

Infrared Molecular Absorption Cross-sections

The folder IR-XSect contains files of infrared cross-sections. The definition and units have been described in articles about the HITRAN compilation. Each molecule is placed in a single file. Within that file are sets of temperature and pressure pairs. The sets have a header that provides information to programs reading the data and also points to a reference for that observation. The sets contain absorption cross-sections that are in equal wavenumber (cm^{-1}) increments, and the intervals can be determined by the minimum and maximum wavenumber and the number of points, namely

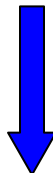
$$\Delta V = \frac{V_{\max} - V_{\min}}{npts - 1}$$

where ν_{\max} is the maximum (final) wavenumber of the set, ν_{\min} is the minimum (initial) wavenumber of the set, and $npts$ is the number of points in the set. The format of the header is given below.

| Cross-section Header Format | | | | | | | | | | | | |
|-----------------------------|--|------------|-----|------|------|--------|-----------|------|-------------|------|----|-----|
| Chemical symbol | | Wavenumber | | No. | Temp | Press | Max | Res. | Common Name | Not | Br | Ref |
| | | Min | Max | Pts. | [K] | [torr] | X-section | | | used | | No |
| 20 | | 10 | 10 | 7 | 7 | 6 | 10 | 5 | 15 | 4 | 3 | 3 |
| 10 | | 20 | 30 | 40 | 50 | 60 | 70 | 80 | 90 | | | |

Note: **Chemical Symbol** is right adjusted; **Res.** is resolution in cm^{-1} for FTS measurements, and in milli-Angstroms for grating measurements in the UV ($\text{xxxm}\text{\AA}$), and **Br** indicates any broadening gas, such as air.

A summary of the molecules represented with their temperature and pressures ranges and spectral coverage is given in the table on the following pages:



Summary of Molecules Represented by Infrared Cross-section Data in HITRAN

| Molecule | Common Name | Temperature Range (K) | Pressure Range (torr) | Number of T,P sets | Spectral Coverage (cm ⁻¹) |
|---|------------------------------|--------------------------|-----------------------------|--------------------------|---|
| SF ₆ | Sulfur hexafluoride | 180-295 | 20-760 | 32 | 925-955 |
| ClONO ₂ | Chlorine nitrate | 189-297 | 0-117 | 25 | 750-830 |
| | | 189-297 | 0-117 | 25 | 1260-1320 |
| | | 213-296 | 0 | 2 | 1680-1790 |
| CCl ₄ | Carbon tetrachloride | 208-297 | 8-760 | 32 | 750-812 |
| N ₂ O ₅ | Dinitrogen pentoxide | 205-293 | 0 | 5 | 540-1380 |
| HNO ₄ | Peroxynitric acid | 220 | 0 | 1 | 780-830 |
| C ₂ F ₆ | Hexafluoroethane, CFC-116 | 181-296 | 25-760 | 43 | 1061-1165 |
| | | 181-296 | 25-760 | 43 | 1220-1285 |
| CCl ₃ F | CFC-11 | 190-296 | 8-760 | 55 | 810-880 |
| | | 190-296 | 8-760 | 55 | 1050-1120 |
| CCl ₂ F ₂ | CFC-12 | 190-296 | 8-760 | 52 | 850-950 |
| | | 190-296 | 8-760 | 52 | 1050-1200 |
| CClF ₃ | CFC-13 | 203-293 | 0 | 6 | 765-805 |
| | | 203-293 | 0 | 6 | 1065-1140 |
| | | 203-293 | 0 | 6 | 1170-1235 |
| CF ₄ | CFC-14 | 180-296 | 8-761 | 55 | 1250-1290 |
| C ₂ Cl ₂ F ₃ | CFC-113 | 203-293 | 0 | 6 | 780-995 |
| | | 203-293 | 0 | 6 | 1005-1232 |
| C ₂ Cl ₂ F ₄ | CFC-114 | 203-293 | 0 | 6 | 815-860 |
| | | 203-293 | 0 | 6 | 870-960 |
| | | 203-293 | 0 | 6 | 1030-1067 |
| | | 203-293 | 0 | 6 | 1095-1285 |
| C ₂ ClF ₅ | CFC-115 | 203-293 | 0 | 6 | 955-1015 |
| | | 203-293 | 0 | 6 | 1110-1145 |
| | | 203-293 | 0 | 6 | 1167-1260 |
| CHCl ₂ F | HCFC-21 | 296 | 1 | 1 | 785-840 |
| CHClF ₂ | HCFC-22 | 181-297 | 0-765 | 29 | 760-860 |
| | | 181-296 | 22-761 | 31 | 1070-1195 |
| | | 253-287 | 0 | 3 | 1060-1210 |
| | | 253-287 | 0 | 3 | 1275-1380 |
| CHCl ₂ CF ₃ | HCFC-123 | 253-287 | 0 | 3 | 740-900 |
| | | 253-287 | 0 | 3 | 1080-1450 |

| | | | | | |
|---|---|---------|--------|----|-----------|
| CHClFCF ₃ | HCFC-124 | 287 | 0 | 1 | 675-715 |
| | | 287 | 0 | 1 | 790-920 |
| | | 287 | 0 | 1 | 1035-1430 |
| CH ₃ CCl ₂ F | HCFC-141b | 253-287 | 0 | 3 | 710-790 |
| | | 253-287 | 0 | 3 | 895-1210 |
| | | 253-287 | 0 | 3 | 1325-1470 |
| CH ₃ CClF ₂ | HCFC-142b | 253-287 | 0 | 3 | 650-705 |
| | | 253-287 | 0 | 3 | 875-1265 |
| | | 253-287 | 0 | 3 | 1360-1475 |
| CHCl ₂ CF ₂ CF ₃ | HCFC-225ca | 253-287 | 0 | 3 | 695-865 |
| | | 253-287 | 0 | 3 | 1010-1420 |
| CClF ₂ CF ₂ CHClF | HCFC-225cb | 253-287 | 0 | 3 | 715-1375 |
| CH ₂ F ₂ | HFC-32 | 203-297 | 0-750 | 17 | 995-1236 |
| | | 203-297 | 0-750 | 17 | 1385-1475 |
| CHF ₂ CF ₃ | HFC-125 | 287 | 0 | 1 | 700-745 |
| | | 287 | 0 | 1 | 840-890 |
| | | 287 | 0 | 1 | 1060-1465 |
| CHF ₂ CHF ₂ | HFC-134 | 203-297 | 0-750 | 9 | 600-1700 |
| CFH ₂ CF ₃ | HFC-134a | 253-287 | 0 | 3 | 815-865 |
| | | 190-296 | 20-760 | 32 | 1035-1130 |
| | | 190-296 | 20-760 | 33 | 1135-1340 |
| | | 253-287 | 0 | 3 | 935-1485 |
| CF ₃ CH ₃ | HFC-143a | 203-297 | 0-750 | 9 | 580-630 |
| | | 203-297 | 0-750 | 9 | 750-1050 |
| | | 203-297 | 0-750 | 9 | 1100-1500 |
| CH ₃ CHF ₂ | HFC-152a | 253-287 | 0 | 3 | 840-995 |
| | | 253-287 | 0 | 3 | 1050-1205 |
| | | 253-287 | 0 | 3 | 1320-1490 |
| SF ₅ CF ₃ | Trifluoromethyl sulfur pentafluoride | 213-323 | 760 | 5 | 599-624 |
| | | 213-323 | 760 | 5 | 676-704 |
| | | 213-323 | 760 | 5 | 740-766 |
| | | 213-323 | 760 | 5 | 860-920 |
| | | 213-323 | 760 | 5 | 1150-1280 |
| | | 213-323 | 760 | 5 | 1280-2600 |

Note: These data are in the main directory. Additional redundant data for CFC-11 and CFC-12 are stored in a supplemental sub-directory.