# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PF1



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## HC(O)F + hν → products

### Primary photochemical transitions

| Reaction | | | $\Delta H°$/kJ·mol$^{-1}$ | $\lambda_{threshold}$/nm |
|---|---|---|---|---|
| HC(O)F + hν | → HF + CO | (1) | 8.7 | 13,800 |
| | → H + FCO | (2) | 458 | 261 |
| | → F + HCO | (3) | 515 | 232 |

### Absorption cross-section data

| Wavelength range/nm | References | Comments |
|---|---|---|
| 200-340 | Rattigan et al., 1994 | (a) |
| 200-370 | Meller and Moortgat, 1992 | (b) |

### Comments

(a) The absorption spectrum of HC(O)F was studied using a purified sample of HC(O)F and recorded by diode array spectroscopy with a resolution of 1.2 nm. The characteristic banded structure was recorded and the absolute cross-section at 230 nm was $\sigma = 6.65 \times 10^{-20}$ cm$^2$ molecule$^{-1}$ using this resolution. The cross-section was independent of temperature in the range 233-318 K, in agreement with the earlier work of Giddings and Innes (1961).

(b) Measurements of the spectrum of HC(O)F at a resolution of 0.02 nm. The spectrum consists of a vibrational progression of many sharp bands, with an origin of structured absorption at 268 nm and a maximum intensity near 210 nm. The maximum value of $\sigma = 1.5 \times 10^{-19}$ cm$^2$ molecule$^{-1}$ was observed at this resolution, which is in reasonable agreement with the earlier work of Giddings and Innes (1961) who reported an absorption coefficient of approximately 50 l mol$^{-1}$ cm$^{-1}$ ($\sigma = 1.9 \times 10^{-19}$ cm$^2$ molecule$^{-1}$) at the maximum.

### Quantum yield data

There are no reported quantum yield data. Klimeck and Berry (1973) have observed infrared laser emission from HF* following flash photolysis of HC(O)F ($\lambda > 165$ nm), indicating the occurrence of reactions (1) and/or (3). Reed et al. (1997) and Maul et al. (1999) have used H-atom photofragment translational spectroscopy in a pulsed molecular beam to study H atoms formed by channel (2) at ~243-247 nm.

## Preferred Values

### Absorption cross-sections for HC(O)F at 298 K

| λ/nm | $10^{20}$ σ/cm$^2$ | λ/nm | $10^{20}$ σ/cm$^2$ | λ/nm | $10^{20}$ σ/cm$^2$ |
|---|---|---|---|---|---|
| 200 | 8.28 | 223 | 6.58 | 245 | 0.67 |
| 201 | 9.75 | 224 | 4.94 | 246 | 0.72 |
| 202 | 8.3 | 225 | 5.33 | 247 | 0.41 |
| 203 | 7.55 | 226 | 4.00 | 248 | 0.48 |
| 204 | 8.52 | 227 | 4.65 | 249 | 0.28 |
| 205 | 10.15 | 228 | 4.43 | 250 | 0.21 |
| 206 | 8.28 | 229 | 4.61 | 251 | 0.15 |
| 207 | 7.41 | 230 | 3.57 | 252 | 0.24 |
| 208 | 8.44 | 231 | 2.55 | 253 | 0.21 |
| 209 | 9.55 | 232 | 3.16 | 254 | 0.07 |
| 210 | 7.76 | 233 | 3.09 | 255 | 0.12 |
| 211 | 7.36 | 234 | 2.98 | 256 | 0.07 |
| 212 | 7.92 | 235 | 2.04 | 257 | 0.05 |
| 213 | 8.56 | 236 | 2.28 | 258 | 0.04 |
| 214 | 9.22 | 237 | 1.24 | 259 | 0.04 |
| 215 | 7.67 | 238 | 1.71 | 260 | 0.04 |
| 216 | 6.51 | 239 | 1.75 | 261 | 0.02 |
| 217 | 7.38 | 240 | 1.55 | 262 | 0.02 |
| 218 | 7.97 | 241 | 0.97 | 263 | 0.02 |
| 219 | 6.28 | 242 | 1.19 | 264 | 0.02 |
| 220 | 6.85 | 243 | 0.57 | 265 | 0.01 |
| 221 | 5.7 | 244 | 0.76 | 266 | 0.01 |
| 222 | 6.07 | | | | |

### Quantum yields for HC(O)F

No recommendation.

*Comments on Preferred Values*

The preferred values for the cross-sections are based on the data for the absolute absorption cross-sections reported by Meller and Moortgat (1992). The listed values are averaged over 1 nm. The cross-sections of Rattigan et al. (1994) are higher than those of Meller and Moortgat (1992) by approximately a factor of 2 at 230 nm. Although the two studies are nominally at comparable resolution, the Rattigan et al. (1994) spectrum does not appear to contain all the features reported by Meller and Moortgat (1992), indicating possible errors.

## References


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