

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 \equiv H₂O). 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 ₂ O | 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 ₂ O | 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 |

| | | | |
|------------------------------------|------|-------------|---------|
| | 26 | 3 – 8465 | 1 019 |
| | 36 | 3 – 6279 | 797 |
| (5) CO | 28 | 3 – 6267 | 770 |
| | 27 | 3 – 6339 | 728 |
| | 38 | 3 – 6124 | 712 |
| | 37 | 1807 – 6197 | 580 |
| | 211 | 0 – 11502 | 336 830 |
| (6) CH ₄ | 311 | 0 – 11319 | 72 420 |
| | 212 | 7 – 6511 | 54 550 |
| | 312 | 959 – 1695 | 4 213 |
| | 66 | 0 – 15928 | 1 787 |
| (7) O ₂ | 68 | 1 – 15853 | 875 |
| | 67 | 0 – 14538 | 11 313 |
| | 46 | 0 – 9274 | 103 701 |
| (8) NO | 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 |
| | 61 | 0 – 19268 | 30 772 |
| (13) OH | 81 | 0 – 329 | 295 |
| | 62 | 0 – 332 | 912 |
| (14) HF | 19 | 24 – 46985 | 10 073 |
| | 29 | 13 – 47365 | 24 303 |
| | 15 | 8 – 34250 | 11 879 |
| (15) HCl | 17 | 8 – 34240 | 11 907 |
| | 25 | 5 – 33284 | 29 994 |
| | 27 | 5 – 33258 | 29 911 |
| | 19 | 13 – 16034 | 3 039 |
| (16) HBr | 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 |
| | 622 | 0 – 4200 | 15 618 |
| (19) OCS | 624 | 0 – 4166 | 6 087 |
| | 632 | 0 – 4056 | 3 129 |
| | 623 | 0 – 4164 | 2 886 |
| | 822 | 0 – 4046 | 1 641 |
| | 126 | 0 – 3100 | 40 670 |
| (20) H ₂ CO | 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 |
| | 124 | 0 – 3424 | 2 955 |
| (23) HCN | 134 | 2 – 3405 | 652 |
| | 125 | 2 – 3420 | 646 |
| (24) CH ₃ Cl | 215 | 0 – 3198 | 107 642 |
| | 217 | 0 – 3198 | 104 854 |
| (25) H ₂ O ₂ | 1661 | 0 – 1731 | 126 983 |
| | 1221 | 604 – 9890 | 12 613 |
| (26) C ₂ H ₂ | 1231 | 613 – 6589 | 285 |
| | 1222 | 1 – 789 | 7 512 |

| | | | |
|--|------|-------------|-----------|
| (27) C₂H₆ | 1221 | 706 – 3001 | 43 592 |
| | 1231 | 725 – 919 | 6 037 |
| (28) PH₃ | 1111 | 0 – 3602 | 22 189 |
| (29) COF₂ | 269 | 696 – 2002 | 168 793 |
| | 369 | 686 – 815 | 15 311 |
| (30) SF₆ | 29 | 580 – 996 | 2 889 065 |
| (31) H₂S | 121 | 2 – 11330 | 36 561 |
| | 141 | 5 – 11227 | 11 352 |
| | 131 | 5 – 11072 | 6 322 |
| (32) HCOOH | 126 | 10 – 1890 | 62 684 |
| (33) HO₂ | 166 | 0 – 3676 | 38 804 |
| (34) O | 6 | 68 – 159 | 2 |
| (35) ClONO₂ | 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) C₂H₄ | 221 | 701 – 3243 | 18 097 |
| | 231 | 2947 – 3181 | 281 |
| (39) CH₃OH | 2161 | 0 – 1408 | 19 897 |
| (40) CH₃Br | 219 | 794 – 1706 | 18 692 |
| | 211 | 796 – 1697 | 18 219 |
| (41) CH₃CN | 2124 | 890 – 946 | 3 572 |
| (42) CF₄ | 29 | 594 – 1313 | 60 033 |
| (43) C₄H₂ | 2211 | 0 – 758 | 124 126 |
| (44) HC₃N | 1224 | 0 – 760 | 180 332 |
| (45) H₂ | 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) SO₃ | 26 | 0 – 2778 | 10 881 |

^aAbbreviated code for isotopologues.

^bIsotopologue 727 (¹⁷O¹²C¹⁷O) 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 SF₆, ClONO₂, and CF₄ have been assigned to the supplemental folder.