# 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_hit08.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 (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 isotopologue | Total number for Molecule |
|---|---|---|---|---|---|---|
| 01 | $H_2O$ | 161 | 0.9973 | 0 – 25233 | 37432 | 69201 |
| | | 181 | $1.999\ 10^{-3}$ | 0 – 14519 | 9753 | |
| | | 171 | $3.719\ 10^{-4}$ | 10 – 14473 | 6992 | |
| | | 162 | $3.107\ 10^{-4}$ | 0 – 22708 | 13238 | |
| | | 182 | $6.230\ 10^{-7}$ | 0 – 3825 | 1611 | |
| | | 172 | $1.158\ 10^{-7}$ | 1234 – 1599 | 175 | |
| 02 | $CO_2$ | 626 | 0.9842 | 352 – 12785 | 128170 | 314919 |
| | | 636 | $1.106\ 10^{-2}$ | 438 – 12463 | 49777 | |
| | | 628 | $3.947\ 10^{-3}$ | 0 – 11423 | 79958 | |
| | | 627 | $7.339\ 10^{-4}$ | 0 – 8271 | 19264 | |
| | | 638 | $4.434\ 10^{-5}$ | 489 – 6745 | 26737 | |
| | | 637 | $8.246\ 10^{-6}$ | 583 – 6769 | 2953 | |
| | | 828 | $3.957\ 10^{-6}$ | 491 – 8161 | 7118 | |
| | | 827 | $1.472\ 10^{-6}$ | 626 – 5047 | 821 | |
| | | 838 | $4.446\ 10^{-8}$ | 4599 – 4888 | 121 | |
| 03 | $O_3$ | 666 | 0.9929 | 0 – 5787 | 249456 | 409686 |
| | | 668 | $3.982\ 10^{-3}$ | 0 – 2768 | 44302 | |
| | | 686 | $1.991\ 10^{-3}$ | 1 – 2740 | 18887 | |
| | | 667 | $7.405\ 10^{-4}$ | 0 – 2122 | 65106 | |
| | | 676 | $3.702\ 10^{-4}$ | 0 – 2101 | 31935 | |
| 04 | $N_2O$ | 446 | 0.9903 | 0 – 7797 | 33074 | 47843 |
| | | 456 | $3.641\ 10^{-3}$ | 5 – 5086 | 4222 | |
| | | 546 | $3.641\ 10^{-3}$ | 4 – 4704 | 4592 | |
| | | 448 | $1.986\ 10^{-3}$ | 542 – 4672 | 4250 | |
| | | 447 | $3.693\ 10^{-4}$ | 550 – 4430 | 1705 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| 05 | CO | 26 | 0.9865 | 3 – 8465 | 917 | 4477 |
| | | 36 | $1.108\ 10^{-2}$ | 3 – 6279 | 780 | |
| | | 28 | $1.978\ 10^{-3}$ | 3 – 6267 | 760 | |
| | | 27 | $3.679\ 10^{-4}$ | 3 – 6339 | 728 | |
| | | 38 | $2.222\ 10^{-5}$ | 3 – 6124 | 712 | |
| | | 37 | $4.133\ 10^{-6}$ | 1807 – 6197 | 580 | |
| 06 | $CH_4$ | 211 | 0.9883 | 0 – 9200 | 212061 | 290091 |
| | | 311 | $1.110\ 10^{-2}$ | 0 – 6070 | 28793 | |
| | | 212 | $6.158\ 10^{-4}$ | 7 – 6511 | 45024 | |
| | | 312 | $6.918\ 10^{-6}$ | 959 – 1695 | 4213 | |
| 07 | $O_2$ | 66 | 0.9953 | 0 – 15928 | 1432 | 6428 |
| | | 68 | $3.991\ 10^{-3}$ | 1 – 15852 | 670 | |
| | | 67 | $7.422\ 10^{-4}$ | 0 – 14537 | 4326 | |
| 08 | NO | 46 | 0.9940 | 0 – 9274 | 103701 | 105079 |
| | | 56 | $3.654\ 10^{-3}$ | 1609 – 2061 | 699 | |
| | | 48 | $1.993\ 10^{-3}$ | 1602 – 2039 | 679 | |
| 09 | $SO_2$ | 626 | 0.9457 | 0 – 4093 | 57963 | 58250 |
| | | 646 | $4.195\ 10^{-2}$ | 2463 – 2497 | 287 | |
| 10 | $NO_2$ | 646 | 0.9916 | 0 – 3075 | 104223 | 104223 |
| 11 | $NH_3$ | 446 | 0.9959 | 0 – 5295 | 27994 | 29084 |
| | | 456 | $3.661\ 10^{-3}$ | 0 – 5180 | 1090 | |
| 12 | $HNO_3$ | 146 | 0.9891 | 0 – 1770 | 487254 | 487254 |
| 13 | OH | 61 | 0.9975 | 0 – 19268 | 30769 | 31976 |
| | | 81 | $2.000\ 10^{-3}$ | 0 – 329 | 295 | |
| | | 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 |
| | | 17 | 0.2422 | 20 – 10995 | 289 | |
| 16 | HBr | 19 | 0.5068 | 16 – 9759 | 651 | 1293 |
| | | 11 | 0.4931 | 16 – 9758 | 642 | |
| 17 | HI | 17 | 0.9998 | 12 – 8488 | 806 | 806 |
| 18 | ClO | 56 | 0.7559 | 0 – 1208 | 5721 | 11501 |
| | | 76 | 0.2417 | 0 – 1200 | 5780 | |
| 19 | OCS | 622 | 0.9374 | 0 – 4200 | 15618 | 29242 |
| | | 624 | $4.158\ 10^{-2}$ | 0 – 4166 | 6087 | |
| | | 632 | $1.053\ 10^{-2}$ | 0 – 4056 | 3124 | |
| | | 623 | $7.399\ 10^{-3}$ | 509 – 4164 | 2787 | |
| | | 822 | $1.880\ 10^{-3}$ | 0 – 4046 | 1626 | |
| 20 | $H_2CO$ | 126 | 0.9862 | 0 – 3100 | 36121 | 37050 |
| | | 136 | $1.108\ 10^{-2}$ | 0 – 73 | 562 | |
| | | 128 | $1.978\ 10^{-3}$ | 0 – 48 | 367 | |
| 21 | HOCl | 165 | 0.7558 | 1 – 3800 | 8877 | 16276 |
| | | 167 | 0.2417 | 1 – 3800 | 7399 | |
| 22 | $N_2$ | 44 | 0.9927 | 1992 – 2626 | 120 | 120 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 23 | HCN | 124<br>134<br>125 | 0.9851<br>$1.107\ 10^{-2}$<br>$3.622\ 10^{-3}$ | 0 – 3424<br>2 – 3405<br>2 – 3420 | 2955<br>652<br>646 | 4253 |
| 24 | $CH_3Cl$ | 215<br>217 | 0.7489<br>0.2395 | 0 – 3173<br>0 – 3162 | 100279<br>95892 | 196171 |
| 25 | $H_2O_2$ | 1661 | 0.9950 | 0 – 1731 | 126983 | 126983 |
| 26 | $C_2H_2$ | 1221<br>1231 | 0.9776<br>$2.197\ 10^{-2}$ | 604 – 9890<br>613 – 6589 | 11055<br>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** |
| 31 | $H_2S$ | 121<br>141<br>131 | 0.9499<br>$4.214\ 10^{-2}$<br>$7.498\ 10^{-3}$ | 2 – 4257<br>5 – 4172<br>5 – 4099 | 12330<br>4894<br>3564 | 20788 |
| 32 | HCOOH | 126 | 0.9839 | 10 – 1890 | 62684 | 62684 |
| 33 | $HO_2$ | 166 | 0.9951 | 0 – 3676 | 38804 | 38804 |
| 34 | O | 6 | 0.9976 | 68 – 159 | 2 | 2 |
| **35** | **$ClONO_2$** | **5646**<br>**7646** | **0.7496**<br>**0.2397** | **763 – 798**<br>**765 – 791** | **21988**<br>**10211** | **32199** |
| 36 | $NO^+$ | 46 | 0.9940 | 1634 – 2531 | 1206 | 1206 |
| 37 | HOBr | 169<br>161 | 0.5056<br>0.4919 | 0 – 316<br>0 – 316 | 2177<br>2181 | 4358 |
| 38 | $C_2H_4$ | 221<br>231 | 0.9773<br>$2.196\ 10^{-2}$ | 701 – 3243<br>2947 – 3181 | 18097<br>281 | 18378 |
| 39 | $CH_3OH$ | 2161 | 0.9859 | 0 – 1408 | 19897 | 19897 |
| 40 | $CH_3Br$ | 219<br>211 | 0.5010<br>0.4874 | 794 – 1706<br>796 – 1697 | 18692<br>18219 | 36911 |
| 41 | $CH_3CN$ | 2124 | 0.9739 | 890 – 946 | 3572 | 3572 |
| **42** | **$CF_4$** | **29** | **0.9889** | **594 – 1313** | **60033** | **60033** |

Note: Highlighted molecules ($SF_6$, $ClONO_2$, and $CF_4$) have been assigned to the supplemental folder [see text in *JQSRT* **110,** 533-572 (2009)].