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, $01_{\text{hit}}08.\text{par}$ is the file for all the water-vapor line parameters in HITRAN ($1 \equiv H_2O$). When these files are combined and sorted on wavenumber, one obtains the full HITRAN database (HITRAN08.par), given in the higher-level directory HITRAN2008/

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.

Molecule Number Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm ⁻¹)	Number of lines per isotopo- logue	Total number for Molecule
01 H ₂ O	161 181 171 162 182 172	0.9973 1.999 10 ⁻³ 3.719 10 ⁻⁴ 3.107 10 ⁻⁴ 6.230 10 ⁻⁷ 1.158 10 ⁻⁷	$0-25233 \\ 0-14519 \\ 10-14473 \\ 0-22708 \\ 0-3825 \\ 1234-1599$	37432 9753 6992 13238 1611 175	69201
02 CO ₂	626 636 628 627 638 637 828 827 838	0.9842 1.106 10 ⁻² 3.947 10 ⁻³ 7.339 10 ⁻⁴ 4.434 10 ⁻⁵ 8.246 10 ⁻⁶ 3.957 10 ⁻⁶ 1.472 10 ⁻⁶ 4.446 10 ⁻⁸	352 - 12785 438 - 12463 0 - 11423 0 - 8271 489 - 6745 583 - 6769 491 - 8161 626 - 5047 4599 - 4888	128170 49777 79958 19264 26737 2953 7118 821 121	314919
03 O ₃	666 668 686 667 676	0.9929 $3.982 ext{ } 10^{-3}$ $1.991 ext{ } 10^{-3}$ $7.405 ext{ } 10^{-4}$ $3.702 ext{ } 10^{-4}$	$0-5787 \\ 0-2768 \\ 1-2740 \\ 0-2122 \\ 0-2101$	249456 44302 18887 65106 31935	409686
04 N ₂ O	446 456 546 448 447	0.9903 3.641 10 ⁻³ 3.641 10 ⁻³ 1.986 10 ⁻³ 3.693 10 ⁻⁴	0 - 7797 $5 - 5086$ $4 - 4704$ $542 - 4672$ $550 - 4430$	33074 4222 4592 4250 1705	47843

05 CO 26 36 1.108 10 ² 28 1.978 10 ³ 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6279 3.6210 3.62210 3.62210 3.62310 3.6							
05 CO			26	0.9865	3 - 8465	917	
10			36	1.108 10 ⁻²	3 - 6279	780	
10	0.5	00	28	$1.978 \ 10^{-3}$	3 - 6267	760	4.477
38	05	CO					4477
37							
06 CH4 211							
06 CH4 311			31	4.133 10	1007 - 0197	360	
06 CH4 312 212 6.918 10⁻6 6.518 10⁻4 959 − 1695 45024 4213 290091 07 O₂ 66 0.9953 67 0 − 15928 7.422 10⁻4 1432 0 − 14537 4326 08 NO 56 3.654 10⁻3 48 1.993 10⁻3 1609 − 2061 1609 − 2061 699 699 105079 09 SO₂ 626 646 0.9457 4.195 10⁻2 0 − 4093 2463 − 2497 57963 287 58250 10 NO₂ 646 0.9916 0 − 3075 104223 104223 11 NH₃ 446 456 0.9959 3.661 10⁻³ 0 − 5295 0 − 5295 27994 29084 29084 12 HNO₃ 146 0.9891 0 − 1770 487254 487254 13 OH 81 2.000 10⁻³ 0 − 329 295 31976 13 OH 81 2.000 10⁻³ 0 − 329 295 31976 15 HCI 15 0.7576 20 − 13459 324 613 16 HBr 19 0.5068 16 − 9759 651			211	0.9883	0 - 9200	212061	
10 NO2 646 0.9916 0.9959 0.9529 0.	0.6	CII	311	$1.110 \ 10^{-2}$	0 - 6070	28793	200001
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	06	CH ₄	212	$6.158 \cdot 10^{-4}$	7 - 6511	45024	290091
$\begin{array}{c} 07 \ {\rm O_2} \\ 07 \ {\rm O_2} \\ 08 \\ 07 \\ 07 \\ 02 \\ 08 \\ 07 \\ 09 \\ 08 \\ 00 \\ 08 \\ 00 \\ 09 \\ 00 \\ 09 \\ 00 \\ 00$							
07 O2 68							
67 7.422 10 ⁻⁴ 0 - 14537 4326 08 NO 56 3.654 10 ⁻³ 1609 - 2061 699 105079 679 09 SO2 626 646 4.195 10 ⁻² 2463 - 2497 287 58250 10 NO2 646 0.9916 0 - 3075 104223 104223 11 NH3 446 0.9959 0 - 5295 27994 29084 29084 12 HNO3 146 0.9891 0 - 1770 487254 487254 487254 487254 13 OH 81 2.000 10 ⁻³ 0 - 329 295 31976 295 31976 14 HF 19 0.9998 41 - 11536 107 107 107 15 HCI 15 0.7576 20 - 13459 324 613 324 613 16 HBr 19 0.5068 16 - 9759 651 10995 289 613 613 16 HBr 19 0.5068 16 - 9759 651 1293 1293 16 HBr 19 0.5068 16 - 9759 651 1293 1293 17 HI 17 0.9998 12 - 8488 806 806 806 18 CIO 56 0.7559 0 - 1208 5721 0 - 1200 5780 11501 11501 19 OCS 632 1.053 10 ⁻² 0 - 4056 3124 29242 620 623 7.399 10 ⁻³ 509 - 4164 2787 623 7.399 10 ⁻³ 509 - 4164 2787 623 7.399 10 ⁻³ 509 - 4164 2787 623 7.399	0.5						6.420
08 NO 56 3.654 10 ⁻³ 1609 - 2061 699 105079 103701 699 105079 09 SO2 626 646 4.195 10 ⁻² 2463 - 2497 287 58250 10 NO2 646 0.9916 0 - 3075 104223 104223 11 NH3 446 0.9959 0 - 5295 27994 456 3.661 10 ⁻³ 0 - 5180 1090 29084 29084 1090 29084 12 HNO3 146 0.9891 0 - 1770 487254 487254 487254 13 OH 81 2.000 10 ⁻³ 0 - 329 295 31976 62 1.554 10 ⁻⁴ 0 - 332 912 30769 295 31976 107 14 HF 19 0.9998 41 - 11536 107 107 107 15 HCl 15 0.7576 20 - 13459 324 613 613 16 HBr 19 0.5068 16 - 9759 651 17 0.2422 20 - 10995 289 651 1293 17 HI 0.4931 16 - 9758 642 1293 1293 18 ClO 56 0.7559 0 - 1208 5721 1501 11501 18 ClO 632 1.053 10 ⁻² 0 - 4056 3124 29242 623 7.399 10 ⁻³ 509 - 4164 2787 822 1.880 10 ⁻³ 0 - 4046 1626 126 0.9862 0 - 3100 36121 29242 623 7.399 10 ⁻³ 509 - 4164 2787 822 1.880 10 ⁻³ 0 - 4046 1626 20 H ₂ CO 136 1.108 10 ⁻² 0 - 73 562 37050 128 1.978 10 ⁻³ 0 - 448 367 16276 0.2417 1 - 3800 7399 16276 21 HOCI 165 0.7558 1-3800 7399 16276 16276 0.2417 1 - 3800 7399 16276	07	O_2					6428
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			67	7.422 10-4	0 – 14537	4326	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			46	0.9940	0 - 9274	103701	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	08	NO					105079
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		110					105075
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$							
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	09	SO_2					58250
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0)	502	646	4.195 10-2	2463 – 2497	287	20220
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	10	NO_2	646	0.9916	0 - 3075	104223	104223
12 HNO ₃ 146 0.9891 0 - 1770 487254 487254 61 0.9975 0 - 19268 30769 62 1.554 10 ⁻⁴ 0 - 332 912 14 HF 19 0.9998 41 - 11536 107 107 15 HCl 15 0.7576 20 - 13459 324 613 16 HBr 19 0.5068 16 - 9759 651 1293 17 HI 17 0.9998 12 - 8488 806 806 18 ClO 56 0.7559 0 - 1208 5721 11501 622 0.9374 0 - 4200 5780 11501 622 0.9374 0 - 4200 5780 11501 622 0.9374 0 - 4200 15618 624 4.158 10 ⁻² 0 - 4166 6087 624 4.158 10 ⁻² 0 - 4166 6087 822 1.880 10 ⁻³ 509 - 4164 2787 822 1.880 10 ⁻³ 0 - 4046 1626 20 H ₂ CO 136 1.108 10 ⁻² 0 - 73 562 37050 128 1.978 10 ⁻³ 0 - 48 367 21 HOCl 165 0.7558 1 - 3800 8877 16276	1 1	NILL	446	0.9959	0 - 5295	27994	20004
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	11	NH ₃	456	$3.661\ 10^{-3}$	0 - 5180	1090	29084
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	12	HNO ₃	146		0 - 1770	487254	487254
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			61	0.9975	0 – 19268	30769	
62 1.554 10-4 0 - 332 912 14 HF 19 0.9998 41 - 11536 107 107 15 HCl 15 0.7576 20 - 13459 324 613 16 HBr 17 0.2422 20 - 10995 289 613 16 HBr 19 0.5068 16 - 9759 651 1293 17 HI 17 0.9998 12 - 8488 806 806 18 ClO 56 0.7559 0 - 1208 5721 11501 622 0.9374 0 - 1200 5780 11501 624 4.158 10-2 0 - 4166 6087 623 7.399 10-3 509 - 4164 2787 822 1.880 10-3 0 - 4046 1626 20 H2CO 136 1.108 10-2 0 - 73 562 37050 128 1.978 10-3 0 - 48 367 21 HOCl 165 0.7558 1 - 3800 7399 16276	13	OH					31076
14 HF 19 0.9998 41 – 11536 107 107 15 HCl 15	13	OH					31770
15 HCl							
16 HBr	14	HF	19	0.9998	41 – 11536	107	107
17 0.2422 20 - 10995 289 16 HBr 19 0.5068 16 - 9759 651 1293 17 HI 17 0.9998 12 - 8488 806 806 18 CIO 56 0.7559 0 - 1208 5721 1501 622 0.9374 0 - 1200 5780 11501 624 4.158 10 ⁻² 0 - 4166 6087 623 7.399 10 ⁻³ 509 - 4164 2787 822 1.880 10 ⁻³ 0 - 4046 1626 19 OCS 632 1.053 10 ⁻² 0 - 4046 1626 20 H ₂ CO 136 1.108 10 ⁻² 0 - 73 562 37050 128 1.978 10 ⁻³ 0 - 48 367 21 HOCI 165 0.7558 1 - 3800 8877 7399 16276	1.5	IIC1	15	0.7576	20 - 13459	324	612
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	13	нсі	17	0.2422	20 - 10995	289	013
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			19	0.5068	16 – 9759	651	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	16	HBr					1293
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1.7	TIT					007
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1/	Ш					806
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	18	ClO					11501
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10		76	0.2417	0 - 1200	5780	11501
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			622	0 9374	0 – 4200	15618	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$							
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10	OCS					20242
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	19	OCB					L)L4L
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$							
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			822	1.000 10	0 – 4040	1020	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			126	_	0 - 3100	36121	
21 HOCl 165 0.7558 1 - 3800 8877 16276	20	H_2CO	136	$1.108\ 10^{-2}$	0 - 73	562	37050
21 HOCl 165 0.7558 1 - 3800 8877 16276			128	1.978 10 ⁻³	0 - 48	367	
21 HOC1 167 0.2417 1 – 3800 7399 ^{162/6}			165	0.7558	1 _ 3800	8877	
	21	HOCl					16276
$22 N_2$ 44 0.9927 $1992 - 2626$ 120 120		.					4.50
	22	N ₂	44	0.9927	1992 – 2626	120	120

		10.4	0.0051	0 2121	2075	
	HON	124	0.9851	0 - 3424	2955	40.50
23	HCN	134	$1.107 \ 10^{-2}$	2 - 3405	652	4253
		125	3.622 10 ⁻³	2 - 3420	646	
24	CH-C1	215	0.7489	0 - 3173	100279	196171
24	CH ₃ Cl	217	0.2395	0 - 3162	95892	1901/1
25	H_2O_2	1661	0.9950	0 - 1731	126983	126983
26	CII	1221	0.9776	604 – 9890	11055	11240
26	C_2H_2	1231	$2.197 \cdot 10^{-2}$	613 - 6589	285	11340
27	C_2H_6	1221	0.9770	706 - 3001	22402	22402
28	PH_3	1111	0.9995	770 - 3602	20099	20099
29	COF_2	269	0.9865	725 - 2002	70601	70601
30	SF ₆	29	0.9502	580 – 996	2889065	2889065
		121	0.9499	2 - 4257	12330	
31	H_2S	141	$4.214\ 10^{-2}$	5 - 4172	4894	20788
		131	$7.498\ 10^{-3}$	5 - 4099	3564	
32	НСООН	126	0.9839	10 - 1890	62684	62684
33	HO_2	166	0.9951	0 - 3676	38804	38804
34	0	6	0.9976	68 – 159	2	2
25	CIONO	5646	0.7496	763 – 798	21988	22100
35	ClONO ₂	7646	0.2397	765 – 791	10211	32199
36	NO ⁺	46	0.9940	1634 - 2531	1206	1206
27	HOD	169	0.5056	0 - 316	2177	4250
37	HOBr	161	0.4919	0 - 316	2181	4358
20	C II	221	0.9773	701 - 3243	18097	10270
38	C_2H_4	231	2.196 10 ⁻²	2947 - 3181	281	18378
39	CH ₃ OH	2161	0.9859	0 - 1408	19897	19897
40	CH ₃ Br	219	0.5010	794 - 1706	18692	36911
40	СПЗВІ	211	0.4874	796 – 1697	18219	30911
41	CH ₃ CN	2124	0.9739	890 – 946	3572	3572
42	CF ₄	29	0.9889	594 – 1313	60033	60033

Note: Highlighted molecules (SF₆, ClONO₂, and CF₄) have been assigned to the supplemental folder [see text in *JQSRT* **110**, 533-572 (2009)].