Gas-phase rate coefficient of OH + cyclohexene oxide measured from 251–373 K

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Supplementary information

This section includes additional information on the infrared cross section measurements as well as tabulated kinetic data obtained as part of this study.

FTIR measurements:

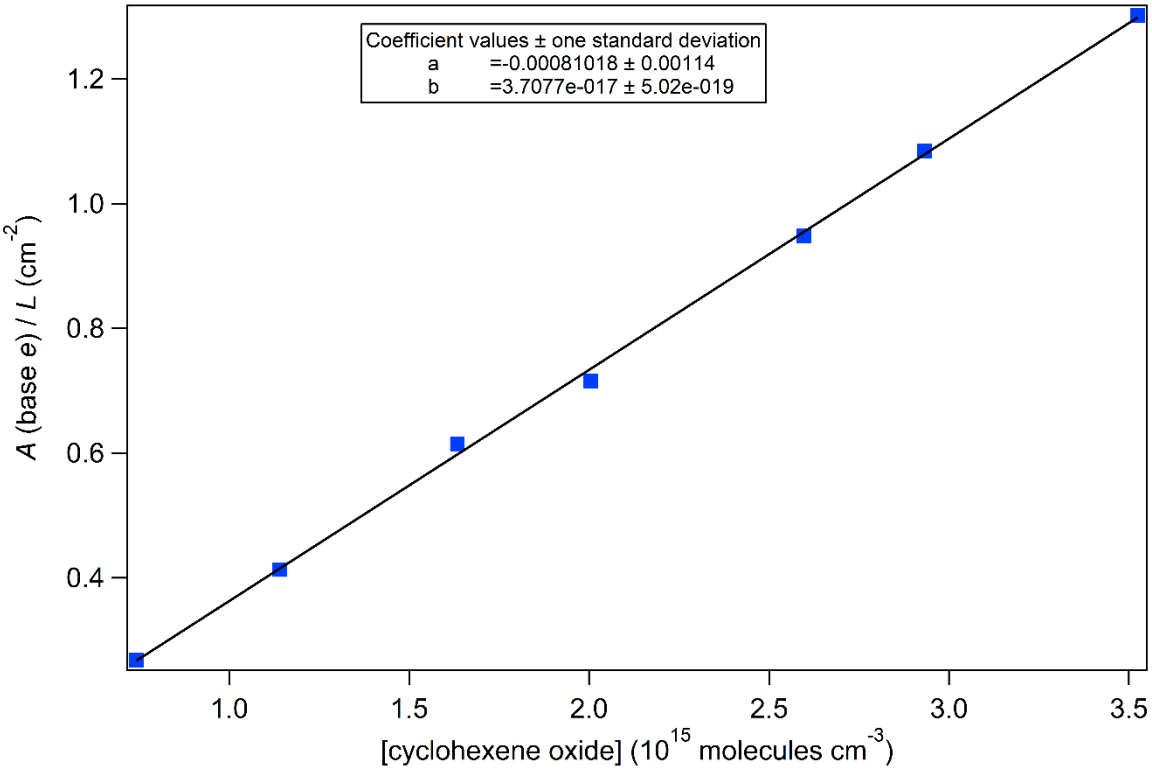

Figure S1: Integrated band intensity measurement of the absorption band of cyclohexene oxide situated between 2800 and 3100 cm^{-1}.

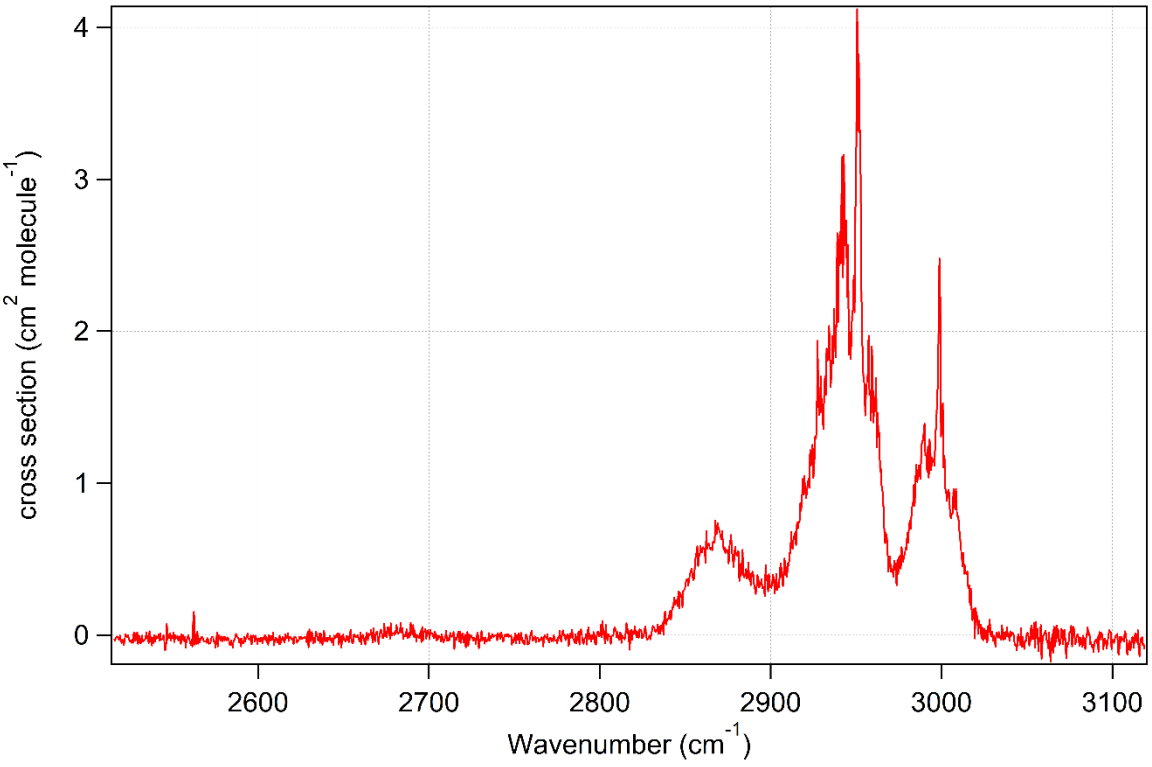

Figure S2: Infrared cross section in the C–H stretch region of the absorption spectrum

Kinetic measurements:

T (K)	P (Torr)	OH source	[OH precursor] (10^{14} molecule cm^{-3})	Photolysis laser fluence (mJ cm^{-2} $pulse^{-1}$)	$[OH]_0$ (10^{11} molecule cm^{-3})	[cyclohexene oxide] (10^{15} molecule cm^{-3})	k' range (s^{-1})	k_d (s^{-1})	(10^{-12}
251	101	HNO_3	6.8	6	1.08	0.34–1.11	2709–11179	164	
253	101	HNO_3	6.7	8	1.38	0.36–0.96	3263–8857	157	
257	101	HNO_3	8.8	11	2.44	0.56–1.31	5029–11268	194	
259	101	HNO_3	11.4	11	3.17	0.33–1.23	2793–9613	244	
263	100	H_2O_2	0.4	11	1.00	0.62–3.15	5328–22626	68	
268	100	H_2O_2	0.5	1	0.14	0.98–3.45	7265–26307	85	
273	100	H_2O_2	0.7	9	1.46	1.0–3.22	7101–23671	116	
274	100	H_2O_2	1.3	1	0.44	0.87–4.72	6504–37165	210	
278	100	H_2O_2	0.8	1	0.27	0.9–4.64	7341–31951	127	
281	100	H_2O_2	1.4	3	1.00	1.19–6.37	8616–43355	235	
282	100	H_2O_2	1.3	2	0.52	1.42–3.50	10170–23206	207	
285	100	H_2O_2	1.5	2	0.72	1.39–3.70	10606–25135	245	
298	100	HNO_3	26.2	9	6.25	1.08–7.58	7497–51156	366	
298	100	H_2O_2	2.1	4	1.82	1.09–7.74	7687–50778	360	
308	100	H_2O_2	1.8	1	0.27	1.06–7.76	6662–47311	305	
335	100	H_2O_2	2.9	56	38.6	0.70–2.16	4793–12777	516	
338	100	H_2O_2	2.8	58	36.4	0.45–3.11	3717–18208	505	
358	100	H_2O_2	1.8	58	23.0	0.62–3.07	3896–18745	327	
373	100	H_2O_2	2.5	58	33.0	0.61–2.95	4119–17606	479	

Table S1: Absolute rate coefficient data and experimental conditions measured using the PLP–LIF apparatus in this work. [OH precursor] is calculated from $k_d/k(T)_{OH}$, where $k(T)_{OH}$ is the temperature-dependent rate coefficient of OH + OH precursor (H_2O_2 or HNO_3)

[Cyclohexene oxide] $\times 10^{13}$molecule/cm^3	**Reference**	**k/k$_{ref}$±error[a]**	**k$_{ref}$**$\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} [b]	**k**$\times 10^{-12}$ cm^3 molecule^{-1} s^{-1} [c]
2.40	1-propanol	1.16±0.01	5.86±0.60	6.79±0.70
2.40	1-propanol	1.20±0.01	5.86±0.60	7.01±0.70

Table S2: Summary of the results from the relative rate study for reaction of cyclohexene-oxide with OH radical at 295±2K.