

NO_2							
Cartesian Coordinates (Å)							
N	-0.00000	-0.00000	0.31848				
O	-0.00000	1.09171	-0.13933				
O	-0.00000	-1.09171	-0.13933				
Vibrational wavenumbers (cm^{-1})							
780.7	1437.7	1753.8					
Rotational Constants (GHz):				247.5663	13.2553	12.5817	

5-OH							
Cartesian Coordinates (Å)							
N	0.02738	0.00315	0.03707				
C	-0.37942	-0.63575	1.16624				
N	0.61759	-1.14301	1.86601				
C	1.73965	-0.82046	1.21123				
C	1.47590	0.04086	0.00797				
H	-1.41885	-0.71797	1.44008				
H	1.86818	-0.35140	-0.93288				
H	-0.55221	0.56245	-0.55859				
H	1.90318	1.66969	0.97897				
O	2.01326	1.35216	0.07915				
H	2.71854	-1.12175	1.54701				
Vibrational wavenumbers (cm^{-1})							
115.9	297.1	333.9	423.1	538.4	598.8	630.9	789.4
823.9	894.1	933.4	1029.9	1047.4	1122.4	1186.7	1235.5
1258.6	1309.1	1334.3	1422.3	1477.0	1534.2	3058.5	3246.7
3255.8	3712.9	3854.0					
Rotational Constants (GHz):				7.6341	3.7595	2.8521	

2a-RO_2							
Cartesian Coordinates (Å)							
N	-0.02068	0.21149	0.22042				
C	-0.47463	-0.45964	1.38663				
N	0.69522	-0.79225	2.16920				
C	1.69498	-0.63427	1.41121				
C	1.38245	-0.07733	0.03850				
H	2.70622	-0.84747	1.73717				
H	1.58599	-0.81470	-0.74056				
H	-0.60932	0.13048	-0.59196				
H	1.84125	1.77941	0.24849				
O	2.14187	1.05035	-0.29994				
H	-1.22626	0.07689	1.96105				
O	-1.19826	-1.72355	1.08374				
O	-0.52970	-2.48122	0.27228				
Vibrational wavenumbers (cm^{-1})							
108.7	124.7	210.0	288.1	368.7	418.9	427.6	544.2
591.0	711.5	796.7	831.8	873.0	933.7	985.1	1038.6
1065.5	1140.7	1162.2	1226.7	1277.5	1292.5	1326.0	1377.1
1385.8	1428.8	1451.1	1728.5	3078.6	3133.3	3195.2	3645.6
3860.8							
Rotational Constants (GHz):				4.3663	1.6376	1.5174	

2s-RO_2							
Cartesian Coordinates (Å)							
N	0.00305	0.01028	0.00595				
C	-0.45831	-0.25049	1.31137				
N	0.63465	-0.86708	2.03053				
C	1.66652	-0.73497	1.30978				
C	1.44668	0.00262	0.00369				
H	-1.37867	-0.82706	1.36513				
H	2.64237	-1.07268	1.63742				
H	1.84264	-0.52699	-0.86211				
H	-0.46800	0.70268	-0.55000				
H	1.68922	1.75936	0.73096				
O	2.07144	1.25691	0.00013				
O	-0.86331	0.97337	2.08272				
O	0.03212	1.90542	2.05153				
Vibrational wavenumbers (cm^{-1})							
131.9	158.7	216.4	320.0	376.1	429.8	486.4	564.5
615.4	661.6	783.2	853.6	871.7	919.6	981.4	1039.6
1068.8	1108.8	1160.4	1239.6	1286.7	1309.0	1326.7	1373.5
1392.9	1438.3	1466.7	1723.1	3102.6	3136.3	3197.8	3665.9
3771.9							
Rotational Constants (GHz):				3.2462	2.1914	1.7943	

4a-RO_2							
Cartesian Coordinates (Å)							
N	0.00716	-0.01854	-0.00679				
C	-0.41455	-0.73935	1.07738				
N	0.47686	-1.15404	1.89054				
C	1.74102	-0.81527	1.29160				
C	1.45405	-0.00335	-0.00192				
H	-1.47435	-0.89743	1.23423				
H	1.87194	-0.49941	-0.87546				
H	-0.51986	0.01528	-0.86037				
H	1.52654	1.80878	0.66637				
O	1.98690	1.28825	0.00418				
H	2.39480	-0.26957	1.97023				
O	2.50469	-2.01845	1.00860				
O	1.91915	-2.76027	0.11485				
Vibrational wavenumbers (cm^{-1})							
82.3	134.8	222.7	283.6	345.0	381.2	425.4	487.6
569.5	683.9	777.6	881.2	936.8	978.0	994.1	1066.7
1073.9	1132.3	1153.9	1217.1	1263.5	1293.4	1314.4	1358.4
1395.1	1434.6	1468.2	1690.4	3118.9	3125.4	3206.0	3682.3
3868.9							
Rotational Constants (GHz):				3.0972	2.0725	1.6072	

4s-RO_2							
Cartesian Coordinates (Å)							
N	0.08681	-0.15602	-0.11014				
C	-0.33055	-0.56922	1.12567				
N	0.55571	-1.02350	1.92200				
C	1.80556	-0.92358	1.21549				
C	1.54422	-0.07661	-0.08441				
H	-1.38204	-0.52894	1.38029				
H	2.19658	-1.90939	0.96636				
H	1.96985	-0.55925	-0.96032				
H	-0.42450	0.54309	-0.62150				
H	1.95972	1.57783	0.81188				
O	2.02072	1.22491	-0.08414				
O	2.84602	-0.37905	2.05014				
O	2.53434	0.79273	2.52771				
Vibrational wavenumbers (cm^{-1})							
69.2	187.4	266.8	319.2	380.5	466.5	504.5	537.8
595.4	682.6	802.1	880.8	894.0	988.3	999.2	1044.7
1087.4	1120.5	1177.5	1221.5	1266.3	1298.4	1338.6	1359.5
1390.1	1453.2	1476.7	1695.4	3105.8	3129.9	3208.8	3656.6
3769.8							
Rotational Constants (GHz):				3.2829	2.2757	1.6586	

TS4a

Cartesian Coordinates (Å)			
N	0.03012	-0.00986	-0.01901
C	-0.36900	-0.78134	1.02354
N	0.61075	-1.02253	1.91118
C	1.70738	-0.81894	1.22551
C	1.48378	0.02322	-0.01891
H	2.69040	-0.99606	1.63724
H	1.90925	-0.41632	-0.91780
H	-0.50623	0.07419	-0.86274
H	1.65640	1.75459	0.83113
O	2.01227	1.31912	0.05278
H	-1.41387	-0.92885	1.24635
O	0.02451	-2.67914	0.13676
O	1.26135	-2.63306	0.01262

Vibrational wavenumbers (cm^{-1})							
206.9 *i*	146.2	182.9	222.6	282.9	344.0	372.3	469.0
511.1	605.2	624.7	840.7	874.0	917.8	939.9	954.5
1041.0	1107.6	1157.9	1196.1	1268.5	1290.5	1304.9	1373.5
1436.7	1452.1	1478.2	1547.6	3126.3	3231.7	3255.3	3691.8
3863.9							

Rotational Constants (GHz):	3.9116	1.7861	1.6896

TS4s

Cartesian Coordinates (Å)			
N	0.36343	0.30736	0.15499
C	-0.04799	-0.43402	1.18699
N	0.79938	-1.40341	1.53421
C	1.91240	-1.13220	0.88216
C	1.71821	-0.10372	-0.21492
H	-1.02767	-0.31889	1.62322
H	2.79215	-1.75282	0.95756
H	1.70670	-0.57532	-1.20328
H	-0.11644	1.09409	-0.23846
H	2.83011	1.21728	0.59277
O	2.63664	0.92904	-0.30650
O	2.40148	0.50599	2.41082
O	1.28194	0.75975	2.88299

Vibrational wavenumbers (cm^{-1})							
136.3 *i*	84.3	142.7	219.3	253.1	340.8	406.8	427.9
565.6	569.0	593.8	769.4	875.2	890.5	915.0	927.4
1060.8	1110.2	1182.7	1204.5	1254.9	1289.2	1308.2	1363.1
1438.1	1445.6	1496.8	1555.5	3034.0	3241.2	3258.4	3713.0
3792.9							

Rotational Constants (GHz):	2.7910	2.3631	1.8121

TS5a							
Cartesian Coordinates (Å)							
N	-0.05254	0.05341	0.14875				
C	-0.38356	-0.93490	0.94989				
N	0.68876	-1.55291	1.62695				
C	1.73089	-0.97977	1.17084				
C	1.41061	0.05530	0.12426				
H	2.73126	-1.22677	1.50048				
H	1.74241	-0.30637	-0.85890				
H	-0.53201	-0.27158	-0.90139				
H	1.72116	1.93218	-0.19866				
O	1.99058	1.27826	0.44826				
H	-1.39788	-1.14257	1.24679				
O	-0.88012	-1.23962	-1.69032				
O	-0.90875	-2.19783	-0.84671				
Vibrational wavenumbers (cm^{-1})							
941.8 *i*	96.3	122.3	183.7	235.9	257.5	367.7	432.3
587.0	614.4	713.5	824.7	885.4	936.5	976.5	1005.6
1039.5	1089.0	1175.8	1222.7	1267.9	1303.1	1335.6	1349.8
1417.4	1438.8	1557.3	1679.7	1807.8	3004.2	3218.7	3268.7
3893.0							
Rotational Constants (GHz):				3.6416	1.6425	1.3036	

TS5s							
Cartesian Coordinates (Å)							
N	-0.00431	-0.00558	-0.05086				
C	-0.38481	-0.67266	1.01158				
N	0.65477	-1.22060	1.79592				
C	1.72611	-0.82212	1.23253				
C	1.46567	0.00243	-0.00988				
H	-1.40689	-0.95556	1.19942				
H	2.71196	-1.06810	1.60583				
H	1.84237	-0.52456	-0.89000				
H	-0.47133	1.07888	0.07919				
H	1.67970	1.79570	0.68313				
O	2.04255	1.26539	-0.03238				
O	-0.99858	1.31083	1.98019				
O	-0.85103	2.01349	0.92221				
Vibrational wavenumbers (cm^{-1})							
893.6 *i*	104.3	113.7	171.0	234.4	393.8	402.6	445.3
542.9	619.6	716.4	801.6	875.8	918.3	976.2	995.3
1053.0	1101.3	1162.0	1241.3	1285.5	1303.0	1330.2	1342.7
1420.1	1433.0	1558.7	1675.1	1812.6	3073.1	3210.7	3271.4
3843.0							
Rotational Constants (GHz):				2.9885	2.0548	1.4963	

TS6a							
Cartesian Coordinates (Å)							
N	0.02244	0.00727	-0.00093				
C	-0.35998	-1.05877	0.70133				
N	0.63428	-1.70163	1.28455				
C	1.75101	-1.05424	0.89653				
C	1.45255	0.01726	-0.02005				
H	-1.39496	-1.35603	0.77580				
H	1.81041	-0.55490	-1.07852				
H	-0.56598	0.57392	-0.58348				
H	2.52491	1.42585	-0.78220				
O	2.06883	1.25583	0.04260				
H	2.70990	-1.24624	1.34424				
O	2.61202	-2.33660	-0.85294				
O	2.39807	-1.54475	-1.81506				
Vibrational wavenumbers (cm^{-1})							
723.9 *i*	110.8	140.4	211.0	266.9	285.5	359.0	409.9
528.9	618.9	658.0	748.3	784.5	902.6	916.9	951.9
1022.5	1144.1	1185.7	1192.3	1264.2	1317.3	1328.6	1373.9
1382.0	1450.7	1514.6	1568.3	1632.0	3246.6	3281.0	3697.8
3890.0							
Rotational Constants (GHz):				2.6955	1.9757	1.4655	

TS7s							
Cartesian Coordinates (Å)							
N	1.44292	-1.37200	-1.07956				
C	0.30882	-1.12226	-1.79401				
N	-0.61760	-0.45012	-1.23438				
C	-0.19464	-0.09268	0.08263				
C	1.44335	-0.51613	0.10955				
H	0.20767	-1.51753	-2.79692				
H	-0.73828	-0.63144	0.85723				
H	1.58386	-1.09250	1.02837				
H	2.31807	-1.47771	-1.56626				
H	1.43053	1.49000	-0.34477				
O	2.22241	0.54113	0.03507				
O	-0.28584	1.23085	0.42957				
O	0.44971	1.99348	-0.43786				
Vibrational wavenumbers (cm^{-1})							
1420.9 *i*	98.3	242.2	395.5	431.4	477.5	512.3	591.4
630.9	680.4	715.1	862.1	887.3	926.4	980.3	1007.2
1037.9	1070.0	1137.3	1150.7	1181.4	1214.2	1302.8	1342.1
1371.9	1390.3	1443.3	1704.5	1792.6	3046.5	3120.3	3208.1
3642.4							
Rotational Constants (GHz):				3.4172	2.3497	1.7398	

TS8s							
Cartesian Coordinates (Å)							
N	-1.60468	0.46721	-0.27073				
C	-0.71913	1.50855	-0.39769				
N	0.43988	1.53461	0.12141				
C	0.85031	0.42179	0.83354				
C	-1.25927	-0.67041	0.51232				
H	-1.05523	2.33993	-1.00722				
H	0.95121	0.49621	1.90999				
H	-1.30764	-0.49252	1.59046				
H	-2.15155	0.25532	-1.09190				
H	0.93495	-1.43700	-0.89833				
O	-1.19657	-1.78157	0.02705				
O	1.83589	-0.35940	0.34390				
O	1.55449	-0.70081	-1.01430				
Vibrational wavenumbers (cm^{-1})							
110.0 *i*	64.6	130.4	226.5	301.5	372.4	398.7	431.7
477.0	513.5	628.4	707.3	763.3	846.9	924.2	967.5
992.3	1063.6	1083.1	1174.2	1215.8	1378.7	1383.0	1427.9
1450.3	1458.7	1702.4	1720.8	3059.7	3182.2	3185.5	3615.2
3736.3							
Rotational Constants (GHz):				2.7809	2.1076	1.4990	

PC5a							
Cartesian Coordinates (Å)							
N	0.01823	-0.00876	-0.10939				
C	-0.46579	-0.48122	0.96893				
N	0.33509	-0.35132	2.14210				
C	1.38218	0.24712	1.73230				
C	1.34792	0.47725	0.24429				
H	2.20633	0.51234	2.38109				
H	2.06606	-0.21587	-0.22124				
H	-0.94032	-0.19610	-1.57611				
H	1.57297	1.89197	-1.04651				
O	1.60346	1.79886	-0.09286				
H	-1.43392	-0.95956	1.02115				
O	-1.63512	-0.42953	-2.24991				
O	-2.53357	-1.09383	-1.56272				
Vibrational wavenumbers (cm^{-1})							
36.9	55.9	63.8	126.5	196.7	262.4	277.3	371.1
582.9	616.5	728.3	788.8	876.5	926.7	972.9	1023.6
1034.2	1072.9	1190.3	1217.4	1268.2	1292.8	1308.7	1339.6
1440.9	1611.7	1633.5	1701.9	2981.6	3214.8	3218.3	3237.9
3890.3							
Rotational Constants (GHz):				3.6171	1.1297	0.8838	

PC5s								
Cartesian Coordinates (Å)								
N	-0.54306	-0.52989	-0.11552					
C	-0.54577	-1.77103	0.16031					
N	0.71858	-2.42169	0.20381					
C	1.55057	-1.49051	-0.05965					
C	0.86058	-0.19112	-0.36535					
H	-1.44276	-2.33962	0.36451					
H	2.61985	-1.64954	-0.10020					
H	0.93729	-0.02217	-1.45380					
H	-1.59355	0.82029	-0.16290					
H	0.71097	1.61481	0.22171					
O	1.32919	0.87822	0.36808					
O	-0.92254	2.53734	-0.15970					
O	-1.96712	1.75319	-0.21688					
Vibrational wavenumbers (cm^{-1})								
62.7	87.5	135.6	186.0	206.9	290.6	377.4	583.8	
608.7	661.8	785.0	835.3	878.2	922.7	983.2	1018.0	
1035.2	1076.3	1204.4	1256.4	1289.6	1301.1	1326.0	1344.2	
1487.0	1612.2	1659.5	1707.0	2950.5	3021.6	3219.7	3226.4	
3628.5								
Rotational Constants (GHz):				4.3082	1.2814	1.0162		

PC6a								
Cartesian Coordinates (Å)								
N	-1.47927	1.18999	0.61032					
C	-1.60810	-0.06510	0.10255					
N	-0.44025	-0.58666	-0.14039					
C	0.50149	0.35465	0.21809					
C	-0.14349	1.45799	0.68427					
H	-2.56267	-0.53311	-0.06304					
H	0.13249	-2.07299	-0.76092					
H	-2.21461	1.81531	0.88429					
H	1.19812	2.70576	1.15747					
O	0.24163	2.65451	1.16139					
H	1.55477	0.16503	0.11322					
O	1.90880	-2.48920	-0.97715					
O	0.65647	-2.86083	-1.09554					
Vibrational wavenumbers (cm^{-1})								
43.5	55.4	59.5	146.8	229.6	271.6	315.9	418.4	
548.2	679.5	683.2	706.2	798.5	825.4	831.1	957.5	
1044.1	1127.5	1147.2	1178.8	1273.4	1299.1	1311.1	1431.3	
1520.2	1571.0	1653.2	1675.4	3066.1	3278.5	3283.3	3700.6	
3910.4								
Rotational Constants (GHz):				4.7375	0.9691	0.8045		

M7s							
Cartesian Coordinates (Å)							
N	0.21666	-1.35705	-0.52171				
C	-0.61094	-0.63155	-1.31260				
N	-1.20540	0.39944	-0.85266				
C	-0.88509	0.69393	0.46308				
C	0.46544	-0.74913	0.78038				
H	-0.76525	-0.95392	-2.33503				
H	-1.65374	0.51489	1.21073				
H	-0.09171	-1.23655	1.58967				
H	0.98374	-1.85109	-0.94780				
H	1.44954	1.45325	0.24050				
O	1.58043	-0.24245	1.00913				
O	-0.28504	1.85491	0.77501				
O	0.80126	2.10533	-0.09870				
Vibrational wavenumbers (cm^{-1})							
61.4	151.2	212.1	250.9	360.1	370.5	446.6	470.4
549.3	580.5	650.8	774.2	840.8	938.9	996.4	1004.8
1011.9	1044.3	1103.7	1185.5	1213.8	1348.1	1380.7	1416.0
1452.9	1486.8	1529.1	1708.2	3010.1	3145.5	3202.3	3518.5
3641.3							
Rotational Constants (GHz):				3.0273	2.3098	1.6577	

M8s							
Cartesian Coordinates (Å)							
N	-1.71555	0.70646	0.19864				
C	-0.49897	1.34972	-0.05560				
N	0.69929	0.79558	-0.07228				
C	0.98424	-0.41083	0.25639				
C	-2.12451	-0.51876	-0.25503				
H	-0.56460	2.41790	-0.19887				
H	0.32970	-1.18505	0.64657				
H	-1.35986	-1.04758	-0.84171				
H	-2.45331	1.25896	0.61027				
H	3.95614	-0.48219	-0.22484				
O	-3.22211	-0.97245	-0.04664				
O	2.23313	-0.91618	0.21479				
O	3.16404	0.06523	-0.22611				
Vibrational wavenumbers (cm^{-1})							
52.6	85.2	90.5	125.1	196.3	223.3	282.4	299.2
413.1	519.7	634.6	664.5	699.6	786.9	813.6	943.3
1043.3	1055.9	1177.0	1240.3	1308.7	1375.4	1403.7	1445.9
1460.7	1502.3	1579.6	1808.5	3019.4	3152.8	3216.5	3605.3
3847.3							
Rotational Constants (GHz):				5.8009	0.9149	0.8038	

4H-4ol							
Cartesian Coordinates (Å)							
N	0.00580	0.00505	0.01352				
C	-0.30849	-0.73512	0.99625				
N	0.75992	-1.25628	1.79607				
C	1.80503	-0.78096	1.24445				
C	1.46154	0.00899	0.00906				
H	2.80615	-0.97531	1.60616				
H	1.76953	-0.58623	-0.86625				
H	1.62113	1.78397	-0.69844				
O	2.03735	1.27602	0.00055				
H	-1.32778	-0.98194	1.26091				
Vibrational wavenumbers (cm^{-1})							
192.7	244.7	370.7	584.7	619.9	783.8	872.0	907.6
970.6	1001.8	1021.7	1060.2	1190.1	1218.4	1292.9	1311.4
1337.6	1433.2	1618.6	1704.1	2966.8	3213.8	3221.8	3886.4
Rotational Constants (GHz):				8.0850	3.9370	2.8620	

5-ol							
Cartesian Coordinates (Å)							
N	-1.04031	-1.46167	-0.37930				
C	0.02442	-1.98513	-1.05992				
N	1.13997	-1.41989	-0.70800				
C	0.80717	-0.48170	0.24556				
C	-0.53918	-0.50520	0.45075				
H	-0.09085	-2.76854	-1.78967				
H	-2.00716	-1.71636	-0.45928				
H	-0.90460	0.80514	1.76587				
O	-1.39623	0.17157	1.24294				
H	1.54525	0.14315	0.71828				
Vibrational wavenumbers (cm^{-1})							
211.7	310.7	411.7	519.8	678.7	686.0	697.3	805.6
818.2	933.4	1045.0	1107.8	1144.0	1177.7	1294.8	1305.8
1419.6	1520.3	1561.7	1660.0	3262.1	3267.3	3702.4	3916.2
Rotational Constants (GHz):				9.5200	3.7114	2.6704	

Z-FMF							
Cartesian Coordinates (Å)							
N	-0.57433	0.39376	-0.00023				
C	-0.01105	-0.84381	-0.00005				
N	1.24455	-1.12609	-0.00005				
C	2.18039	-0.09939	-0.00010				
C	-1.94740	0.59518	-0.00016				
H	-0.73132	-1.65542	0.00009				
H	3.20948	-0.47896	0.00018				
H	-2.20665	1.66357	-0.00018				
H	0.07184	1.17659	-0.00049				
O	-2.76188	-0.28312	0.00027				
O	1.96606	1.09670	0.00026				
Vibrational wavenumbers (cm^{-1})							
93.5	115.0	192.2	262.4	271.4	456.6	484.1	779.3
840.8	854.9	1026.8	1046.6	1074.4	1087.8	1097.1	1265.5
1386.9	1428.7	1441.6	1484.7	1661.2	1751.9	1847.4	3020.5
3048.5	3184.3	3512.8					
Rotational Constants (GHz):				8.3563	1.5380	1.2989	

E-FMF							
Cartesian Coordinates (Å)							
N	0.56391	0.06587	-1.05395				
C	-0.02128	-0.04303	0.16837				
N	0.66170	0.03157	1.23985				
C	-0.07507	-0.00580	2.43103				
C	-0.11517	-0.05214	-2.25077				
H	-1.10053	-0.20464	0.15696				
H	0.50971	-0.40606	3.27004				
H	-1.19098	-0.24328	-2.11517				
H	1.55853	0.23964	-1.09341				
O	0.41452	0.04505	-3.32015				
O	-1.20544	0.38281	2.56720				
Vibrational wavenumbers (cm^{-1})							
100.7	105.4	153.0	246.2	318.7	335.9	481.4	613.4
748.7	801.7	1032.8	1048.1	1068.2	1098.6	1235.3	1310.8
1346.7	1410.4	1433.5	1498.8	1700.3	1803.2	1853.0	3004.3
3032.0	3107.0	3608.0					
Rotational Constants (GHz):				14.6836	1.0554	0.9908	

4a-ROONO								
Cartesian Coordinates (Å)								
N	-1.12610	1.90690	0.86465					
C	-1.07679	1.92606	-0.50140					
N	-0.52413	0.93377	-1.08285					
C	0.00618	0.09959	-0.02643					
C	-0.43620	0.72520	1.33058					
H	-1.52880	2.75024	-1.03981					
H	0.42253	0.96583	1.95360					
H	-1.21688	2.73841	1.41831					
H	-2.07101	-0.26245	1.64114					
O	-1.24645	-0.10954	2.10819					
H	-0.35023	-0.92877	-0.10335					
O	1.41142	-0.07596	-0.12918					
O	2.02957	1.17735	-0.00610					
N	2.42794	1.58600	-1.33253					
O	2.93795	2.62211	-1.26745					
Vibrational wavenumbers (cm^{-1})								
53.1	70.0	100.4	192.9	239.8	268.3	299.5	351.2	
385.3	459.5	488.8	545.5	575.0	696.0	773.5	824.4	
877.6	970.5	984.8	1025.9	1060.0	1074.5	1085.0	1124.6	
1153.9	1257.2	1289.3	1302.0	1358.9	1385.5	1443.5	1470.5	
1688.4	1822.5	3097.3	3126.1	3200.8	3690.6	3867.9		
Rotational Constants (GHz):				2.6916	0.9325	0.8349		

4s-ROONO								
Cartesian Coordinates (Å)								
N	-1.89865	1.13622	-0.99540					
C	-1.58903	1.59430	0.25489					
N	-0.55393	1.10605	0.81803					
C	0.01559	0.17849	-0.13350					
C	-0.75977	0.37114	-1.48824					
H	-2.23096	2.32280	0.73429					
H	-0.09766	-0.84819	0.21844					
H	-1.08888	-0.58201	-1.89439					
H	-2.43608	1.69154	-1.63837					
H	0.51782	1.67049	-2.14929					
O	-0.07282	1.00648	-2.51641					
O	1.42329	0.28736	-0.23888					
O	1.76588	1.61459	-0.53424					
N	2.16540	2.24800	0.72345					
O	2.41918	3.35241	0.51764					
Vibrational wavenumbers (cm^{-1})								
50.2	87.2	95.7	209.0	256.8	291.3	337.2	394.3	
419.9	491.6	523.3	537.0	588.2	690.3	794.9	825.4	
878.7	897.3	990.8	1020.4	1044.1	1093.3	1096.4	1121.5	
1186.3	1262.3	1296.0	1328.6	1359.5	1373.7	1453.4	1474.8	
1693.0	1844.1	3088.4	3125.4	3204.6	3662.8	3834.3		
Rotational Constants (GHz):				2.3582	1.0392	0.9282		

4a-RO							
Cartesian Coordinates (Å)							
N	0.02468	0.02145	0.05063				
C	-0.42336	-0.70303	1.13620				
N	0.44213	-1.12749	1.96014				
C	1.74684	-0.76623	1.42167				
C	1.46688	0.00142	0.03046				
H	-1.49029	-0.84727	1.26060				
H	1.87253	-0.57198	-0.79992				
H	-0.49072	0.02858	-0.81181				
H	1.61601	1.83738	0.58161				
O	2.04248	1.25935	-0.05585				
H	2.24847	-0.03778	2.07867				
O	2.56858	-1.78148	1.15745				
Vibrational wavenumbers (cm^{-1})							
65.2	221.3	311.7	346.0	383.0	492.0	550.3	597.1
693.0	727.5	889.3	965.7	1006.9	1013.9	1112.2	1134.7
1147.1	1169.5	1262.9	1301.1	1305.4	1365.7	1445.1	1460.0
1712.8	2958.1	3121.9	3192.2	3665.8	3861.6		
Rotational Constants (GHz):				3.7219	3.2466	2.0028	

4s-RO							
Cartesian Coordinates (Å)							
N	-0.11969	-0.26275	-0.08258				
C	-0.47604	-0.57380	1.21624				
N	0.45765	-0.78665	2.05110				
C	1.69428	-0.57440	1.30484				
C	1.28229	0.06116	-0.07244				
H	-1.52583	-0.65956	1.46727				
H	2.15856	-1.56498	1.10282				
H	1.80542	-0.39588	-0.91388				
H	-0.73263	0.30788	-0.64044				
H	2.31472	1.65856	0.27412				
O	1.44942	1.45436	-0.09029				
O	2.67286	0.08242	1.93892				
Vibrational wavenumbers (cm^{-1})							
91.0	226.8	272.0	342.2	472.8	497.4	581.7	642.4
787.9	826.6	868.1	978.9	994.0	1057.6	1064.2	1125.7
1143.1	1170.4	1224.1	1258.2	1328.0	1362.2	1405.3	1462.8
1702.1	2851.9	3071.0	3205.4	3649.4	3857.7		
Rotational Constants (GHz):				3.8964	3.4469	2.0938	

TS12a							
Cartesian Coordinates (Å)							
N	-0.02976	0.12393	-0.01958				
C	-0.57236	-0.28962	1.18784				
N	0.18560	-0.66031	2.12556				
C	1.56341	-0.71167	1.71887				
C	1.38131	-0.00649	-0.06886				
H	-1.65098	-0.23676	1.28659				
H	1.79547	-0.78050	-0.70207				
H	-0.56475	0.01134	-0.86457				
H	1.58126	1.86307	0.19254				
O	2.07239	1.14830	-0.22315				
H	2.15461	0.12198	2.13528				
O	2.12057	-1.81673	1.53020				
Vibrational wavenumbers (cm^{-1})							
430.8 *i*	73.6	250.4	316.5	345.6	389.8	473.7	533.1
606.3	707.4	872.3	939.2	974.9	1000.8	1017.9	1094.7
1142.3	1215.1	1303.4	1344.8	1378.1	1436.2	1453.7	1470.5
1741.7	2941.7	3183.3	3189.6	3637.2	3847.6		
Rotational Constants (GHz):				3.7948	2.9833	1.9615	

TS12s							
Cartesian Coordinates (Å)							
N	-0.11050	0.04028	0.02250				
C	-0.45348	-0.62950	1.17954				
N	0.47076	-1.11871	1.89461				
C	1.75971	-0.65204	1.40642				
C	1.30496	-0.01473	-0.17805				
H	-1.50522	-0.73864	1.41712				
H	2.44423	-1.46965	1.14245				
H	1.59257	-0.79993	-0.87371				
H	-0.60884	0.86395	-0.27010				
H	2.03246	1.68612	0.25685				
O	1.90542	1.14958	-0.53264				
O	2.27873	0.35179	2.00920				
Vibrational wavenumbers (cm^{-1})							
312.1 *i*	86.7	237.7	302.1	372.5	403.2	420.4	497.6
618.2	715.8	871.9	948.4	971.1	1003.1	1089.8	1146.8
1165.1	1207.9	1295.7	1337.3	1370.2	1382.8	1426.1	1455.5
1713.9	2989.9	3117.0	3191.1	3650.5	3819.4		
Rotational Constants (GHz):				4.0870	3.2517	2.0571	

TS13a							
Cartesian Coordinates (Å)							
N	0.00546	-0.01119	-0.00379				
C	-0.48309	-0.14506	1.25538				
N	0.26545	-0.52595	2.20823				
C	1.85242	-0.81596	1.25170				
C	1.44932	0.00704	0.00071				
H	-1.52873	0.08386	1.44972				
H	1.84443	-0.47840	-0.88762				
H	-0.51763	0.45058	-0.72549				
H	1.75987	1.72432	0.84976				
O	1.98319	1.29980	0.01734				
H	2.52144	-0.27682	1.94104				
O	1.90601	-2.05558	1.16303				
Vibrational wavenumbers (cm^{-1})							
567.4 *i*	101.3	221.5	320.6	340.4	365.6	458.0	493.7
594.5	633.0	846.0	926.5	944.2	970.4	1060.4	1107.8
1173.4	1245.1	1263.4	1298.9	1367.1	1426.2	1465.0	1488.9
1676.0	2969.2	3141.2	3143.0	3680.4	3855.8		
Rotational Constants (GHz):				3.6570	3.0726	2.1347	

TS13s							
Cartesian Coordinates (Å)							
N	-0.05865	-0.06972	-0.03875				
C	-0.40614	-0.00879	1.27556				
N	0.44023	-0.25752	2.18621				
C	1.90961	-0.67058	1.16637				
C	1.38670	-0.08084	-0.17337				
H	-1.43618	0.20819	1.54826				
H	1.80559	-1.75628	1.28361				
H	1.66803	-0.72959	-1.00551				
H	-0.59647	0.44707	-0.71412				
H	2.52133	1.33787	0.36905				
O	1.90271	1.19120	-0.36364				
O	2.89120	-0.08457	1.67597				
Vibrational wavenumbers (cm^{-1})							
531.4 *i*	108.5	305.6	325.6	358.1	485.4	511.6	551.2
589.5	749.3	818.7	888.4	941.7	1012.6	1053.0	1142.9
1181.4	1217.2	1260.7	1321.4	1378.3	1415.6	1456.6	1493.7
1688.8	3015.4	3070.7	3148.8	3649.5	3688.6		
Rotational Constants (GHz):				3.9761	3.2394	2.1024	

TS14a							
Cartesian Coordinates (Å)							
N	0.00222	-0.00419	0.00312				
C	-0.41011	-0.97257	0.85254				
N	0.48079	-1.53680	1.59722				
C	1.70767	-0.92538	1.23978				
C	1.45314	0.00312	0.00254				
H	-1.46017	-1.23315	0.90041				
H	1.83591	-0.50924	-0.88273				
H	-0.55002	0.32510	-0.76705				
H	1.98077	1.62115	0.90115				
O	2.03893	1.25264	0.01461				
H	1.56502	0.32544	2.37707				
O	2.81590	-1.26501	1.61147				
Vibrational wavenumbers (cm^{-1})							
1080.7 *i*	114.4	256.1	315.7	339.5	431.3	471.6	526.1
577.7	594.4	672.9	724.9	842.5	910.0	1008.6	1028.2
1111.8	1151.5	1191.9	1264.0	1302.5	1355.1	1434.6	1481.3
1625.7	1705.5	3077.7	3204.4	3689.3	3822.8		
Rotational Constants (GHz):				3.6462	3.4900	1.9186	

TS14s							
Cartesian Coordinates (Å)							
N	0.01915	-0.07098	-0.06971				
C	-0.32327	-0.58630	1.13114				
N	0.62708	-1.02748	1.88673				
C	1.81743	-0.77252	1.16456				
C	1.45084	-0.02474	-0.16193				
H	-1.36572	-0.62756	1.41936				
H	1.81852	-2.33007	0.47497				
H	1.80956	-0.53254	-1.05850				
H	-0.60388	0.42345	-0.67917				
H	2.76033	1.27173	0.37232				
O	1.92701	1.28962	-0.11041				
O	2.94905	-0.76177	1.61068				
Vibrational wavenumbers (cm^{-1})							
1062.6 *i*	77.2	245.7	254.0	314.8	413.5	457.8	482.3
544.4	578.2	688.5	798.7	847.8	893.4	1009.8	1054.7
1101.2	1128.4	1193.5	1229.4	1344.4	1368.0	1376.8	1493.0
1622.0	1726.4	3073.8	3214.0	3708.8	3819.0		
Rotational Constants (GHz):				3.8125	3.4912	2.0464	

TS15a							
Cartesian Coordinates (Å)							
N	1.63831	1.97932	-0.29636				
C	1.20831	0.72936	0.01377				
N	0.06972	0.32131	0.44197				
C	-1.10401	1.01645	0.34840				
C	1.00879	3.19492	-0.10086				
H	2.00005	-0.00922	-0.08502				
H	0.96472	3.91271	-0.90505				
H	2.56249	2.02057	-0.69317				
H	-0.60866	3.60277	0.80812				
O	0.29587	3.35717	1.02666				
H	-1.80652	0.76200	1.15528				
O	-1.43021	1.77200	-0.54753				
Vibrational wavenumbers (cm^{-1})							
220.8 *i*	100.5	118.0	176.6	211.6	252.3	317.3	433.4
512.5	561.0	749.9	874.3	972.4	985.8	1061.3	1090.6
1220.9	1230.3	1314.6	1421.0	1444.0	1486.0	1542.7	1681.2
1738.8	3008.3	3140.1	3228.1	3628.4	3820.7		
Rotational Constants (GHz):				3.7877	2.8693	1.9895	

TS16a							
Cartesian Coordinates (Å)							
N	0.18415	-0.14220	-0.13945				
C	-0.59921	-1.11145	0.47921				
N	-0.25858	-1.76232	1.56849				
C	0.69425	-1.27578	2.37956				
C	1.46575	0.02433	0.18813				
H	-1.50168	-1.37311	-0.05547				
H	2.10953	-0.83459	0.28553				
H	-0.27332	0.62456	-0.61055				
H	2.89080	1.25683	0.19737				
O	1.98279	1.21279	-0.10648				
H	0.95788	-1.92279	3.21932				
O	1.28923	-0.17125	2.24632				
Vibrational wavenumbers (cm^{-1})							
311.1 *i*	177.2	241.1	287.4	353.6	395.0	476.3	528.5
563.1	662.1	723.8	888.7	917.9	945.8	1027.9	1155.8
1200.9	1277.5	1317.7	1351.4	1411.7	1444.9	1477.5	1517.8
1626.6	3079.0	3201.8	3232.8	3595.5	3904.1		
Rotational Constants (GHz):				5.0048	2.5379	1.7680	

TS16s							
Cartesian Coordinates (Å)							
N	-0.05099	-1.71912	-1.60360				
C	-0.63886	-0.78619	-0.80529				
N	0.02959	0.15332	-0.18886				
C	1.37791	0.03514	-0.12923				
C	1.23145	-1.59354	-2.05592				
H	-1.71742	-0.82017	-0.74205				
H	1.82498	-0.79502	0.40888				
H	1.66640	-2.44353	-2.57198				
H	-0.60881	-2.47577	-1.95810				
H	1.48562	1.89107	-0.19576				
O	1.91396	-0.56424	-1.72754				
O	2.06095	1.16488	0.06643				
Vibrational wavenumbers (cm^{-1})							
503.6 *i*	158.8	272.8	369.3	438.2	467.3	526.6	579.1
610.4	628.6	646.0	810.3	964.0	1007.6	1057.3	1084.5
1174.4	1245.5	1325.0	1363.1	1399.1	1477.6	1506.9	1531.1
1630.5	3143.8	3149.9	3208.3	3667.8	3830.8		
Rotational Constants (GHz):				5.2290	2.7062	1.8615	

TS17a							
Cartesian Coordinates (Å)							
N	-1.01652	0.75308	-0.28800				
C	0.24149	1.19426	-0.07956				
N	1.12146	0.54805	0.58251				
C	2.10189	-0.34303	0.38331				
C	-1.46990	-0.50287	0.00807				
H	0.41704	2.19819	-0.46672				
H	-0.82968	-1.15852	0.57907				
H	-1.67625	1.38108	-0.71911				
H	-3.08678	-1.49849	0.11864				
O	-2.82081	-0.57921	0.08486				
H	2.64651	-0.58130	1.30848				
O	2.39001	-0.86316	-0.67896				
Vibrational wavenumbers (cm^{-1})							
192.7 *i*	85.3	128.0	172.1	198.3	298.3	395.3	442.2
514.7	643.2	714.7	770.4	920.7	1009.4	1042.6	1108.1
1227.4	1252.9	1299.0	1411.4	1421.4	1470.9	1586.5	1719.8
1744.0	3001.9	3100.7	3226.3	3637.4	3913.8		
Rotational Constants (GHz):				6.3386	1.3716	1.2245	

TS17s							
Cartesian Coordinates (Å)							
N	-1.44209	0.03770	0.58610				
C	-0.17997	0.03184	1.20226				
N	0.88077	-0.00265	0.49266				
C	2.05166	-0.03311	0.02229				
C	-1.72363	0.01029	-0.75131				
H	-0.22834	0.05883	2.29040				
H	2.98629	-0.03493	0.57874				
H	-2.81166	0.02381	-0.92692				
H	-2.23939	0.06536	1.19813				
H	1.37793	-0.06399	-1.71628				
O	-0.93078	-0.02449	-1.66569				
O	2.25922	-0.06865	-1.31041				
Vibrational wavenumbers (cm^{-1})							
208.9 *i*	109.9	117.5	219.9	256.0	323.7	397.7	560.1
616.0	655.3	701.1	818.8	873.6	955.5	1010.4	1083.1
1184.3	1271.7	1327.0	1394.8	1451.4	1516.6	1561.2	1701.3
1780.0	2977.2	3087.4	3128.3	3659.1	3710.3		
Rotational Constants (GHz):				4.6960	2.0609	1.4323	

TS18a							
Cartesian Coordinates (Å)							
N	0.12900	-0.02016	0.11686				
C	-0.27055	1.26316	0.26077				
N	0.54881	2.24618	0.35795				
C	-0.03535	3.50534	0.38687				
C	1.43287	-0.43774	-0.11460				
H	-1.35252	1.39579	0.30253				
H	1.93437	-1.11141	0.56235				
H	-0.58746	-0.72329	0.17444				
H	3.01597	0.28242	-0.89857				
O	2.09030	0.17006	-1.11965				
H	0.61422	4.25328	0.86447				
O	-1.11084	3.81027	-0.07196				
Vibrational wavenumbers (cm^{-1})							
352.9 *i*	67.6	70.3	133.9	197.0	214.1	290.6	331.6
512.8	524.8	724.6	849.9	991.7	1039.1	1067.2	1132.7
1223.0	1246.3	1315.9	1387.7	1423.0	1462.6	1541.5	1667.3
1776.9	3009.7	3105.8	3228.1	3641.6	3893.4		
Rotational Constants (GHz):				7.2787	1.4143	1.2670	

TS19a							
Cartesian Coordinates (Å)							
N	0.42430	0.27177	0.03621				
C	-0.30117	1.35372	0.41929				
N	0.28419	2.54851	0.30828				
C	-0.42876	3.65345	0.68871				
C	1.67842	0.32471	-0.44176				
H	-1.30332	1.19651	0.79022				
H	2.16482	-0.59954	-0.71766				
H	-0.00340	-0.63476	0.11411				
H	1.56165	2.20158	-0.21695				
O	2.29001	1.45450	-0.56907				
H	0.14050	4.58418	0.55861				
O	-1.56264	3.64937	1.12502				
Vibrational wavenumbers (cm^{-1})							
715.8 *i*	98.4	202.2	228.7	343.6	443.3	496.8	664.8
695.3	702.8	768.1	808.1	905.8	1024.9	1073.2	1136.8
1210.2	1250.5	1318.8	1357.7	1422.0	1516.1	1551.2	1642.0
1737.0	1919.2	3016.9	3221.2	3230.6	3671.2		
Rotational Constants (GHz):				7.7141	1.6087	1.3311	

TS20							
Cartesian Coordinates (Å)							
N	0.05007	-0.15978	0.07343				
C	-0.44743	-0.77434	-1.05219				
N	0.38053	-1.24772	-1.89009				
C	2.28425	-0.97797	0.78622				
C	1.47175	-0.06545	-0.06158				
H	-1.52347	-0.86524	-1.17008				
H	1.85916	-1.97800	0.96469				
H	1.45083	-0.67648	-1.23250				
H	-0.45674	0.55785	0.56290				
H	2.81255	1.19346	0.32650				
O	1.93198	1.21272	-0.07702				
O	3.36373	-0.63982	1.20625				
Vibrational wavenumbers (cm^{-1})							
1919.0 *i*	102.1	161.2	252.6	319.3	380.3	417.3	507.3
545.1	583.6	706.3	857.8	928.1	954.0	1036.8	1117.1
1146.3	1231.0	1278.7	1316.3	1366.8	1443.5	1462.7	1661.9
1779.0	1808.6	3002.1	3160.0	3655.8	3727.5		
Rotational Constants (GHz):				5.4181	1.8679	1.6621	

TS21							
Cartesian Coordinates (Å)							
N	-0.10462	0.22579	0.14126				
C	-0.75520	-0.48837	1.11685				
N	-0.24416	-1.25180	1.99131				
C	1.93867	-0.56769	1.09398				
C	1.29182	0.01124	-0.16791				
H	-1.83600	-0.33870	1.12007				
H	1.03747	-1.27217	1.70258				
H	1.39062	-0.75131	-0.95139				
H	-0.66172	0.64812	-0.57927				
H	2.50679	1.48119	0.07284				
O	1.90890	1.16977	-0.61442				
O	2.96495	-0.17600	1.54335				
Vibrational wavenumbers (cm^{-1})							
1782.1 *i*	73.1	143.0	177.3	290.6	327.3	441.4	463.4
495.9	596.7	713.8	790.6	898.4	953.6	1036.5	1146.8
1180.2	1201.8	1283.7	1324.4	1342.1	1416.3	1510.2	1657.0
1697.7	1883.2	3005.3	3095.0	3676.2	3820.0		
Rotational Constants (GHz):				4.1564	2.4931	1.6358	

M12a							
Cartesian Coordinates (Å)							
N	-0.50255	0.94849	-0.07532				
C	-1.41226	-0.01180	0.21006				
N	-1.23879	-1.24854	0.51806				
C	-0.14293	-2.02004	0.27256				
C	0.86625	0.86347	-0.10109				
H	-2.42483	0.37891	0.23257				
H	1.33223	-0.05392	-0.43517				
H	-0.86889	1.88330	-0.17308				
H	2.37934	1.96017	-0.45021				
O	1.43758	2.07304	-0.32322				
H	-0.01251	-2.80970	1.02628				
O	0.58717	-1.96339	-0.70154				
Vibrational wavenumbers (cm^{-1})							
103.1	154.1	187.0	197.8	272.2	276.8	424.5	454.1
596.2	642.6	722.5	858.8	941.3	1002.2	1052.9	1109.0
1227.6	1261.9	1305.6	1416.7	1421.5	1476.2	1588.3	1682.5
1720.5	3011.2	3158.6	3186.8	3618.6	3925.3		
Rotational Constants (GHz):				4.9629	1.8797	1.4210	

M12s							
Cartesian Coordinates (Å)							
N	-1.26993	-0.00000	0.46860				
C	-0.11419	-0.00000	1.27495				
N	1.17713	0.00000	1.04142				
C	1.98909	0.00000	0.03223				
C	-1.53382	0.00000	-0.85563				
H	-0.40552	-0.00000	2.31753				
H	3.04852	0.00000	0.26141				
H	-2.61202	0.00000	-1.05614				
H	-2.10578	-0.00000	1.02994				
H	0.79197	-0.00000	-1.47742				
O	-0.72862	0.00000	-1.77426				
O	1.76307	-0.00000	-1.26273				
Vibrational wavenumbers (cm^{-1})							
56.9	109.8	217.5	320.6	378.5	493.4	498.4	651.9
684.6	712.1	826.1	855.9	947.4	972.9	996.0	1129.6
1251.1	1326.1	1425.7	1450.5	1472.2	1527.5	1582.8	1617.0
1754.1	3035.9	3122.0	3176.4	3190.4	3640.0		
Rotational Constants (GHz):				4.0121	2.5739	1.5680	

M13							
Cartesian Coordinates (Å)							
N	0.05039	-0.18066	-0.17358				
C	-0.63939	0.49422	-1.13519				
N	-0.12223	1.26452	-1.98953				
C	1.98617	-0.86419	1.08770				
C	1.46159	0.00066	-0.04872				
H	-1.72030	0.33271	-1.14666				
H	1.94395	-0.32767	-0.98063				
H	-0.43369	-0.65131	0.57170				
H	1.67589	1.86849	-0.50481				
O	1.86476	1.31053	0.25555				
H	3.04250	-0.67869	1.34281				
O	1.31451	-1.66608	1.67010				
Vibrational wavenumbers (cm^{-1})							
73.3	121.4	156.8	221.3	254.9	381.0	389.2	415.4
556.4	649.7	746.6	846.2	922.2	1031.8	1089.0	1137.4
1220.0	1242.8	1273.0	1379.8	1393.1	1419.4	1523.6	1698.7
1859.8	2985.5	2994.6	3072.3	3655.8	3836.0		
Rotational Constants (GHz):				5.6860	1.8663	1.4804	

M16a							
Cartesian Coordinates (Å)							
N	0.00537	0.00024	0.00839				
C	-0.60363	-1.20771	0.31631				
N	0.01171	-2.10401	1.06193				
C	1.20893	-1.81923	1.49287				
C	1.45252	-0.00552	0.01094				
H	-1.61280	-1.37336	-0.02690				
H	1.87178	-0.50970	-0.86466				
H	-0.38846	0.51662	-0.76138				
H	1.59177	1.72865	0.76904				
O	1.95238	1.26821	0.00527				
H	1.75602	-2.46820	2.15695				
O	1.89232	-0.68109	1.17270				
Vibrational wavenumbers (cm^{-1})							
144.2	226.3	339.7	421.7	504.8	549.4	591.8	620.4
669.5	679.5	702.3	923.4	964.6	1040.9	1088.8	1139.7
1195.0	1260.6	1335.7	1346.6	1365.2	1423.5	1445.3	1488.2
1531.8	3052.7	3231.1	3253.7	3633.5	3845.7		
Rotational Constants (GHz):				5.6929	2.7370	1.9235	

M16s							
Cartesian Coordinates (Å)							
N	-0.02813	-1.28533	1.96032				
C	-0.59671	-0.43465	1.06779				
N	0.06270	0.27413	0.23138				
C	1.48037	0.07516	0.21659				
C	1.35594	-1.31340	2.09737				
H	-1.67891	-0.37335	1.09694				
H	1.75855	-0.73961	-0.45718				
H	1.76713	-1.65658	3.03396				
H	-0.60027	-1.87243	2.53715				
H	1.56556	1.95301	0.02767				
O	2.00015	-0.27806	1.52974				
O	2.13397	1.20815	-0.18246				
Vibrational wavenumbers (cm^{-1})							
126.5	257.0	290.6	379.1	438.0	493.8	524.4	600.0
634.6	675.7	894.0	954.8	964.3	982.3	1042.0	1163.8
1208.3	1242.0	1328.4	1358.2	1398.5	1435.4	1443.3	1531.6
1698.5	3057.5	3175.5	3226.9	3699.2	3867.5		
Rotational Constants (GHz):				5.5608	2.7805	1.9338	

M17a							
Cartesian Coordinates (Å)							
N	-0.70731	0.01479	-0.80028				
C	-0.60714	-0.02927	0.54025				
N	0.54437	-0.02776	1.12745				
C	0.49716	-0.00840	2.51592				
C	0.34749	0.14282	-1.66700				
H	-1.55381	-0.06565	1.07533				
H	1.34234	-0.02284	-1.28115				
H	-1.62680	-0.00076	-1.20971				
H	0.73740	0.05693	-3.52756				
O	0.01499	-0.17544	-2.94421				
H	1.48165	-0.20656	2.96351				
O	-0.47044	0.21213	3.20746				
Vibrational wavenumbers (cm^{-1})							
44.6	110.9	150.3	241.6	279.1	297.1	368.9	447.0
558.1	650.8	693.5	861.0	986.6	1036.5	1064.4	1143.2
1216.2	1261.2	1304.4	1364.1	1413.4	1435.2	1596.0	1639.3
1766.2	3012.2	3137.5	3224.5	3652.3	3919.8		
Rotational Constants (GHz):				14.9127	1.0880	1.0183	

M17s							
Cartesian Coordinates (Å)							
N	-1.58457	-0.00000	-0.01798				
C	-0.40340	-0.00000	0.70747				
N	0.77900	0.00000	0.12529				
C	1.87845	0.00000	0.79846				
C	-1.79263	-0.00000	-1.37651				
H	-0.54434	0.00000	1.78529				
H	1.97351	0.00000	1.88125				
H	-2.87433	0.00000	-1.59653				
H	-2.42365	-0.00000	0.53478				
H	2.88139	-0.00000	-0.77561				
O	-0.95261	0.00000	-2.23721				
O	3.06326	-0.00000	0.17130				
Vibrational wavenumbers (cm^{-1})							
35.2	118.4	161.0	247.7	267.2	349.3	482.7	563.8
571.1	598.7	661.1	830.2	884.6	999.1	1003.0	1152.2
1178.9	1305.4	1329.6	1376.7	1433.7	1499.6	1565.5	1578.0
1814.3	2959.1	3124.2	3142.1	3668.2	3816.6		
Rotational Constants (GHz):				6.3625	1.4237	1.1634	

M18a								
Cartesian Coordinates (Å)								
N	-0.92926	0.00000	1.00623					
C	-0.71421	-0.00000	-0.32641					
N	0.52759	0.00001	-0.77831					
C	0.68188	0.00000	-2.14576					
C	0.01714	0.00000	1.96989					
H	-1.58941	-0.00001	-0.96455					
H	-0.28399	0.00001	3.00356					
H	-1.88525	0.00001	1.31827					
H	1.35151	-0.00002	0.65975					
O	1.29442	-0.00001	1.67065					
H	1.73944	0.00002	-2.44464					
O	-0.20987	-0.00001	-2.96879					
Vibrational wavenumbers (cm^{-1})								
85.3	174.2	190.9	282.1	319.0	467.8	468.7	511.2	
696.9	770.0	854.7	889.3	983.7	1012.2	1038.4	1095.3	
1219.5	1311.4	1341.7	1421.7	1494.4	1528.8	1571.3	1622.0	
1740.6	2814.3	3015.2	3191.9	3268.2	3667.2			
Rotational Constants (GHz):				7.7931	1.5545	1.2960		

M19a								
Cartesian Coordinates (Å)								
N	0.11258	-1.62343	-0.19885					
C	-0.64185	-0.54229	0.19520					
N	-0.12993	0.72287	0.11935					
C	-0.84479	1.82199	0.49996					
C	1.38150	-1.61528	-0.68681					
H	-1.63911	-0.68882	0.56520					
H	1.74559	-2.62326	-0.92349					
H	-0.32976	-2.52177	-0.11448					
H	0.81485	0.81046	-0.23613					
O	2.05461	-0.61110	-0.84996					
H	-0.27830	2.75405	0.37115					
O	-1.97536	1.77600	0.93092					
Vibrational wavenumbers (cm^{-1})								
74.0	111.5	172.1	250.7	331.9	380.3	412.0	435.5	
615.6	762.8	784.2	868.7	969.9	991.0	1041.0	1107.6	
1211.7	1285.5	1366.8	1427.1	1443.2	1559.4	1595.3	1741.5	
1781.9	3025.3	3032.7	3299.0	3538.7	3670.9			
Rotational Constants (GHz):				7.9506	1.4693	1.2401		

M20							
Cartesian Coordinates (Å)							
N	0.03411	-0.04857	-0.20174				
C	-0.86130	0.96620	-0.52645				
N	-0.65167	2.18182	-0.79204				
C	2.03536	-1.24176	0.27127				
C	1.38050	-0.03753	-0.07472				
H	-1.88112	0.58863	-0.53582				
H	3.13373	-1.18564	0.36384				
H	0.33138	2.42825	-0.75538				
H	-0.34105	-0.97062	-0.02116				
H	2.96002	0.99409	-0.16503				
O	2.01526	1.12104	-0.28581				
O	1.41435	-2.29526	0.45900				
Vibrational wavenumbers (cm^{-1})							
67.6	183.7	199.6	275.1	278.2	396.6	433.8	519.7
614.8	697.6	781.0	856.6	879.8	889.7	1095.7	1115.7
1210.0	1247.1	1357.9	1408.7	1447.3	1513.0	1613.6	1668.0
1731.5	2955.5	3141.7	3564.3	3580.8	3858.5		
Rotational Constants (GHz):				5.9734	1.7824	1.3727	

M21							
Cartesian Coordinates (Å)							
N	0.05007	0.26130	-0.00024				
C	-0.77070	0.49213	-1.08570				
N	-0.45540	0.86506	-2.25182				
C	1.99255	-0.57309	1.14503				
C	1.46875	0.24739	-0.07718				
H	-1.81967	0.31597	-0.85520				
H	0.54070	1.04210	-2.35647				
H	1.81292	-0.23983	-0.99244				
H	-0.37034	-0.01558	0.86937				
H	1.67544	2.03265	0.63549				
O	2.07947	1.50333	-0.05689				
O	2.86849	-1.34570	1.14226				
Vibrational wavenumbers (cm^{-1})							
49.2	97.7	165.5	179.8	281.7	352.6	388.1	423.1
448.1	581.9	699.1	853.4	892.5	1013.1	1079.0	1099.2
1184.9	1251.3	1266.2	1312.7	1426.5	1438.0	1524.1	1735.3
1986.8	3071.1	3133.0	3514.1	3658.3	3862.5		
Rotational Constants (GHz):				5.8822	1.5375	1.3737	

P5								
	Cartesian Coordinates (Å)							
N	-0.13412	-0.06248	-0.03011					
C	-0.47014	-0.84780	1.01178					
N	0.46352	-1.16340	1.85451					
C	1.61436	-0.55084	1.35962					
C	1.29627	0.10877	-0.00750					
H	-1.49415	-1.18074	1.12456					
H	1.75412	-0.46024	-0.82450					
H	-0.71561	0.09237	-0.83170					
H	2.42346	1.53875	0.56914					
O	1.69201	1.44107	-0.05003					
O	2.68706	-0.45123	1.88838					
	Vibrational wavenumbers (cm^{-1})							
98.3	247.2	291.1	303.8	442.8	545.6	575.6	669.7	
775.2	854.8	920.5	1020.9	1045.6	1128.0	1162.5	1197.8	
1251.6	1347.2	1372.8	1390.1	1498.2	1616.1	1860.7	3026.8	
3211.9	3704.0	3816.0						
	Rotational Constants (GHz):			3.9571	3.5955	1.9988		

E2-RO_2							
	Cartesian Coordinates (Å)						
N	1.78178	-0.33107	-0.25874				
C	0.53583	-0.15853	0.27561				
N	-0.48769	-0.66672	-0.26890				
C	-1.74250	-0.37881	0.32456				
C	2.93654	0.17707	0.29374				
H	0.51297	0.43969	1.18743				
H	2.75437	0.74387	1.22053				
H	1.86309	-0.85415	-1.11878				
H	-2.41451	-1.82456	-0.68720				
O	4.02411	0.01951	-0.18408				
H	-1.71596	-0.10644	1.38226				
O	-2.63840	-1.38061	0.13593				
O	-2.30807	0.82115	-0.35631				
O	-1.63237	1.88341	-0.05232				
	Vibrational wavenumbers (cm^{-1})						
52.7	104.3	113.2	135.8	181.6	296.0	313.3	342.7
393.9	403.9	495.6	601.4	642.7	669.9	725.1	886.6
1021.2	1048.1	1072.0	1200.3	1250.4	1276.8	1295.2	1332.0
1349.0	1368.2	1422.2	1450.3	1508.2	1761.1	1850.9	2997.2
3073.6	3106.9	3614.5	3851.8				
	Rotational Constants (GHz):			3.9609	0.6979	0.6143	

E4-RO_2							
Cartesian Coordinates (Å)							
N	1.25142	-0.67568	-0.65350				
C	0.19991	0.02234	-0.02016				
N	-1.05080	-0.53160	-0.39395				
C	-1.97987	-0.45911	0.45964				
C	2.50337	-0.77301	-0.11979				
H	0.39280	0.10299	1.05076				
H	3.18353	-1.35937	-0.75696				
H	1.04449	-1.11562	-1.53344				
H	-3.22809	-1.20930	-0.70476				
O	2.83891	-0.29112	0.93152				
H	-1.88861	-0.05563	1.46590				
O	-3.20572	-0.89197	0.20613				
O	0.26905	1.42097	-0.52249				
O	-0.55836	2.18045	0.12140				
Vibrational wavenumbers (cm^{-1})							
46.1	77.0	129.5	148.2	194.1	211.5	279.0	358.2
419.6	517.7	542.7	582.5	623.6	652.5	831.1	888.4
1038.0	1046.8	1112.0	1124.7	1231.9	1253.9	1273.6	1333.1
1358.4	1381.3	1428.4	1438.9	1542.5	1752.4	1824.9	2997.7
3093.3	3149.6	3666.3	3808.4				
Rotational Constants (GHz):				2.7512	0.9686	0.7993	

Z2-RO_2							
Cartesian Coordinates (Å)							
N	1.26795	0.25059	0.22390				
C	0.66836	-0.85542	-0.33001				
N	-0.57200	-1.12938	-0.35601				
C	-1.52299	-0.31845	0.32113				
C	2.64244	0.40286	0.26390				
H	1.36835	-1.54572	-0.78657				
H	2.93685	1.38645	0.65828				
H	0.68283	1.03783	0.47983				
H	-2.72517	-1.64139	-0.26310				
O	3.42952	-0.43274	-0.08286				
H	-1.21870	0.05408	1.30260				
O	-2.71307	-0.96000	0.41627				
O	-1.78067	0.92474	-0.47683				
O	-1.01612	1.90379	-0.10613				
Vibrational wavenumbers (cm^{-1})							
55.3	101.9	144.8	150.7	229.3	255.0	313.8	371.1
414.3	445.0	547.4	595.4	675.3	738.4	834.3	883.2
996.1	1036.7	1045.4	1117.1	1209.4	1251.9	1292.8	1327.7
1363.7	1399.4	1440.5	1449.5	1541.4	1744.2	1846.0	3014.8
3068.9	3196.3	3520.0	3841.2				
Rotational Constants (GHz):				3.5166	0.9142	0.7594	

Z4-RO$_2$							
Cartesian Coordinates (Å)							
N	1.43862	-0.78440	-0.18310				
C	0.13559	-0.26151	-0.06093				
N	-0.76413	-1.08876	-0.78254				
C	-2.01979	-0.93032	-0.66775				
C	2.41757	-0.53764	0.73525				
H	-0.11314	-0.08841	0.98871				
H	3.35679	-1.06084	0.49922				
H	1.60110	-1.41606	-0.94846				
H	-2.11373	0.75327	0.20968				
O	2.27805	0.16513	1.70309				
H	-2.67652	-1.65194	-1.14164				
O	-2.69915	0.00692	-0.02901				
O	0.19684	1.12139	-0.64604				
O	-0.76454	1.87085	-0.20941				
Vibrational wavenumbers (cm^{-1})							
55.7	100.2	126.4	190.7	230.1	248.7	303.3	393.2
431.1	514.6	561.2	597.2	755.6	786.5	812.1	869.3
1030.8	1047.5	1066.1	1126.2	1238.7	1249.8	1291.8	1329.3
1381.6	1406.8	1433.1	1464.7	1532.8	1732.7	1824.0	3003.0
3078.2	3188.0	3511.4	3664.3				
Rotational Constants (GHz):				3.0316	1.0776	0.9192	

TS25							
Cartesian Coordinates (Å)							
N	-1.09142	-0.29686	0.20363				
C	-0.13216	0.31811	0.97096				
N	1.07468	-0.13998	1.25093				
C	1.77875	-0.72186	0.33025				
C	-2.39030	0.14945	0.12988				
H	-0.53632	1.06541	1.64444				
H	-2.59449	0.99000	0.81209				
H	-0.81609	-1.03615	-0.42613				
H	1.90340	-1.78391	-1.25756				
O	-3.21918	-0.33299	-0.59140				
H	2.84421	-0.84502	0.49075				
O	1.23711	-1.52395	-0.61831				
O	1.75649	1.03847	-0.82568				
O	0.69792	1.59263	-0.46862				
Vibrational wavenumbers (cm^{-1})							
257.1 *i*	75.3	136.6	157.6	193.8	218.5	289.3	319.0
333.2	388.0	444.4	571.8	590.8	627.5	741.8	793.6
966.9	1001.7	1047.9	1085.4	1198.0	1249.9	1279.6	1305.4
1361.4	1406.8	1446.0	1465.7	1590.0	1622.5	1838.0	2995.2
3176.3	3182.3	3621.5	3884.0				
Rotational Constants (GHz):				2.8125	1.0683	0.9716	

TS26							
Cartesian Coordinates (Å)							
N	-1.48771	-0.47909	-0.21636				
C	-0.27673	-0.27123	0.38183				
N	0.77987	-0.88775	-0.10505				
C	1.92828	-0.48197	0.39004				
C	-2.68654	-0.04146	0.29366				
H	-0.33533	0.10966	1.39880				
H	-2.58057	0.44700	1.27538				
H	-1.49355	-0.90454	-1.13162				
H	2.85051	-1.24520	-1.03379				
O	-3.73806	-0.18128	-0.26650				
H	2.07292	-0.13246	1.40771				
O	3.05994	-0.87716	-0.16761				
O	1.62871	1.47137	-0.16101				
O	0.38077	1.59475	-0.16236				
Vibrational wavenumbers (cm^{-1})							
227.0 *i*	74.4	119.4	157.7	199.8	213.5	309.0	389.5
402.8	432.7	494.0	524.2	621.7	637.2	685.7	712.5
989.3	1044.0	1072.2	1170.0	1231.6	1290.4	1316.4	1330.2
1381.9	1392.4	1406.3	1462.9	1588.5	1628.4	1842.3	2995.6
3125.7	3156.4	3621.5	3817.9				
Rotational Constants (GHz):				4.0614	0.8060	0.7019	

TS27							
Cartesian Coordinates (Å)							
N	-1.47112	-0.31486	-0.38532				
C	-0.18131	-0.40097	0.05563				
N	0.74293	-0.77570	-0.81517				
C	1.97414	-0.66042	-0.41195				
C	-2.55422	-0.10267	0.43300				
H	-0.07218	-0.47564	1.13259				
H	-2.28310	-0.07082	1.50013				
H	-1.62762	-0.32495	-1.38268				
H	3.25008	-0.66048	1.00104				
O	-3.67733	0.02734	0.03071				
H	2.77166	-0.70880	-1.14482				
O	2.32290	-0.86642	0.86960				
O	1.74820	1.44134	-0.21341				
O	0.55959	1.50511	0.16773				
Vibrational wavenumbers (cm^{-1})							
237.6 *i*	77.5	125.2	159.0	203.4	217.5	291.6	300.4
380.5	429.0	442.9	548.1	575.1	620.9	719.2	777.2
965.6	1026.3	1049.6	1127.2	1230.9	1257.7	1273.1	1309.9
1347.3	1399.6	1424.3	1464.8	1603.3	1612.8	1840.4	2997.1
3161.2	3182.6	3617.7	3891.8				
Rotational Constants (GHz):				3.6994	0.8667	0.7822	

TS28							
Cartesian Coordinates (Å)							
N	1.17368	-0.52906	0.52410				
C	0.39823	-0.38601	-0.61362				
N	-0.85905	-0.74212	-0.72876				
C	-1.66326	-0.53884	0.29238				
C	2.53402	-0.30523	0.52794				
H	0.99075	-0.27244	-1.51074				
H	2.97408	-0.45294	1.52604				
H	0.73876	-0.73881	1.40526				
H	-3.13275	-0.70275	-0.83137				
O	3.17574	0.00152	-0.43801				
H	-1.40771	-0.60106	1.34707				
O	-2.96893	-0.68429	0.11928				
O	-1.27181	1.44984	0.34549				
O	-0.18243	1.61377	-0.24474				
Vibrational wavenumbers (cm^{-1})							
244.2 *i*	55.6	120.9	139.6	203.8	232.8	246.6	347.6
394.0	444.1	516.7	535.8	585.4	646.3	677.4	829.3
993.4	1023.9	1036.8	1082.2	1146.5	1222.7	1291.8	1372.2
1394.6	1402.1	1440.7	1477.6	1579.9	1609.6	1839.5	3001.7
3133.1	3226.0	3668.3	3807.3				
Rotational Constants (GHz):				3.6663	0.9567	0.8489	

TS29e							
Cartesian Coordinates (Å)							
N	1.12289	0.65537	0.55247				
C	-0.18190	0.55418	0.98340				
N	-0.83990	-0.56790	1.03341				
C	-1.19645	-1.40518	0.11128				
C	1.88935	-0.28536	-0.11159				
H	-0.46568	1.33865	1.67360				
H	2.89061	0.11325	-0.33709				
H	1.54051	1.56391	0.66226				
H	-1.30840	-0.04099	-1.37059				
O	1.54855	-1.39753	-0.39638				
H	-1.36317	-2.43449	0.41740				
O	-1.46053	-1.13320	-1.09755				
O	-0.96761	1.81902	-0.49898				
O	-1.20825	1.22029	-1.62146				
Vibrational wavenumbers (cm^{-1})							
736.5 *i*	53.8	77.4	121.1	189.3	220.5	241.5	283.2
325.5	366.3	521.2	576.0	621.7	692.2	866.3	894.7
995.7	1034.7	1048.9	1070.6	1142.6	1248.2	1279.8	1329.0
1400.1	1433.0	1466.5	1533.4	1613.7	1712.5	1783.9	1865.4
3000.0	3166.9	3187.2	3656.3				
Rotational Constants (GHz):				2.0198	1.5617	1.2578	

TS29z							
Cartesian Coordinates (Å)							
N	1.38514	-0.60442	-0.19259				
C	0.11271	-0.48959	0.26229				
N	-0.78597	-1.34597	-0.21204				
C	-2.06852	-1.20003	-0.02425				
C	2.46338	0.06685	0.35416				
H	0.00937	-0.07640	1.26195				
H	2.19444	0.65448	1.24491				
H	1.53959	-1.13305	-1.03884				
H	-2.10500	0.84088	0.16698				
O	3.57017	0.00235	-0.09602				
H	-2.67244	-2.10177	-0.10744				
O	-2.71415	-0.13152	0.19826				
O	-0.23631	1.40814	-0.35842				
O	-1.39541	1.87169	-0.02487				
Vibrational wavenumbers (cm^{-1})							
837.0 *i*	64.2	85.4	123.2	190.9	213.4	269.6	306.2
326.4	427.7	481.0	548.9	618.5	698.3	760.7	833.6
1040.8	1056.8	1114.9	1168.1	1217.1	1257.7	1309.8	1333.8
1342.3	1402.9	1435.5	1486.0	1609.9	1692.3	1749.8	1854.1
3011.4	3139.1	3148.4	3617.9				
Rotational Constants (GHz):				3.2362	0.9306	0.7453	

TS30e							
Cartesian Coordinates (Å)							
N	0.57829	0.21773	-0.37538				
C	0.04841	0.08657	0.86157				
N	-0.94872	-0.79335	1.17780				
C	-1.35460	-1.66954	0.33158				
C	1.90268	0.66838	-0.45705				
H	0.60409	0.47943	1.70441				
H	2.13419	1.10009	-1.44197				
H	-0.21465	1.11553	-0.86200				
H	-0.22771	-1.24666	-1.09481				
O	2.72219	0.56518	0.41206				
H	-2.14231	-2.35262	0.63135				
O	-0.93001	-1.90092	-0.88999				
O	-1.15127	1.75772	0.62544				
O	-1.02039	1.97248	-0.62303				
Vibrational wavenumbers (cm^{-1})							
1013.3 *i*	66.1	84.6	136.8	173.2	208.0	218.2	304.4
342.7	483.4	535.0	591.4	669.6	790.4	839.2	872.5
1032.2	1045.6	1057.3	1105.4	1150.0	1230.1	1276.3	1345.0
1362.1	1401.3	1432.3	1464.4	1515.7	1681.2	1823.1	1836.1
3010.8	3187.2	3195.2	3446.4				
Rotational Constants (GHz):				1.9377	1.3717	1.0249	

TS30z							
Cartesian Coordinates (Å)							
N	1.03607	-0.14426	0.70138				
C	-0.21490	-0.19805	1.11284				
N	-1.09119	-1.14716	0.74092				
C	-1.93094	-1.03739	-0.20659				
C	1.58504	-1.14293	-0.11242				
H	-0.50689	0.47147	1.91375				
H	1.16039	-2.14162	0.07141				
H	1.26194	0.95796	0.40661				
H	-1.48283	0.72187	-0.76256				
O	2.47444	-0.93510	-0.88345				
H	-2.60069	-1.86057	-0.42524				
O	-2.10199	-0.00727	-0.99720				
O	-0.45074	1.94449	-0.03673				
O	0.81813	2.14303	-0.09050				
Vibrational wavenumbers (cm^{-1})							
614.3 *i*	41.0	118.6	125.3	148.9	176.8	217.4	253.0
383.5	388.8	470.7	584.5	670.0	708.5	827.9	878.8
980.1	1041.6	1056.1	1068.0	1182.8	1267.9	1282.2	1344.9
1395.3	1419.1	1454.2	1492.4	1618.0	1753.0	1810.5	1905.9
3006.7	3182.7	3204.3	3395.4				
Rotational Constants (GHz):				1.8811	1.3837	0.9960	

TS31							
Cartesian Coordinates (Å)							
N	1.41179	-0.37224	0.18138				
C	0.88346	0.87187	-0.04560				
N	-0.29832	1.27866	0.21370				
C	-1.26156	0.44554	0.76075				
C	2.73712	-0.67599	-0.06752				
H	1.59260	1.56958	-0.47731				
H	2.96934	-1.72586	0.16461				
H	0.78203	-1.08295	0.52764				
H	-1.98404	-1.17590	0.04466				
O	3.54817	0.10124	-0.48778				
H	-1.91496	0.96206	1.46319				
O	-1.15191	-0.83371	0.85663				
O	-2.56395	0.44482	-0.62680				
O	-2.75648	-0.80491	-0.78883				
Vibrational wavenumbers (cm^{-1})							
909.3 *i*	32.3	89.1	133.3	166.4	239.4	256.0	275.0
402.6	475.0	615.8	684.3	719.1	775.0	783.9	831.8
1030.0	1045.3	1079.4	1091.2	1098.6	1136.6	1239.5	1362.1
1373.4	1394.2	1440.8	1502.1	1561.6	1720.2	1843.1	1928.3
3012.0	3113.7	3190.7	3581.8				
Rotational Constants (GHz):				4.2771	0.7668	0.7302	

TS32							
Cartesian Coordinates (Å)							
N	1.10408	0.16492	0.05045				
C	0.61709	-1.05257	-0.09538				
N	-0.65659	-1.35038	-0.18115				
C	-1.60753	-0.65030	0.38241				
C	2.49436	0.32907	0.08003				
H	1.32759	-1.86690	-0.20285				
H	2.77514	1.38010	0.23475				
H	0.37684	1.16903	0.10803				
H	-2.87761	-1.34403	-0.78402				
O	3.30427	-0.54654	-0.05023				
H	-1.49316	-0.16822	1.34556				
O	-2.85428	-0.84241	0.03995				
O	-1.53918	1.46503	-0.26762				
O	-0.44391	2.09531	0.02928				
Vibrational wavenumbers (cm^{-1})							
1013.5 *i*	67.7	91.5	123.2	166.2	207.8	241.1	266.9
292.0	389.1	417.1	484.7	560.7	672.5	718.3	872.4
1032.0	1049.9	1072.1	1113.4	1164.0	1253.1	1280.0	1317.8
1366.3	1400.1	1423.5	1454.9	1588.6	1672.9	1790.8	1853.8
3027.3	3173.9	3195.4	3808.4				
Rotational Constants (GHz):				2.7918	0.9990	0.7492	

TS33							
Cartesian Coordinates (Å)							
N	-1.92057	-0.21499	0.33656				
C	-0.68001	0.31921	0.16337				
N	0.27464	0.02404	0.94943				
C	1.51571	0.59360	0.65675				
C	-3.01113	0.09304	-0.44997				
H	-0.57868	1.00942	-0.67444				
H	-2.77484	0.81988	-1.24283				
H	-2.05494	-0.87476	1.08987				
H	2.47901	0.39319	-0.97759				
O	-4.09841	-0.38206	-0.28602				
H	2.09877	0.82559	1.54711				
O	1.76445	1.20491	-0.43292				
O	2.53173	-0.98996	0.25245				
O	2.97784	-0.69185	-0.90414				
Vibrational wavenumbers (cm^{-1})							
901.9 *i*	46.6	103.6	120.4	124.2	211.3	275.4	306.2
324.0	476.4	595.9	606.6	675.7	721.3	744.6	807.7
1036.1	1052.4	1071.3	1101.0	1126.9	1237.3	1305.0	1344.7
1363.1	1376.4	1429.7	1499.7	1585.0	1730.3	1851.1	1918.6
3001.3	3117.4	3120.9	3609.1				
Rotational Constants (GHz):				4.7907	0.6109	0.6023	

TS34e							
Cartesian Coordinates (Å)							
N	1.06928	-0.07365	-0.59989				
C	0.29039	-0.52057	0.37216				
N	-0.98008	-0.90660	0.14517				
C	-2.05394	-0.25351	0.16493				
C	2.44892	-0.17886	-0.41037				
H	0.74204	-0.85682	1.30060				
H	3.00624	0.57210	-0.98767				
H	0.71982	1.06112	-0.79662				
H	-3.09435	-1.73455	-0.32145				
O	2.98631	-1.01455	0.26304				
H	-2.12320	0.80129	0.41063				
O	-3.22599	-0.80332	-0.10771				
O	-0.08175	1.73480	0.85579				
O	0.29611	2.17334	-0.28871				
Vibrational wavenumbers (cm^{-1})							
883.1 *i*	55.6	88.2	108.1	163.5	187.9	211.8	225.5
285.7	370.0	456.2	500.5	600.6	640.3	705.0	832.4
1004.5	1046.2	1056.2	1098.6	1136.9	1255.9	1285.6	1342.5
1366.7	1396.3	1427.6	1442.5	1591.4	1789.8	1816.8	1841.0
3024.4	3171.2	3187.5	3813.8				
Rotational Constants (GHz):				2.5573	0.9811	0.7657	

TS34z							
Cartesian Coordinates (Å)							
N	1.10476	-0.27730	0.69889				
C	-0.13865	0.14050	0.77887				
N	-1.16835	-0.50334	0.13575				
C	-2.29314	0.08952	0.11065				
C	1.43510	-1.46180	0.03475				
H	-0.37261	0.87997	1.53894				
H	0.68181	-2.25640	0.13444				
H	1.73099	0.71518	0.31444				
H	-3.11034	-1.30824	-0.80939				
O	2.47919	-1.61932	-0.53112				
H	-2.49352	1.08032	0.51633				
O	-3.35519	-0.44583	-0.44926				
O	0.42994	1.96914	-0.35966				
O	1.69467	1.81406	-0.29532				
Vibrational wavenumbers (cm^{-1})							
1051.4 *i*	47.3	88.3	104.2	122.0	163.9	206.1	216.8
320.1	441.3	484.0	563.3	623.7	651.4	685.2	791.9
994.3	1044.4	1052.5	1094.7	1189.3	1247.2	1285.7	1365.0
1387.0	1392.9	1414.7	1459.8	1624.9	1716.6	1785.7	1856.3
3015.7	3138.4	3142.6	3791.8				
Rotational Constants (GHz):				2.2083	1.0104	0.7534	

TS35							
Cartesian Coordinates (Å)							
N	1.38608	-0.73082	-0.48145				
C	0.13468	-0.25179	-0.05538				
N	-0.87421	-1.20697	-0.35813				
C	-2.05574	-0.99724	0.22595				
C	2.56498	-0.30555	0.06783				
H	0.18375	0.12076	0.96986				
H	3.43747	-0.81178	-0.37238				
H	1.38321	-1.43484	-1.20000				
H	-1.60589	1.19543	0.34815				
O	2.64903	0.51885	0.93929				
H	-2.77543	-1.81109	0.11399				
O	-2.39291	0.03549	0.83881				
O	-0.21746	0.88007	-0.90937				
O	-1.04736	1.76978	-0.29535				
Vibrational wavenumbers (cm^{-1})							
474.2 *i*	59.3	114.5	174.2	211.2	238.9	334.5	360.0
429.4	467.3	542.1	561.1	696.7	802.7	829.1	864.5
995.2	1046.4	1047.1	1085.4	1123.7	1256.4	1297.7	1332.7
1391.2	1413.2	1434.5	1460.2	1532.3	1652.2	1827.8	2408.9
3005.2	3090.3	3101.8	3659.8				
Rotational Constants (GHz):				3.0757	1.0935	0.9537	

TS36							
Cartesian Coordinates (Å)							
N	1.47126	0.92322	0.30875				
C	0.48011	0.13651	0.87088				
N	-0.55664	-0.19244	0.29013				
C	-1.64799	-0.62207	-0.36164				
C	2.61413	1.30708	0.96993				
H	0.71132	-0.15620	1.90091				
H	2.66014	0.92584	2.00258				
H	1.35627	1.22835	-0.64721				
H	-2.45413	-2.20851	-0.97331				
O	3.47299	1.98579	0.47913				
H	-2.51769	0.00283	-0.13391				
O	-1.87906	-1.96283	-0.23484				
O	-1.44444	-0.33828	-1.87606				
O	-2.26637	-1.02971	-2.59522				
Vibrational wavenumbers (cm^{-1})							
223.2 *i*	55.0	72.7	119.9	134.3	177.7	259.9	312.1
391.8	399.8	487.4	572.8	605.0	649.4	717.7	736.3
994.6	1032.9	1048.5	1164.1	1215.3	1255.1	1264.1	1293.8
1323.4	1353.9	1442.7	1460.8	1558.2	1837.2	2002.4	2992.8
3041.7	3047.0	3611.6	3748.5				
Rotational Constants (GHz):				4.5766	0.6174	0.5573	

TS37							
Cartesian Coordinates (Å)							
N	1.39220	-0.28240	-0.19087				
C	0.19628	0.29449	0.31515				
N	-0.95502	-0.24848	-0.10651				
C	-2.01400	-0.84889	-0.29809				
C	2.51775	-0.41715	0.56934				
H	0.26826	0.38183	1.39810				
H	3.35786	-0.83755	-0.00499				
H	1.43139	-0.50857	-1.16939				
H	-2.93227	0.66449	-0.89591				
O	2.59752	-0.13262	1.73657				
H	-2.18773	-1.91077	-0.11522				
O	-3.12195	-0.27796	-0.78963				
O	0.29931	1.78174	-0.15776				
O	-0.84947	2.34194	-0.29089				
Vibrational wavenumbers (cm^{-1})							
217.6 *i*	36.6	62.7	88.9	123.2	180.6	220.7	287.5
406.2	445.1	516.7	542.8	649.3	664.9	690.4	793.6
1010.6	1035.5	1044.4	1092.9	1207.4	1228.3	1253.4	1313.1
1318.1	1376.7	1432.8	1474.3	1550.8	1821.4	1983.1	2997.5
3101.9	3123.1	3666.9	3769.3				
Rotational Constants (GHz):				2.9057	0.9387	0.7634	

PC29e							
Cartesian Coordinates (Å)							
N	1.33356	0.55784	0.82310				
C	0.12752	0.34372	1.47070				
N	-0.71740	-0.56402	1.26581				
C	-0.80530	-1.43488	0.21378				
C	2.06065	-0.34231	0.07932				
H	-0.06567	1.07087	2.25352				
H	2.95355	0.12123	-0.36483				
H	1.71487	1.48464	0.90851				
H	-1.42825	0.52182	-1.30847				
O	1.78862	-1.50461	-0.05594				
H	-0.62812	-2.48343	0.46809				
O	-1.19025	-1.10174	-0.88866				
O	-0.83850	2.17202	-0.71506				
O	-1.53233	1.47523	-1.57832				
Vibrational wavenumbers (cm^{-1})							
29.9	39.2	86.3	93.9	127.4	166.4	223.0	236.1
271.3	319.6	402.6	565.1	589.3	725.9	749.7	900.0
981.7	998.3	1040.0	1049.4	1088.7	1247.3	1285.6	1406.4
1436.8	1473.4	1541.9	1606.8	1740.9	1783.6	1858.8	3015.4
3087.5	3160.7	3227.8	3658.6				
Rotational Constants (GHz):				2.0269	1.2402	1.0581	

PC29z							
Cartesian Coordinates (Å)							
N	1.63064	-0.68632	-0.13561				
C	0.31368	-0.72950	0.16219				
N	-0.38981	-1.76745	-0.09745				
C	-1.74733	-1.68152	0.11286				
C	2.44600	0.40284	0.14426				
H	-0.08225	0.17221	0.63468				
H	1.90513	1.22910	0.62831				
H	2.05192	-1.48164	-0.59591				
H	-2.18918	0.97778	-0.28194				
O	3.61063	0.42350	-0.12566				
H	-2.20647	-2.64252	0.37055				
O	-2.43889	-0.68978	-0.01172				
O	-0.92341	2.18474	0.29695				
O	-2.02822	1.95285	-0.36459				
Vibrational wavenumbers (cm^{-1})							
39.6	49.0	72.3	113.1	129.9	168.7	179.2	248.2
262.4	327.1	348.7	481.9	614.0	688.3	760.6	805.4
1044.6	1064.1	1081.2	1129.1	1224.8	1284.1	1332.0	1363.0
1423.8	1447.8	1505.1	1597.4	1680.7	1765.0	1857.1	3025.1
3063.2	3095.9	3317.0	3602.3				
Rotational Constants (GHz):				1.9557	0.9089	0.6302	

PC30e							
Cartesian Coordinates (Å)							
N	0.76235	-0.16927	-0.32743				
C	0.37748	-0.46172	0.88171				
N	-0.71785	-1.20304	1.18783				
C	-1.35746	-1.81373	0.24297				
C	1.99262	0.50999	-0.45028				
H	0.94613	-0.09785	1.73408				
H	2.05989	1.08819	-1.38275				
H	-0.59051	1.06796	-0.96774				
H	-0.30008	-1.24445	-1.17502				
O	2.89262	0.45271	0.33776				
H	-2.22534	-2.41033	0.50415				
O	-1.08925	-1.82851	-1.03214				
O	-1.30954	2.10362	0.35312				
O	-1.25648	1.79114	-0.91780				
Vibrational wavenumbers (cm^{-1})							
34.4	49.4	60.8	74.4	118.5	167.9	192.0	220.4
237.7	319.6	470.1	523.0	599.8	760.5	863.4	954.1
1032.9	1058.5	1082.3	1107.6	1159.6	1252.9	1305.9	1382.1
1409.1	1432.2	1460.4	1525.1	1577.5	1675.1	1820.6	3019.7
3155.8	3182.5	3240.7	3425.1				
Rotational Constants (GHz):				1.6023	1.2961	0.9015	

PC30z							
Cartesian Coordinates (Å)							
N	0.44696	-0.98292	0.84881				
C	-0.53766	-0.27581	1.26142				
N	-1.77656	-0.22166	0.69958				
C	-2.07193	0.49058	-0.30858				
C	0.27525	-1.84759	-0.23871				
H	-0.39702	0.31443	2.16551				
H	-0.53123	-2.58826	-0.10386				
H	1.78497	0.15971	0.51707				
H	-0.38067	1.36193	-0.63322				
O	0.98832	-1.83283	-1.20155				
H	-3.07935	0.45452	-0.70710				
O	-1.30127	1.32102	-0.97532				
O	1.30903	1.81188	-0.14971				
O	2.24349	1.01577	0.28134				
Vibrational wavenumbers (cm^{-1})							
39.7	68.1	90.0	103.2	146.8	154.0	208.3	235.9
287.8	371.6	427.8	622.5	719.9	747.0	766.8	842.9
1015.7	1023.1	1046.6	1070.2	1118.4	1266.2	1304.8	1393.8
1404.4	1437.2	1466.3	1578.9	1673.7	1750.8	1832.9	2975.2
3130.4	3154.5	3197.2	3437.7				
Rotational Constants (GHz):				1.6720	1.4418	1.0411	

PC31							
Cartesian Coordinates (Å)							
N	-1.67441	-0.39104	0.00001				
C	-1.46858	0.94786	0.00006				
N	-0.33712	1.56981	0.00003				
C	0.84259	0.86404	-0.00008				
C	-2.94911	-0.95532	-0.00002				
H	-2.38234	1.53308	0.00018				
H	-2.91316	-2.05362	0.00001				
H	-0.84791	-0.97767	0.00005				
H	2.61801	-0.94071	-0.00003				
O	-3.96397	-0.32294	-0.00006				
H	1.73379	1.49751	-0.00032				
O	0.96788	-0.35730	0.00009				
O	4.06271	0.17583	-0.00001				
O	3.59875	-1.05178	-0.00001				
Vibrational wavenumbers (cm^{-1})							
20.5	54.9	59.0	103.4	110.8	111.4	209.9	222.0
260.4	293.1	456.6	500.2	649.4	780.1	828.9	860.6
1038.0	1045.8	1067.9	1109.9	1112.2	1263.7	1272.9	1389.6
1438.4	1441.2	1484.6	1584.9	1642.7	1713.3	1854.6	3027.8
3099.6	3186.8	3387.4	3536.9				
Rotational Constants (GHz):				5.0561	0.5365	0.4850	

PC32								
Cartesian Coordinates (Å)								
N	1.03790	-0.00300	-0.12197					
C	0.57250	-1.17547	0.12413					
N	-0.71354	-1.54798	-0.09977					
C	-1.69485	-0.80322	0.21253					
C	2.42516	0.16376	0.06773					
H	1.23012	-1.96413	0.48714					
H	2.68908	1.20974	0.27837					
H	0.15133	1.46148	-0.44550					
H	-2.91889	-1.91725	-0.64923					
O	3.24923	-0.70331	-0.01666					
H	-1.62410	0.12054	0.78644					
O	-2.93024	-1.10717	-0.12397					
O	-1.18651	2.32883	0.48452					
O	-0.33435	2.33615	-0.51032					
Vibrational wavenumbers (cm^{-1})								
55.0	57.3	81.0	93.2	127.5	140.7	199.1	229.0	
239.6	316.9	364.3	494.7	680.0	680.8	822.6	832.1	
1036.2	1065.4	1075.1	1094.1	1152.5	1277.2	1291.7	1381.5	
1396.4	1430.0	1449.2	1618.9	1636.4	1733.9	1818.3	3022.3	
3081.9	3133.5	3137.0	3798.4					
Rotational Constants (GHz):				1.7944	1.0254	0.6714		

PC33								
Cartesian Coordinates (Å)								
N	2.45309	0.36834	-0.07789					
C	1.13457	0.08967	0.05529					
N	0.24211	0.97213	-0.17419					
C	-1.07399	0.55105	-0.12327					
C	3.46852	-0.52943	0.21026					
H	0.90203	-0.92419	0.38480					
H	3.09285	-1.50289	0.56117					
H	2.71871	1.28851	-0.40129					
H	-3.16132	-0.83505	-0.26035					
O	4.62780	-0.26532	0.08628					
H	-1.78217	1.32809	0.18067					
O	-1.45373	-0.56388	-0.42444					
O	-4.27205	0.42371	0.45922					
O	-4.12843	-0.77020	-0.06532					
Vibrational wavenumbers (cm^{-1})								
19.8	49.7	62.9	92.6	106.7	138.5	186.9	217.2	
278.1	317.0	357.5	485.6	618.0	672.3	755.5	808.3	
1033.7	1051.0	1085.9	1122.3	1230.0	1266.5	1320.2	1348.6	
1418.4	1433.8	1503.3	1588.2	1686.0	1762.1	1859.4	3007.3	
3086.7	3110.5	3359.5	3604.0					
Rotational Constants (GHz):				8.9413	0.4078	0.3952		

PC34e							
Cartesian Coordinates (Å)							
N	1.00144	-0.20916	-0.18635				
C	0.33325	-1.26874	0.10118				
N	-1.00958	-1.38985	-0.05667				
C	-1.81440	-0.46854	0.28774				
C	2.40256	-0.30973	-0.06385				
H	0.84505	-2.16579	0.44700				
H	2.87132	0.66799	0.11628				
H	0.39619	1.39547	-0.49332				
H	-3.26889	-1.33458	-0.49736				
O	3.04080	-1.31926	-0.17122				
H	-1.54091	0.42918	0.84184				
O	-3.09995	-0.53310	0.01385				
O	-0.70449	2.50996	0.48310				
O	0.08386	2.34644	-0.55020				
Vibrational wavenumbers (cm^{-1})							
54.9	57.2	80.9	93.7	128.2	141.2	199.4	228.9
239.7	316.8	364.2	494.7	680.1	680.7	822.3	832.1
1036.2	1065.4	1075.0	1094.0	1152.4	1277.2	1292.1	1381.4
1396.2	1430.1	1449.7	1619.3	1636.5	1733.9	1818.3	3022.3
3082.1	3133.6	3137.0	3798.4				
Rotational Constants (GHz):				1.7944	1.0254	0.6714	

PC34z							
Cartesian Coordinates (Å)							
N	-0.73060	0.52214	0.23677				
C	0.22523	-0.31054	0.17607				
N	1.55734	0.06129	0.10722				
C	2.39308	-0.87930	-0.07875				
C	-0.47066	1.90430	0.31273				
H	-0.03646	-1.36986	0.16608				
H	0.14220	2.20219	1.17894				
H	-2.35643	-0.22501	0.01531				
H	3.84829	0.28140	-0.04376				
O	-0.94043	2.69379	-0.45119				
H	2.14167	-1.93262	-0.20326				
O	3.68790	-0.66554	-0.14979				
O	-2.46525	-2.04957	-0.06038				
O	-3.08376	-0.89453	-0.08635				
Vibrational wavenumbers (cm^{-1})							
38.4	44.2	56.8	59.8	118.6	140.9	157.6	215.0
237.8	313.0	402.6	548.6	666.2	690.4	697.6	738.9
997.8	1046.8	1053.2	1070.2	1163.1	1267.9	1271.9	1384.3
1391.2	1405.6	1456.5	1602.9	1694.3	1751.5	1844.9	2984.1
3106.9	3128.8	3251.5	3789.9				
Rotational Constants (GHz):				1.8086	0.8056	0.5671	

M22								
Cartesian Coordinates (Å)								
N	0.93349	-0.35749	-0.47453					
C	0.04572	0.45314	0.30316					
N	-1.27456	0.29960	-0.24868					
C	-2.13482	-0.55417	0.41935					
C	1.71508	-1.33171	0.07926					
H	0.10112	0.14485	1.34968					
H	2.40070	-1.77920	-0.65683					
H	1.07730	-0.08648	-1.43249					
H	-0.40732	2.54963	-1.21164					
O	1.66543	-1.68151	1.22927					
H	-2.81986	-1.09909	-0.24417					
O	-2.19858	-0.61151	1.62334					
O	0.40313	1.80604	0.30602					
O	0.49317	2.24789	-1.04215					
Vibrational wavenumbers (cm^{-1})								
27.9	45.9	127.4	146.3	169.0	201.9	271.2	284.8	
330.0	416.5	500.1	561.5	642.0	718.1	770.9	943.8	
996.7	1036.7	1045.7	1081.1	1085.6	1182.3	1214.4	1301.3	
1377.2	1401.9	1420.3	1429.8	1521.2	1703.7	1820.7	2999.4	
3028.0	3096.2	3663.2	3805.4					
Rotational Constants (GHz):				1.6494	1.5781	0.9327		

EE-P5								
Cartesian Coordinates (Å)								
N	-0.45812	0.24637	0.98403					
C	0.58074	-0.16414	0.37205					
N	0.77082	-0.00619	-0.98206					
C	-0.22343	-0.12498	-1.75777					
C	-0.47027	0.13629	2.37532					
H	1.40956	-0.64130	0.89524					
H	-1.21345	-0.45660	-1.45305					
H	-1.45180	-0.17707	2.76166					
O	0.44884	0.40106	3.10380					
O	-0.14340	0.12376	-3.05295					
H	0.75031	0.43280	-3.24637					
Vibrational wavenumbers (cm^{-1})								
78.5	126.7	174.6	184.9	324.7	361.6	485.6	669.9	
687.2	814.2	1027.1	1040.1	1066.6	1075.4	1156.7	1273.2	
1376.6	1399.9	1412.9	1419.8	1665.4	1740.2	1801.9	3005.8	
3115.9	3156.8	3803.3						
Rotational Constants (GHz):				16.1722	1.0964	1.0415		

ZZ-P5

Cartesian Coordinates (Å)			
N	-1.33070	-0.12724	-0.83518
C	-1.24649	-0.13697	0.43362
N	-0.22798	-0.57074	1.24254
C	0.92009	-0.04211	1.37683
C	-0.29282	-0.27615	-1.70898
H	-2.14106	0.13795	0.98831
H	1.58633	-0.44756	2.13193
H	-0.44736	-1.05534	-2.46583
O	0.68271	0.44947	-1.75008
O	1.44217	0.98858	0.74509
H	1.05520	1.08001	-0.15825

Vibrational wavenumbers (cm^{-1})							
109.6	157.5	218.8	236.0	363.8	405.6	652.6	708.5
797.8	822.8	1004.8	1015.8	1048.6	1076.4	1135.1	1272.6
1405.4	1412.9	1449.3	1479.9	1687.1	1738.1	1774.6	3045.2
3139.5	3175.0	3355.8					

Rotational Constants (GHz):			4.2348	2.7392	1.8119	

TSa endo

Cartesian Coordinates (Å)			
N	1.65998	-0.43078	1.18071
C	1.74121	0.04283	-0.13139
N	2.06903	1.35898	-0.12442
C	1.09692	1.74950	0.80384
C	1.29632	0.72658	1.98657
H	1.01735	2.79482	1.07762
H	0.38060	0.56771	2.55122
H	1.19771	-1.30914	1.35169
H	3.09923	1.20368	2.42340
O	2.26456	1.12427	2.89351
H	2.08504	-0.62710	-0.90798
O	0.06534	0.24399	-0.49891
O	-0.20524	1.34856	0.22821

Vibrational wavenumbers (cm^{-1})							
1586.0 *i*	169.5	300.9	327.6	353.4	424.8	511.7	536.9
583.9	630.5	774.0	790.5	869.3	913.5	928.7	986.4
1059.4	1131.0	1142.2	1161.0	1207.6	1225.2	1257.8	1280.4
1307.7	1399.0	1428.1	1451.5	3132.0	3189.5	3216.0	3634.3
3852.9							

Rotational Constants (GHz):			4.1581	2.1193	1.9332	

TSs endo							
Cartesian Coordinates (Å)							
N	2.47575	-1.66100	0.55641				
C	2.25636	-1.36346	-0.76810				
N	0.99539	-0.92311	-0.94735				
C	0.97487	0.00495	0.10739				
C	1.55794	-0.82301	1.32623				
H	2.80102	-1.89144	-1.53835				
H	0.05855	0.55304	0.29319				
H	0.77145	-1.40903	1.79649				
H	3.40232	-1.83025	0.91322				
H	2.70146	0.59844	1.89156				
O	2.17558	-0.08961	2.31425				
O	2.01829	0.98241	-0.16981				
O	3.01873	0.29186	-0.79690				
Vibrational wavenumbers (cm^{-1})							
1459.9 *i*	171.3	280.9	311.5	405.6	466.0	500.7	525.0
613.2	628.4	672.7	772.5	852.5	889.6	931.2	1021.7
1065.1	1104.9	1130.1	1169.8	1211.4	1234.9	1262.9	1308.1
1322.1	1408.5	1430.7	1449.2	3122.4	3185.5	3224.1	3640.6
3809.7							
Rotational Constants (GHz):				3.4409	2.4831	2.1611	

BPRa							
Cartesian Coordinates (Å)							
N	0.29760	-1.06603	0.27929				
C	0.33230	-0.70871	-1.10759				
N	0.83324	0.65434	-1.01911				
C	-0.30782	1.06937	-0.24893				
C	-0.18194	0.12290	0.98135				
H	-0.40156	2.13107	-0.04999				
H	-1.15904	-0.01093	1.44338				
H	-0.15093	-1.94116	0.49848				
H	1.57683	0.48397	1.65852				
O	0.67628	0.56381	1.98251				
H	0.88767	-1.38463	-1.74912				
O	-0.95572	-0.54873	-1.67831				
O	-1.44712	0.63462	-0.99039				
Vibrational wavenumbers (cm^{-1})							
153.8	275.9	307.6	391.5	440.1	511.1	549.5	596.6
765.6	814.9	853.8	897.7	904.8	942.8	984.0	998.1
1043.7	1112.7	1115.8	1145.3	1217.3	1245.3	1274.2	1295.7
1327.0	1364.6	1427.1	1445.1	3111.0	3177.8	3182.6	3628.1
3865.3							
Rotational Constants (GHz):				4.3319	2.1229	1.9034	

BPRs							
Cartesian Coordinates (Å)							
N	0.49759	-1.11138	0.15469				
C	0.47784	-0.57684	-1.16345				
N	-0.95001	-0.34926	-1.30882				
C	-0.96337	0.59300	-0.23550				
C	-0.40130	-0.26698	0.94616				
H	0.95275	-1.18347	-1.92721				
H	-1.88550	1.13797	-0.06724				
H	-1.16906	-0.85173	1.44733				
H	1.38601	-1.34448	0.56977				
H	0.72316	1.18582	1.46898				
O	0.22254	0.49488	1.91904				
O	0.06664	1.53995	-0.54266				
O	1.04259	0.73259	-1.26109				
Vibrational wavenumbers (cm^{-1})							
150.8	309.9	393.7	429.6	510.2	530.6	559.2	628.4
682.9	794.2	861.4	873.7	906.9	917.6	981.5	1031.2
1041.7	1101.4	1132.2	1152.4	1219.1	1237.8	1289.0	1310.3
1326.1	1361.4	1414.6	1462.0	3123.1	3177.4	3182.2	3627.0
3795.5							
Rotational Constants (GHz):				3.6141	2.4667	2.2090	

TS FMF N-inversion							
Cartesian Coordinates (Å)							
N	0.72705	0.15162	-0.73951				
C	-0.49043	-0.17369	-0.16049				
N	-0.72156	-0.04314	1.04886				
C	-0.91152	0.00533	2.37036				
C	0.97390	0.04528	-2.09201				
H	-1.21957	-0.54467	-0.87895				
H	-1.34441	0.96765	2.68603				
H	2.00658	0.32681	-2.34808				
H	1.46746	0.45847	-0.12983				
O	0.16550	-0.30999	-2.90449				
O	-0.65308	-0.88366	3.14802				
Vibrational wavenumbers (cm^{-1})							
217.6 *i*	59.6	127.5	200.5	223.9	359.1	415.0	634.1
671.3	801.3	1005.2	1016.2	1042.8	1070.5	1095.5	1224.1
1391.6	1415.5	1439.7	1539.0	1754.7	1834.2	1970.7	2988.0
3005.6	3135.4	3644.8					
Rotational Constants (GHz):				14.5916	1.0251	0.9980	

TS direct H-abstraction							
Cartesian Coordinates (Å)							
N	0.15043	-1.98036	-0.92115				
C	0.93100	-1.21646	-0.16734				
C	0.22814	-0.03860	0.33920				
N	-1.11589	-0.36202	-0.06638				
C	-1.06717	-1.44144	-0.84930				
H	1.98523	-1.40441	-0.04237				
H	0.56486	0.86638	-0.33483				
H	-1.92984	-1.82973	-1.36631				
H	-1.90798	0.23959	0.06902				
O	0.40299	0.39337	1.63396				
H	0.45769	1.36233	1.62171				
O	0.75430	2.44006	-0.51742				
O	0.54633	2.97120	0.60121				
Vibrational wavenumbers (cm^{-1})							
505.6 *i*	38.9	111.1	136.7	266.5	290.4	355.8	512.7
590.0	613.8	624.5	708.0	749.3	864.4	896.6	901.1
972.6	1115.2	1152.2	1185.9	1259.4	1262.5	1310.3	1360.9
1392.1	1436.6	1501.4	1540.3	1925.2	3253.4	3259.9	3624.8
3692.0							
Rotational Constants (GHz):				4.2413	1.1984	1.1568	

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