Infrared Molecular Absorption Cross-sections

In the folder IR_XSECT\ are placed files of IR cross-sections, the definition and units being described in previous articles on the database.[a] Each portion of the cross-section files, i.e., a set with a temperature and pressure pair, contains a header that points to the reference for that observation and other relevant information. 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 given in the header and the number of points, i.e.,

$$\Delta n = (n_{max} - n_{min})/(npts - 1),$$

where n_{max} is the maximum wavenumber of the set, n_{min} is the minimum wavenumber of the set, and *npts* is the number of points in the set. The new format is quite similar to what we had before, except that the field length for the chemical symbol has been increased from 10 to 20 (there is already one compound that requires 13 characters), the number of points and temperature fields have been reduced from 10 to 7, and the pressure field has been reduced to 6. Previously the last 30 characters were rather undefined, although there was an indicator for the reference. Now we have put in the resolution of the observation. For Fourier transform spectrometer observations (all of the IR data), this will be in wavenumber. For grating spectrometer observations (presently only for some UV data), we employ *xxx*mA (where *xxx* is a number and mA indicates milli-Angstroms). Since some of the experiments were done in air, we have a field in which we put "air" (blank indicates "pure gas"). Finally, there is an integer pointer at the end for the references, which we will manage in the HAWKS software as well as providing an acrobat file (/Documentation/ReferenceTable.pdf) for those not using HAWKS.

Following is the format of the headers in the current edition:

"2000" Cross-section Header format:

Chemical symbol	Wavenumber Minimum	Wavenumber Maximum	Number Of pts.	Temp. [K]	Press. [Torr]	Maximum X-section	Res.	Common Name	Not used	Broad.	Ref No
20	10	10	7	7	6	10	5	15	4	3	3

10 20 30 40 50 60 70 80 90 100

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 (*xxx*mÅ)

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

Molecule	Common Name	Temperature Range (K)	Pressure Range (Torr)	Number of *P,T* sets	Spectral Coverage (cm^{-1})	Reference
SF_6	Sulfur hexafluoride	180-295	20-760	32	925-955	f, j
$ClONO_2$	Chlorine nitrate	213-296	0	2	740–840	e
		213-296	0	2	1240-1340	
		213-296	0	2	1680-1790	
CCl_4	Carbon tetrachloride	208-297	8-760	32	750-812	j
N_2O_5	Dinitrogen pentoxide	233-293	0	4	555-600	d
		233-293	0	4	720-765	
		233-293	0	4	1210-1275	
		233-293	0	4	1680-1765	
C_2F_6	Hexafluoro-Ethane	181-296	25-760	43	1061-1165	j
		181-296	25-760	43	1220-1285	
HNO_4	Pernitric acid	268	0.7	1	770-830	b
CCl_3F	CFC-11	201-296	40-760	55	810-880	j
		201-296	40-760	55	1050-1120	
CCl_2F_2	CFC-12	190-296	7.5-760	52	850-950	j
		190-296	7.5-760	52	1050-1200	
$CClF_3$	CFC-13	203-293	0	6	765-805	c
		203-293	0	6	1065-1140	
		203-293	0	6	1170-1235	
CF_4	CFC-14	180-296	7.5-761	55	1250-1290	j
$C_2Cl_2F_3$	CFC-113	203-293	0	6	780-995	c
		203-293	0	6	1005-1232	
$C_2Cl_2F_4$	CFC-114	203-293	0	6	815-860	c
		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	c
		203-293	0	6	1110-1145	
		203-293	0	6	1167-1260	
$CHCl_2F$	HCFC-21	296	1	1	785-840	b
$CHClF_2$	HCFC-22	181-297	0-764	29	760-860	j
		181-296	0-761	34	1070-1195	i, j
		253-287	0	3	1275-1380	i
$CHCl_2CF_3$	HCFC-123	253-287	0	3	740-900	i
		253-287	0	3	1079-1450	
$CHClFCF_3$	HCFC-124	287	0	1	675-715	i
		287	0	1	790-920	
		287	0	1	1035-1430	
CH_3CCl_2F	HCFC-141b	253-287	0	3	710-790	i
		253-287	0	3	895-1210	
		253-287	0	3	1325-1470	
CH_3CClF_2	HCFC-142b	253-287	0	3	650-705	i
		253-287	0	3	875-1265	
		253-287	0	3	1360-1475	
$CHCl_2CF_2CF_3$	HCFC-225ca	253-287	0	3	695-865	i
		253-287	0	3	1010-1420	
$CClF_2CF_2CHClF$	HCFC-225cb	253-287	0	3	715-1375	i

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

(continued)

Molecule	Common Name	Temperature Range (K)	Pressure Range (Torr)	Number of *P,T* sets	Spectral Coverage (cm^{-1})	Reference
CH_2F_2	HFC-32	203-297	0-750	17	995-1236	h
		203-297	0-750	17	1385-1475	
CHF_2CF_3	HFC-125	287	0	1	700-745	i
		287	0	1	840-890	
		287	0	1	1060-1465	
CHF_2CHF_2	HFC-134	203-297	0-750	9	600-1700	g
CFH_2CF_3	HFC-134a	253-287	0	3	815-865	i
		253-287	0	3	935-1485	i
		190-296	20-760	32	1035-1130	j
		190-296	20-760	34	1135-1340	j
CF_3CH_3	HFC-143a	203-297	0-750	9	580-630	g
		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	i
		253-287	0	3	1050-1205	
		253-287	0	3	1320-1490	

Note: These data are in main directory. Additional data are stored in supplemental sub-directory: $ClONO_2$, 1265-1325 cm^{-1}, 3 *P,T*-sets; CFC-11, 830-860 and 1060-1107 cm^{-1}, 6 *P,T*-sets; CFC-12, 867-937 and 1080-1177 cm^{-1}, 6 *P,T*-sets**.**

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