

Electronic Supplementary Information (ESI)

Atmospheric chemistry of $(\text{CF}_3)_2\text{C}=\text{CH}_2$: OH radicals, Cl atoms and O_3 rate coefficients, oxidation end-products and IR spectra

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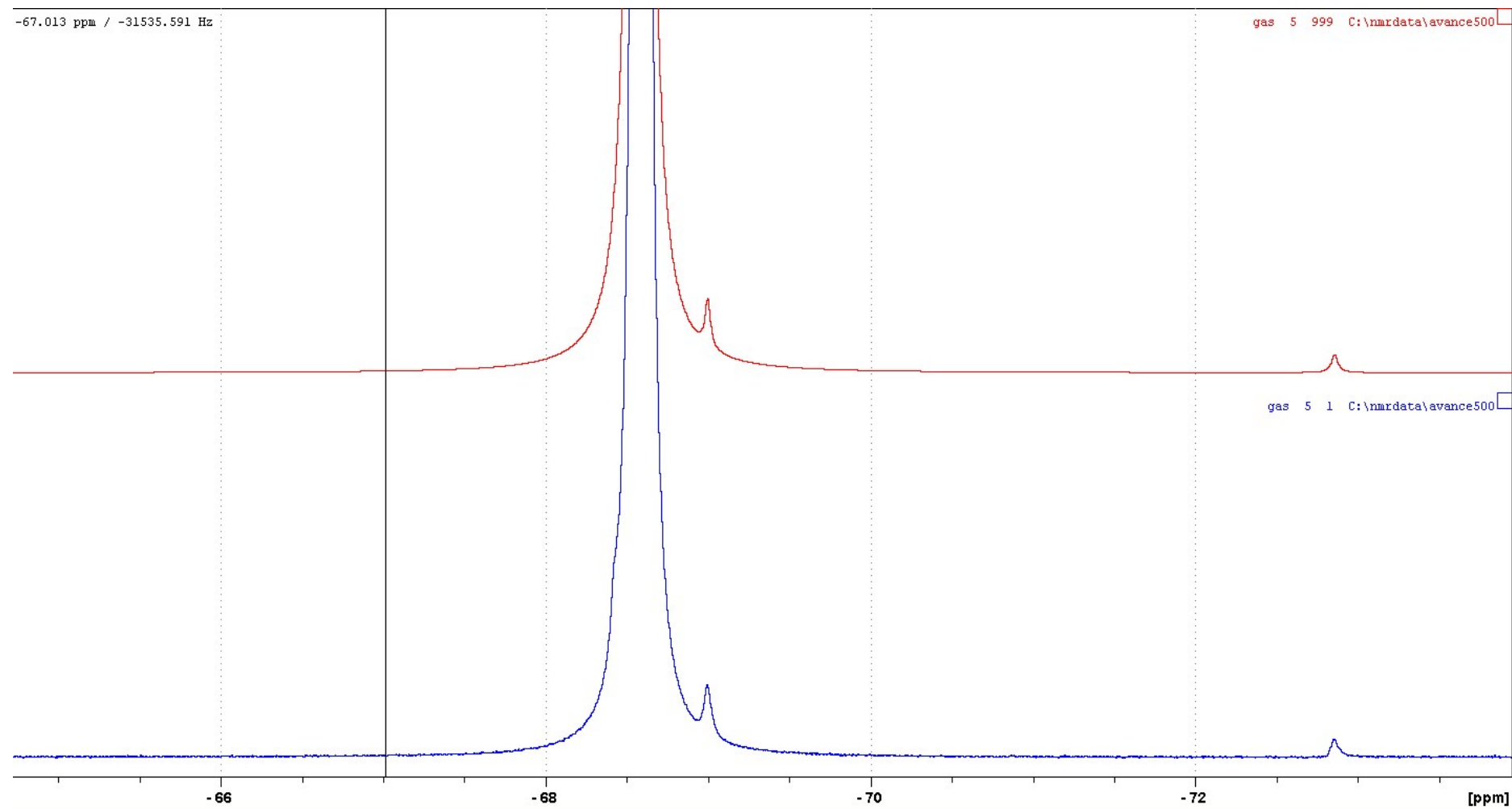
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Figure S1. ^1H and ^{19}F gas-phase NMR spectra of $(\text{CF}_3)_2\text{C}=\text{CH}_2$ and integrated peaks used in purity analysis



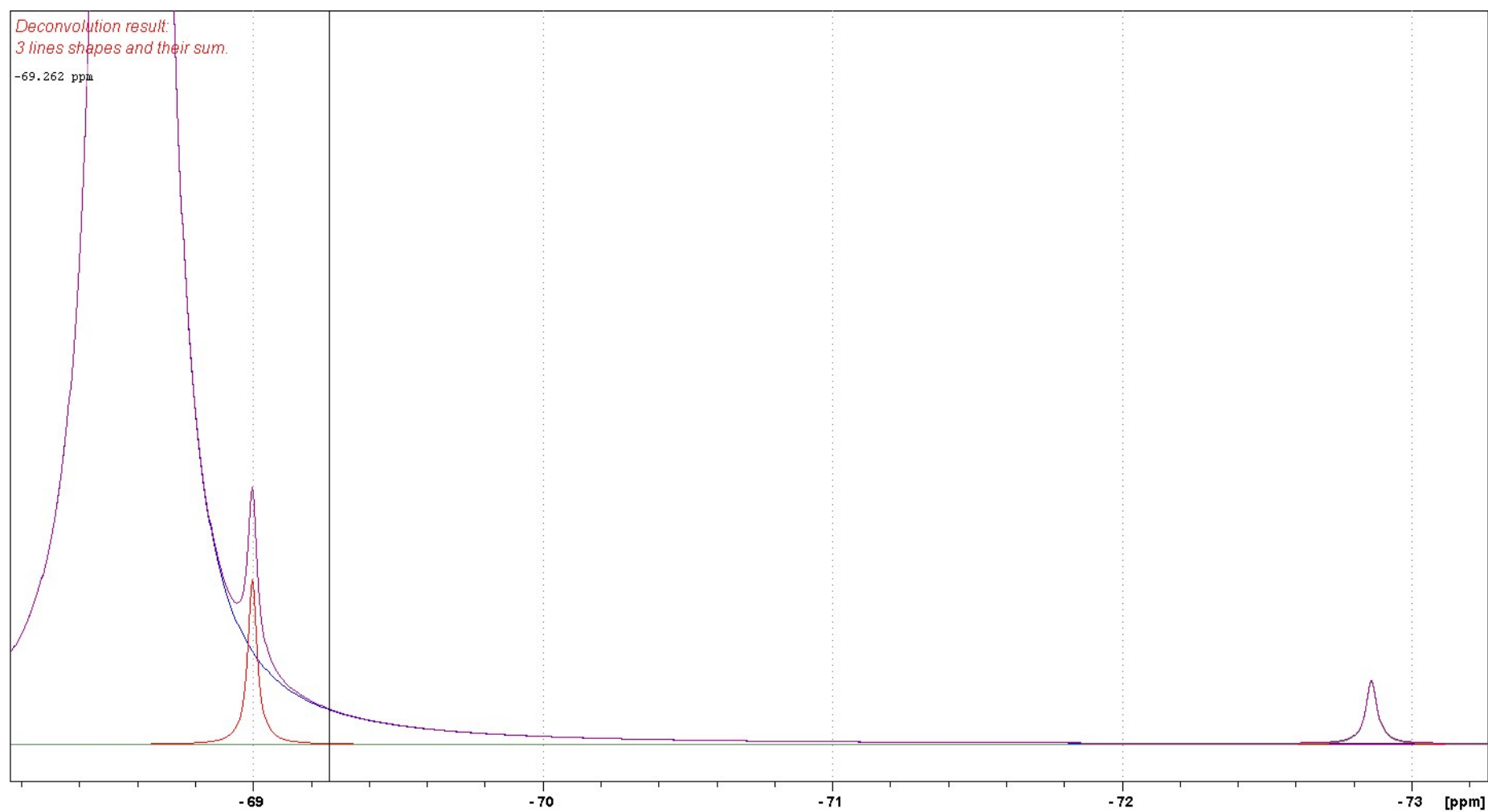


Table S1. ^1H and ^{19}F integrated gas-phase NMR spectra analysis for $(\text{CF}_3)_2\text{C}=\text{CH}_2$. Different ^{19}F analyses correspond to the two scenarios that both detected impurities contain one or two CF_3 groups, respectively. Higher number of CF_3 groups will result in higher purity.

Compound	F-group	^{19}F NMR		F-group	^{19}F NMR		^1H NMR
		Integral	%		Integral	%	%
HFIB	$(\text{CF}_3)_2-$	43.64817	99.41	$(\text{CF}_3)_2-$	43.64817	98.83	98.81
Impurity 1	$(\text{CF}_3)_2-$	0.1785	0.41	$(\text{CF}_3)-$	0.357	0.81	0.89
Impurity 2	$(\text{CF}_3)_2-$	0.080333	0.18	$(\text{CF}_3)-$	0.160667	0.36	0.29
Abundance		43.91	100 %		44.17	100 %	100 %

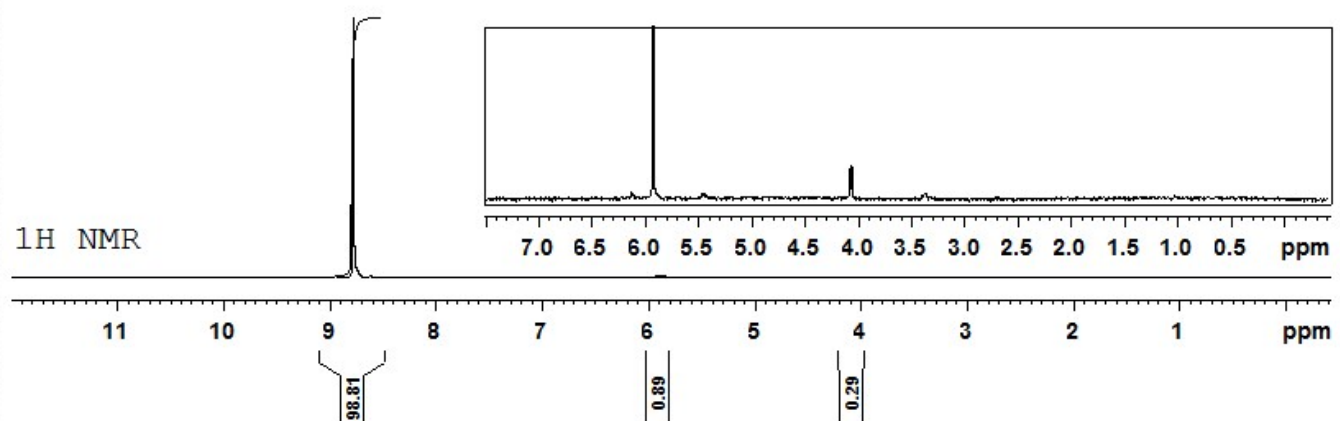
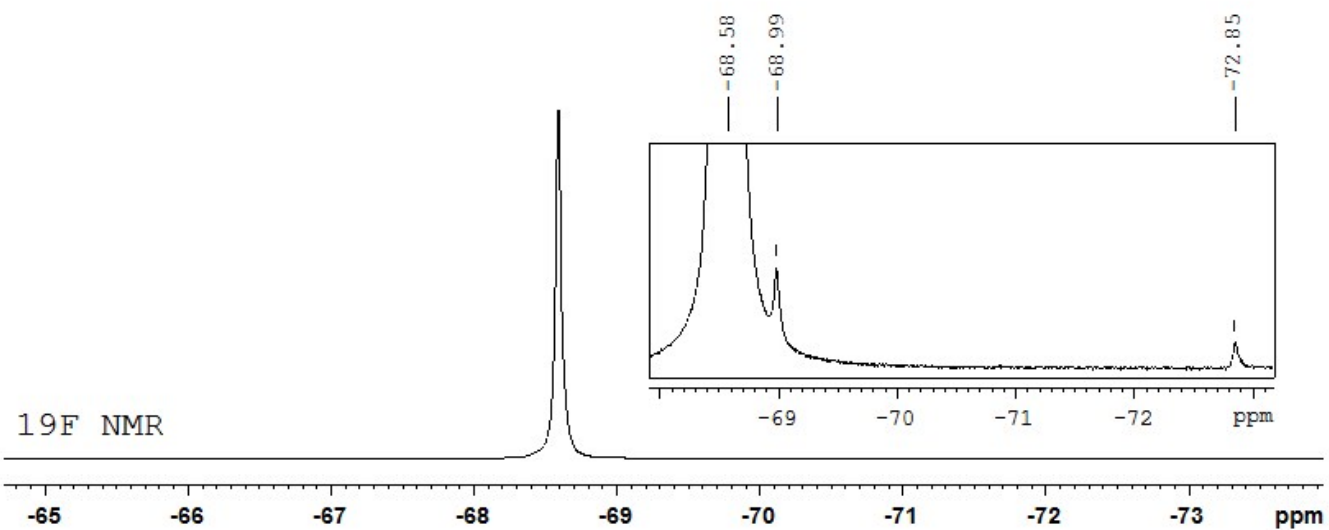


Table S2. Infrared absorption cross-sections of $(\text{CF}_3)_2\text{C}=\text{CH}_2$ at 296 K measured in this work. Cross sections are in units of $\text{cm}^2 \text{ molecule}^{-1}$ (base e).

Wavenumber (cm^{-1})	HFIB IR Cross-Section ($\text{cm}^2 \text{ molecule}^{-1}$)
599.9943	1.212110765599998e-21
600.2354	2.884818919267847e-21
600.4764	3.80160108990536e-21
600.7175	3.858108893870514e-21
600.9585	3.249239143200729e-21
601.1996	2.492945749221335e-21
601.4406	2.320387522886653e-21
601.6817	3.173302648249377e-21
601.9227	4.591938782424489e-21
602.1638	5.328487512001494e-21
602.4048	4.341731926115843e-21
602.6459	1.787748195927467e-21
602.8879	0
603.1281	0
603.3691	0
603.6102	1.965957202658664e-21
603.8512	3.299993291703631e-21
604.0923	2.523635585796168e-21
604.3333	2.764245668115412e-22
604.5744	0
604.8154	0
605.0565	0
605.2975	2.451997798948797e-22
605.5386	5.785877402484067e-22
605.7797	0
606.0208	0
606.2618	0
606.5029	0
606.7439	0
606.985	2.755541702732223e-22
607.226	5.123508943521916e-22
607.4671	6.727257736161028e-22
607.7081	5.794254372122595e-22
607.9492	0
608.1902	0
608.4313	0
608.6724	0
608.9135	0
609.1545	0
609.3956	0
609.6366	0
609.8777	0
610.1187	0
610.3598	0
610.6008	4.961517456082149e-22
610.8419	1.321782933893875e-21
611.0829	8.957478938039303e-22
611.324	0
611.5651	0
611.8062	0
612.0472	0
612.2883	0

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613.0114	2.17905922722192e-21
613.2525	1.505455341437568e-21
613.4935	1.142897891016411e-21
613.7346	8.7820034687691e-22
613.9756	0
614.2167	0
614.4578	0
614.6989	0
614.9399	0
615.181	2.327456509546533e-21
615.422	6.706058124400369e-21
615.6631	8.893953584947138e-21
615.9041	7.983178583326726e-21
616.1452	5.188761128074654e-21
616.3862	2.921464487326913e-21
616.6273	2.789200219775446e-21
616.8683	4.634154300471277e-21
617.1094	7.068472284551393e-21
617.3505	8.491454890253864e-21
617.5916	8.027929236922019e-21
617.8326	6.027817512438902e-21
618.0737	3.578211558768474e-21
618.3147	1.534620422573809e-21
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622.4127	4.975221884482019e-21
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696.1766	4.59825825074829e-21

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696.8997	2.858277152307881e-21
697.1408	6.27192534699318e-22
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