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Experimental Determination of the Global Warming Potential of Carbonyl Fluoride (COF_2)

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This Supporting Information provides additional data and methodological details not included in the main text but essential for the discussion of the study titled "Experimental Determination of the Global Warming Potential of Carbonyl Fluoride (COF_2)." These materials support the interpretation of Fourier Transform Infrared (FTIR) measurements, data processing procedures, and uncertainty analysis applied in this work.

Figure S1 demonstrates the linearity of COF_2 absorbance with pressure. **Figure S2** and **Table S1** provide a band-resolved comparison of the infrared absorption cross-section spectra and integrated absorption cross-sections of COF_2 derived from the PNNL experimental spectrum, the present FTIR measurements, and the HITRAN line-by-line data. **Figures S3** and **S4** present FTIR absorbance spectra associated with atmospheric chemical reactions under humid morning and drier afternoon conditions, respectively, including original, background, and corrected spectra that resolve NF_3 absorption and characteristic reaction-product bands. **Table S2** summarizes the uncertainty budget for the ACS of COF_2 obtained from FTIR measurements, including the equation for the combined relative standard uncertainty and the resulting combined and expanded relative standard uncertainties ($k = 2$).

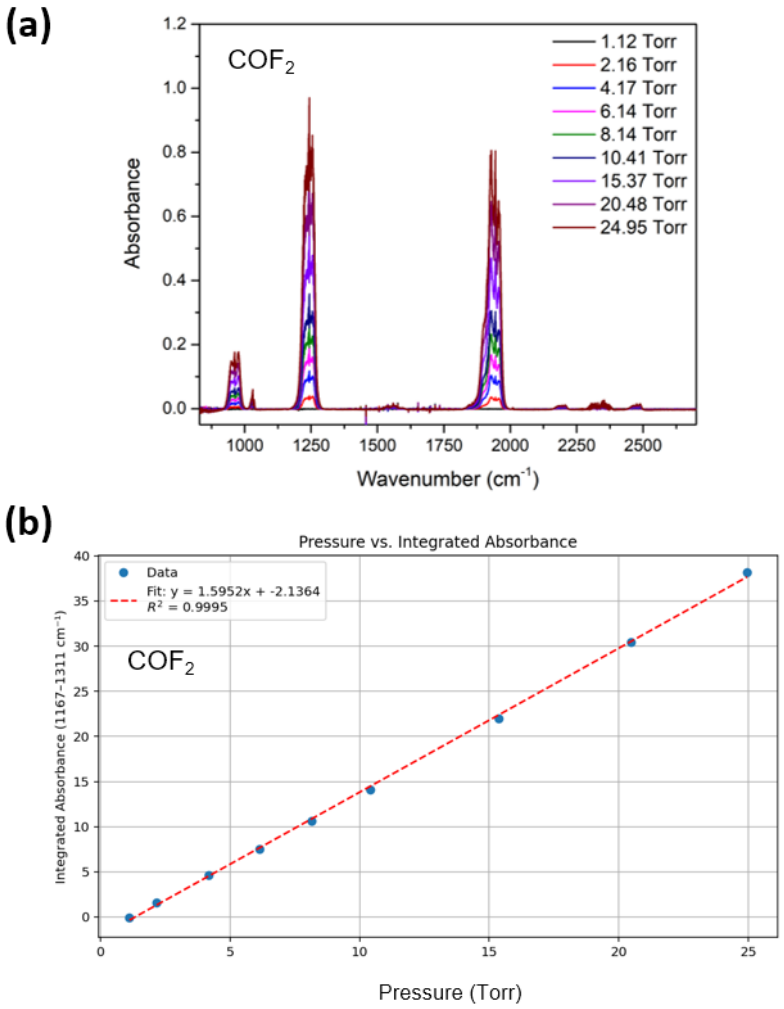

Figure S1. Linearity of COF_2 absorbance with pressure. (a) FTIR spectra of COF_2 at various pressures (from 1.12 to 24.95 Torr) showing the absorbance peaks across different wavenumbers. (b) Integrated absorbance values (1617-1311 cm^{-1}) plotted against pressure, demonstrating a strong linear relationship with a correlation coefficient (R^2) of 0.9995. The red dashed line represents the linear fit with the equation: $y = 1.5952x + 2.1364$.

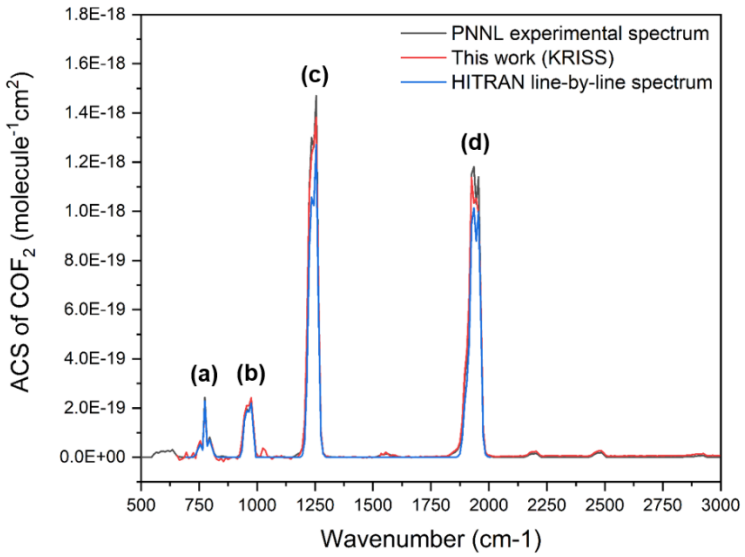

Figure S2. Band-resolved comparison of the infrared absorption cross-section spectra of COF_2 derived from the PNNL experimental spectrum, the present FTIR measurements (KRISS, Korea Research Institute of Standards and Science), and the HITRAN line-by-line data. The annotated regions **(a)**–**(d)** indicate the four infrared bands represented in the HITRAN database, corresponding to 695–865, 925–995, 1175–1305, and 1845–2005 cm^{-1}, respectively. The spectra are shown for qualitative comparison of band-specific differences among the datasets.

Table S1. Band-resolved integrated absorption cross-sections of COF_2 for the four infrared bands represented in the HITRAN database, comparing values derived from the PNNL experimental spectrum, the present FTIR measurements (KRISS, Korea Research Institute of Standards and Science), and the HITRAN line-by-line data. Integrated absorption cross-sections are given in units of cm $molecule^{-1}$. The relative differences—calculated as (Experimental Value – HITRAN) / Experimental Value —are provided for both this work and the PNNL dataset to quantify the band-specific underestimation in the HITRAN line-by-line representation

	Integrated absorption cross-sections (cm $molecule^{-1}$)			
	Band 1 (695-865 cm^{-1})	Band 2 (925-995 cm^{-1})	Band 3 (1175-1305 cm^{-1})	Band 4 (1845-2005 cm^{-1})
PNNL	5.86×10^{-18}	9.67×10^{-18}	6.56×10^{-17}	6.82×10^{-17}
This work (KRISS)	5.29×10^{-18}	1.06×10^{-17}	6.46×10^{-17}	6.74×10^{-17}
HITRAN	5.31×10^{-18}	8.74×10^{-18}	5.28×10^{-17}	5.61×10^{-17}
Relative Difference (PNNL – HITRAN)	9%	10%	19%	18%
Relative Difference (This work – HITRAN)	0%	18%	18%	17%

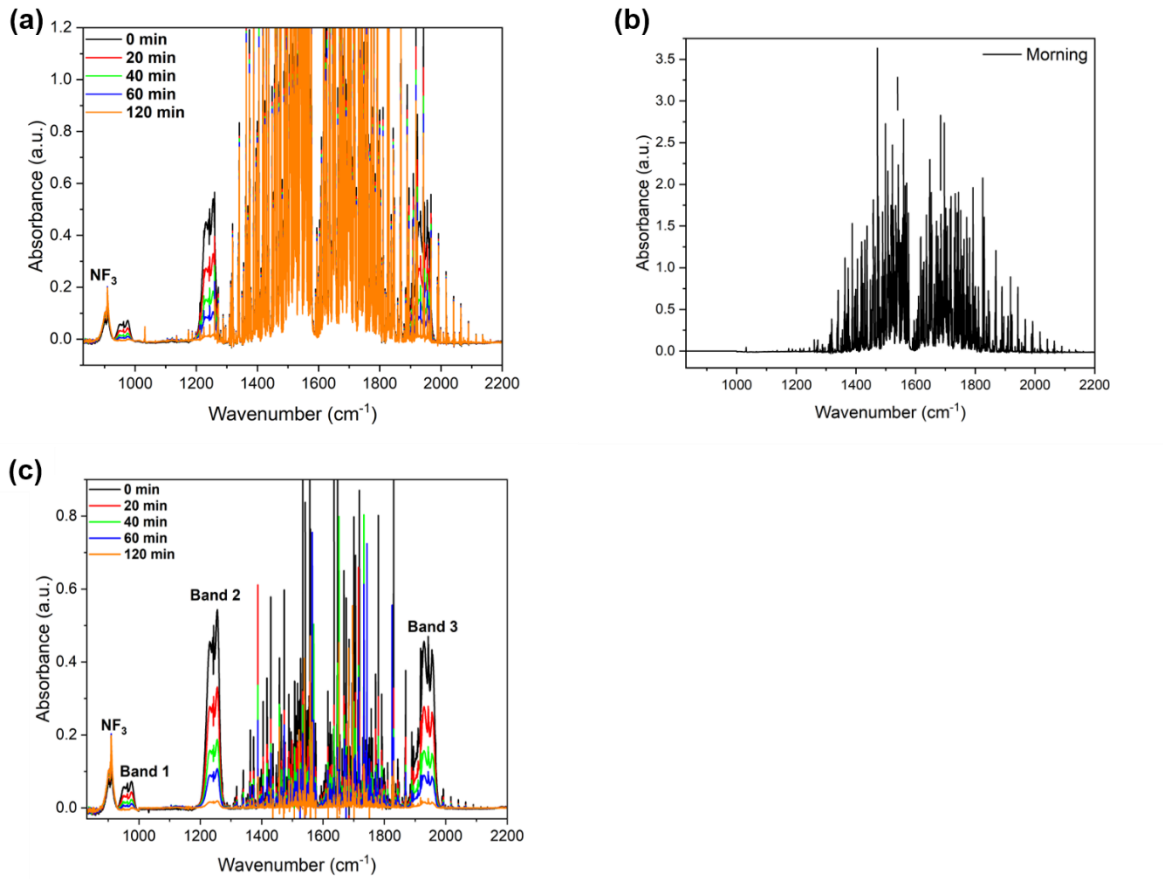

Figure S3. FTIR absorbance spectra associated with the atmospheric chemical reaction under humid morning conditions. (a) Original spectra collected at different reaction times (0–120 min), showing the evolution of absorption features. (b) Background spectrum of atmospheric water vapor recorded in the morning with higher humidity. (c) Corrected spectra obtained by subtracting (b) from (a), clearly resolving NF_3 absorption and three characteristic bands (Band 1–3) of the reaction products.

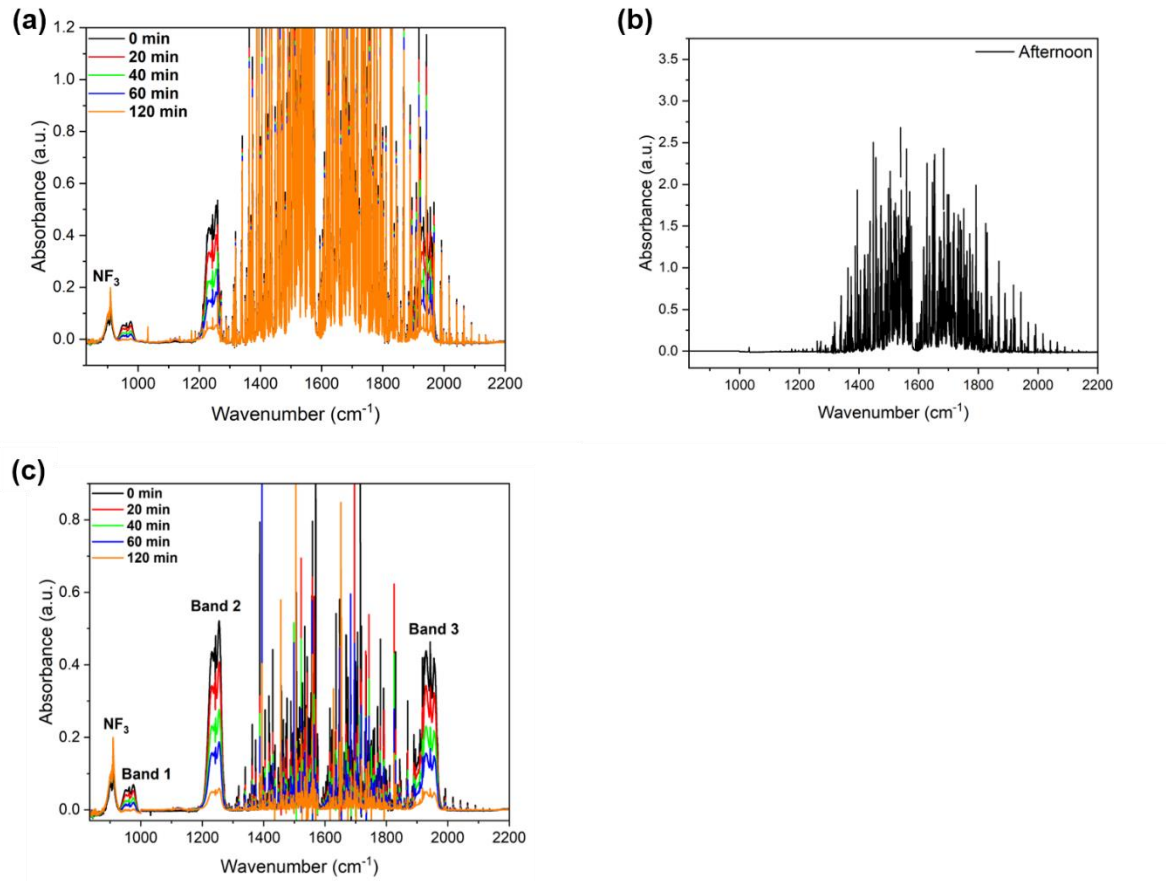

Figure S4. FTIR absorbance spectra associated with the atmospheric chemical reaction under drier afternoon conditions. (a) Original spectra collected at different reaction times (0–120 min), showing the evolution of absorption features. (b) Background spectrum of atmospheric water vapor recorded in the afternoon with lower humidity. (c) Corrected spectra obtained by subtracting (b) from (a), clearly resolving NF_3 absorption and three characteristic bands (Band 1–3) of the reaction products.

Table S2. Uncertainty budget for the ACS of COF_2 obtained from FTIR measurements, including input quantities, relative standard uncertainties, the equation for the combined relative standard uncertainty, and the resulting combined and expanded relative standard uncertainties (k = 2).

Quantity	Symbol	Value (mean)	Standard deviation	Relative uncertainty (RSD %)
Total pressure	P_{Total}	40.244 Torr	0.002 Torr	0.0047 %
Temperature	T	296.770 K	0.014 K	0.059 %
Optical path length	L	2.4000 m	0.0065 m	0.27 %
COF_2 mole fraction	x_{COF2}	3360.0 ppm	33.5 ppm	1.0 %
FTIR transmittance	Tr	0.9950	0.0063	0.63 %
Equation for combined relative standard uncertainty	$\left(\frac{u(\sigma)}{\sigma}\right)^2 = \left(\frac{u(T)}{T}\right)^2 + \left(\frac{u(P_{Total})}{P_{Total}}\right)^2 + \left(\frac{u(x_{COF2})}{x_{COF2}}\right)^2 + \left(\frac{u(L)}{L}\right)^2 + \left(\frac{u(Tr)}{Tr \cdot \ln(1/Tr)}\right)^2$			
Combined relative standard uncertainty (%)	≈ 2.1 %			
Expanded relative standard uncertainty (%, k = 2)	≈ 4.2 %			