By-Molecule Folder

The By-Molecule folder contains files of individual molecules of the HITRAN absorption parameter database. The files use the arbitrary molecule number as the first two characters of a file name. The correspondence for these numbers can be found in several places, such as the file molparam.txt; the table below also illustrates these numbers. For example, 01_hit12.par is the file for all the water-vapor line parameters in HITRAN (1 ≡ H_2O). When these files are combined and sorted on wavenumber, one obtains the full HITRAN database (HITRAN12.par), given in the higher-level directory HITRAN2012/

The purpose of this folder is to provide data for specific molecules for applications such as laboratory experiments, theoretical analysis, or validation. It is recommended that the full HITRAN database be used for most applications, for example atmospheric simulations or modeling.

Molecules and isotopologues represented in line-by-line portion of HITRAN.

Molecule	Isotopologue[a]	Spectral Coverage (cm^{-1})	Number of Transitions
(1) **H_2O**	161	0 – 25711	142 045
	181	0 – 19918	39 903
	171	0 – 19946	27 544
	162	0 – 22708	13 237
	182	0 – 3825	1 611
	172	1234 – 1599	175
(2) **CO_2**	626	345 – 12785	169 292
	636	406 – 12463	70 611
	628	0 – 9558	116 482
	627	0 – 9600	72 525
	638	489 – 6745	26 737
	637	583 – 6769	2 953
	828	491 – 8161	7 118
	827	626 – 5047	821
	727[b]	535 – 6933	5187
	838[b]	4599 – 4888	121
(3) **O_3**	666	0 – 6997	261 886
	668	0 – 2768	44 302
	686	1 – 2740	18 887
	667	0 – 2122	65 106
	676	0 – 2101	31 935
(4) **N_2O**	446	0 – 7797	33 074
	456	5 – 5086	4 222
	546	4 – 4704	4 592
	448	542 – 4672	4 250
	447	550 – 4430	1 705

(5) **CO**	26	3 – 8465	1 019
	36	3 – 6279	797
	28	3 – 6267	770
	27	3 – 6339	728
	38	3 – 6124	712
	37	1807 – 6197	580
(6) **CH_4**	211	0 – 11502	336 830
	311	0 – 11319	72 420
	212	7 – 6511	54 550
	312	959 – 1695	4 213
(7) **O_2**	66	0 – 15928	1 787
	68	1 – 15853	875
	67	0 – 14538	11 313
(8) **NO**	46	0 – 9274	103 701
	56	1609 – 2061	699
	48	1602 – 2039	679
(9) **SO_2**	626	0 – 4093	72 460
	646	0 – 2501	22 661
(10) **NO_2**	646	0 – 3075	104 223
(11) **NH_3**	4111	0 – 7000	45 302
	5111	0 – 5180	1 090
(12) **HNO_3**	146	0 – 1770	903 854
	156	0 – 923	58 108
(13) **OH**	61	0 – 19268	30 772
	81	0 – 329	295
	62	0 – 332	912
(14) **HF**	19	24 – 46985	10 073
	29	13 – 47365	24 303
(15) **HCl**	15	8 – 34250	11 879
	17	8 – 34240	11 907
	25	5 – 33284	29 994
	27	5 – 33258	29 911
(16) **HBr**	19	13 – 16034	3 039
	11	13 – 16032	3 031
	29	7 – 8781	1 455
	21	7 – 8778	1 455
(17) **HI**	17	10 – 13908	3 161
	27	5 – 7625	1 590
(18) **ClO**	56	0 – 1208	5 721
	76	0 – 1200	5 780
(19) **OCS**	622	0 – 4200	15 618
	624	0 – 4166	6 087
	632	0 – 4056	3 129
	623	0 – 4164	2 886
	822	0 – 4046	1 641
(20) **H_2CO**	126	0 – 3100	40 670
	136	0 – 117	2 309
	128	0 – 101	1 622
(21) **HOCl**	165	1 – 3800	8 877
	176	1 – 3800	7 399
(22) **N_2**	44	11 – 9355	1 107
	45	11 – 2578	161
(23) **HCN**	124	0 – 3424	2 955
	134	2 – 3405	652
	125	2 – 3420	646
(24) **CH_3Cl**	215	0 – 3198	107 642
	217	0 – 3198	104 854
(25) **H_2O_2**	1661	0 – 1731	126 983
(26) **C_2H_2**	1221	604 – 9890	12 613
	1231	613 – 6589	285
	1222	1 – 789	7 512

(27) C_2H_6	1221	706 – 3001	43 592
	1231	725 – 919	6 037
(28) PH_3	1111	0 – 3602	22 189
(29) COF_2	269	696 – 2002	168 793
	369	686 – 815	15 311
(30) SF_6	29	580 – 996	2 889 065
(31) H_2S	121	2 – 11330	36 561
	141	5 – 11227	11 352
	131	5 – 11072	6 322
(32) HCOOH	126	10 – 1890	62 684
(33) HO_2	166	0 – 3676	38 804
(34) O	6	68 – 159	2
(35) $ClONO_2$	5646	763 – 798	21 988
	7646	765 – 791	10 211
(36) NO^+	46	1634 – 2531	1 206
(37) HOBr	169	0 – 316	2 177
	161	0 – 316	2 181
(38) C_2H_4	221	701 – 3243	18 097
	231	2947 – 3181	281
(39) CH_3OH	2161	0 – 1408	19 897
(40) CH_3Br	219	794 – 1706	18 692
	211	796 – 1697	18 219
(41) CH_3CN	2124	890 – 946	3 572
(42) CF_4	29	594 – 1313	60 033
(43) C_4H_2	2211	0 – 758	124 126
(44) HC_3N	1224	0 – 760	180 332
(45) H_2	11	15 – 36024	4 017
	12	3 – 36406	5 129
(46) CS	22	1 – 2586	1 088
	24	1 – 1359	396
	32	1 – 1331	396
	23	1 – 156	198
(47) SO_3	26	0 – 2778	10 881

[a]Abbreviated code for isotopologues.

[b]Isotopologue 727 ($^{17}O^{12}C^{17}O$) introduced into HITRAN for the first time in this edition. Isotopologue 838, which existed in the database before but is of lesser terrestrial abundance, has been reassigned as the 10th isotopologue and has the number zero in the corresponding ASCII format transition field.

Note: Molecules SF_6, $ClONO_2$, and CF_4 have been assigned to the supplemental folder.