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 (ten to a line from left to right) 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

$$\Delta\nu = \frac{\nu_{max} - \nu_{min}}{npts - 1}$$

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 Min	Wavenumber Max	No. Pts.	Temp [K]	Press [torr]	Max X-section	Res.	Common Name	Not used	Br	Ref 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 **Br** indicates the broadening gas, such as air.

The \Supplemental folder contains two types of files: (1) some older, redundant cross-section data that have nonetheless been retained, and (2) data that have some small experimental negative cross-sections that were zeroed out for the files in the main directory (some users prefer these files as they do not introduce any bias). The extension for file names is ".xsc" for the former, and ".alt" for the latter.

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_2O_5	Dinitrogen pentoxide	205-293	0	5	540-1380
HNO_4	Peroxynitric acid	220	0	1	780-830
C_2F_6	Hexafluoroethane, CFC-116	181-296	25-760	43	1061-1165
		181-296	25-760	43	1220-1285
CCl_3F	CFC-11	190-296	8-760	55	810-880
		190-296	8-760	55	1050-1120
CCl_2F_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
$C_2Cl_2F_3$	CFC-113	203-293	0	6	780-995
		203-293	0	6	1005-1232
$C_2Cl_2F_4$	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_2ClF_5	CFC-115	203-293	0	6	955-1015
		203-293	0	6	1110-1145
		203-293	0	6	1167-1260
$CHCl_2F$	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
$CHCl_2CF_3$	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_3CCl_2F	HCFC-141b	253-287	0	3	710-790
		253-287	0	3	895-1210
		253-287	0	3	1325-1470
$CHCl_2CF_2CF_3$	HCFC-225ca	253-287	0	3	695-865
		253-287	0	3	1010-1420
$CClF_2CF_2CHClF$	HCFC-225cb	253-287	0	3	715-1375
CH_2F_2	HFC-32	203-297	0-750	17	995-1236
		203-297	0-750	17	1385-1475
CHF_2CF_3	HFC-125	287	0	1	700-745
		287	0	1	840-890
		287	0	1	1060-1465
CHF_2CHF_2	HFC-134	203-297	0-750	9	600-1700
CFH_2CF_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_3CH_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_3CHF_2	HFC-152a	253-287	0	3	840-995
		253-287	0	3	1050-1205
		253-287	0	3	1320-1490
SF_5CF_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
$CH_3C(O)OONO_2$	PAN	295	0.08	1	1650-1901
CH_3CN	Acetonitrile (methyl cyanide)	276-324	760	3	624-784
		276-324	760	3	867-1159
		276-324	760	3	1175-1687
		276-324	760	3	2217-2343
		276-324	760	3	2786-3261
		276-324	760	3	3881-4574
New data introduced since HITRAN2008					
C_2H_6	Ethane	194-297	49-763	14	2545-3315
CH_3OH	Methanol	204-295	50-761	12	877-1167
		204-296	51-761	12	2600-3250
CH_3CN	Acetonitrile	203-297	50-760	12	880-1700
		208-296	50-760	11	2550-3300
C_3H_8	Propane	195-296	40-763	12	2540-3300
CH_3COCH_3	Acetone	194-298	50-700	19	830-1950
		195-296	49-759	12	2615-3300

$CH_3C(O)OONO_2$	PAN	250-295	0	3	560-1400
		250	0	1	1590-2200
CH_3CHO	Acetaldehyde	200-297	50-762	16	2400-3400
CH_3CClF_2	HCFC-142b	223-283	0	7	650-1500
$BrONO_2$	Bromine nitrate	218-296	0	2	770-843
ClOOCl	Chlorine peroxide	225-250	15-33	4	500-835

Notes: These data are in the main directory. Additional redundant data for CFC-11, CFC-12, HFC-125, and HFC-143a are stored in a supplemental sub-directory.