Aerosol Files in HITRAN

Some files in the AEROSOL folder are carried over from previous HITRAN editions. The older files are listed here first, followed by a summary of the new aerosol indices of refraction included in this edition of HITRAN. If you have any questions, please contact Steve Massie at the National Center for Atmospheric Research (NCAR), Boulder, Colorado USA (303-497-1404, massie@ncar.ucar.edu).

File names	Substance
DowningandWilliams.dat	Water
Kou_etal.dat	Water and Ice
Warren.dat	Ice
Shettle.dat	Water, Ice, Sodium Chloride, Sea Salt, Water Soluble Aerosol, Ammonium Sulfate, Carbonaceous Aerosol, Volcanic Dust, Sulfuric Acid, Meteoric Dust, Quartz, Hematite, Sand, and Dust-like Aerosol
PalmerandWilliams.dat	Sulfuric Acid Solutions
Remsberg.dat	Sulfuric Acid and Nitric Acid Solutions
SteeleandHamill.dat	Sulfuric Acid Solutions
Timmermans.dat	Sulfuric Acid Solutions
Toon_etal.dat	H_2O-Ice, Amorphous Nitric Acid Solutions, and Nitric Acid Hydrates
Norman_etal.dat	Aqueous HNO_3/H_2O
Tisdale_etal.dat	Sulfuric Acid Solutions
h2so4t*.biermann	Sulfuric Acid Solutions at 12 Temperatures
h2so4T*.niedziela	Sulfuric Acid Solutions at 8 Temperatures
SutherlandandKhanna.dat	Organic-based Nonvolatile Aerosols
QuerryandTyler.dat	Nitric Acid Solutions
hno3t*.biermann	Nitric Acid Solutions at 7 Temperatures
nad*.niedziela	Nitric Acid Dyhydrate (NAD) at 3 Temperatures
Richwine_etal.dat	Nitric Acid Trihydrate (NAT)
ice*.clapp	Water Ice at 9 Temperatures

Summary of Aerosol Files from Earlier HITRAN Editions

File: **DowningandWilliams.dat**

Data: Real and imaginary indices of refraction for water at 27 C between 10 and 5000 cm^{-1}.

Reference: H.D. Downing and D. Williams, "Optical constants of water in the infrared," *J.Geophys.Res.* **80,** 1656-1661 (1975).

File: **Kou_etal.dat**

Data: Imaginary indices of refraction for water and ice in the 0.67 to 2.5 micron range.

Reference: L. Kou, D. Labrie, and P. Chylek, "Refractive indices of water and ice in the 0.65 to 2.5 micron range," *Appl.Opt.* **32,** 3531-3540 (1993).

File: **Warren.dat**

Data: Real and imaginary indices of refraction of ice at -7 C for the $4.43x10^{-2}$ to 167 micron range, and indices of ice at -1, -5, -20, and -60 C for the 167 to $8.6x10^{6}$ micron range.

Reference: S.G. Warren, "Optical constants of ice from the ultraviolet to the microwave," *Appl.Opt.* **23,** 1206-1225 (1984).

The values here were generated from a program of S.G. Warren.

File: **Shettle.dat**

Data: Real and imaginary indices of refraction for water, ice, sodium chloride, sea salt, water soluble aerosol, ammonium sulfate, carbonaceous aerosol, volcanic dust, sulfuric acid, meteoric dust, quartz, hematite, sand, and dust-like aerosol. The tabulations start at 0.2 microns and extend out to 40 microns (or to longer wavelengths). These indices were used to generate the aerosol models which are incorporated into the LOWTRAN, MODTRAN, and FASCODE computer codes.

References: The data were tabulated by E.P. Shettle of the Naval Research Laboratory.

File: **PalmerandWilliams.dat**

Data: Real and imaginary indices of refraction of sulfuric acid solutions at 25, 38, 50, 75, 84.5, and 95.6% H_2SO_4, by weight.

Reference: K.F. Palmer and D. Williams, "Optical constants of sulfuric acid; Application to the clouds of Venus?," *Appl.Opt.* **14,** 208-219 (1975).

File: **Remsberg.dat**

Data: Real and imaginary indices of refraction of sulfuric acid solutions at 75 and 90% H_2SO_4, by weight, plus the standard deviations of the measurements.

Real and imaginary indices of refraction of nitric acid solutions at 68% HNO_3, by weight, plus the standard deviations of the measurements.

Reference: E.E. Remsberg, D. Lavery, and B. Crawford, "Optical constants for sulfuric and nitric acids," *J.Chem. and Engin.Data* **19,** 263-255 (1974).

File: **SteeleandHamill.dat**

Data: Theoretical equilibrium composition (weight percentage of H_2SO_4) of sulfuric acid solutions, given as a function of temperature and H_2O vapour pressure.

Reference: H.M. Steele and P. Hamill, "Effects of temperature and humidity on the growth and optical properties of sulphuric acid-water droplets in the stratosphere," *J.Aerosol Sci.* **12,** 517-528 (1981).

File: **Timmermans.dat**

Data: Sulfuric acid density (gm/cm^3) values for solutions between 0 and 100% H_2SO_4 (by weight) for temperatures between 0 and 60 C.

Reference: J. Timmermans, The physico-chemical constants of binary systems in concentrated solutions, Interscience, New York, (1960).
The data cited here (from pages 561-562 of Timmermans) are from Domke and Bein (1905).

File: **Toon_etal.dat**

Data: Real and imaginary indices of refraction of H_2O-ice, amorphous nitric acid solutions, and nitric acid hydrates.

Reference: O.B. Toon, M.A. Tolbert, B.G. Koehler, A.M. Middlebrook, and J. Jordan, "The infrared optical constants of H_2O-ice, amorphous acid solutions, and nitric acid hydrates," *J.Geophys.Res.* **99,** 25631-25654 (1994).

Summary of New Aerosol Files for HITRAN2000

The files are organized by temperature, and concentrations are in weight percent. For cases in which there are multiple temperatures, the temperature value of a given file is stated in the file name and in the header text of the file.

The data were obtained by downloading files from several web sites. The web files sometimes show some minor differences from the published papers. Each file cites the published paper which discusses the indices, and each file cites the ascii formatting of the data.

The data were written out in a similar convenient style. The original data were cited in terms of wavenumber. We also give wavelengths (by simply citing 10^4 / wavenumber values). Small negative imaginary indices from the Biermann data sets were set to zero.

Biermann provides on her web site a program which shows how to combine the HNO_3/H_2O and H_2SO_4/H_2O indices into those for the ternary droplet ($HNO_3/H_2SO_4/H_2O$). Tisdale, on Tolbert's web site, provides a program which gives a polynomial fit to the data.

File: **Norman_etal.dat**

Data: Real and imaginary indices of aqueous HNO_3/H_2O at 220 K from 754 to 4700 cm^{-1} for 35, 45, 54, 63, and 70% HNO_3 by weight.

Reference: Norman, M.L., J. Qian, R.E. Miller, and D.R. Worsnop, "Infrared complex refractive indices of supercooled liquid HNO_3/H_2O aerosols," *J.Geophys.Res.* **104,** 30571-30584 (1999).

Email contact person: R.E. Miller (remiller@unc.edu)
ftp://frenchie.chem.unc.edu/ri/

File: **Tisdale_etal.dat**

Data: Real and imaginary indices of liquid H_2SO_4/H_2O at 215 K from 499 to 6996 cm^{-1} as a function of the H_2SO_4 concentration by weight.

Reference: Tisdale, R.T., D.L. Glandorf, M.A. Tolbert, and O.B. Toon, "Infrared optical constants of low-temperature H_2SO_4 solutions representative of stratospheric sulfate aerosols," *J.Geophys.Res.* **103,** 25353-25370 (1998).

Email contact person: M. Tolbert (tolbert@spot.colorado.edu)
http://cires.colorado.edu/people/tolbert.group/data/saoc/

Files: **h2so4t*.biermann**

Data: Real indices of liquid H_2SO_4/H_2O from 0 to 16382 cm-1 and imaginary indices from 432 to 5028 cm^{-1} at 12 temperatures (213 to 293K) as a function of the H_2SO_4 concentration by weight.

Reference: Biermann, U.M., B.P. Luo, and Th. Peter, "Absorption Spectra and Optical Constants of Binary and Ternary Solutions of H_2SO_4, HNO_3, and H_2O in the Mid Infrared at Atmospheric Temperatures," *J.Phys.Chem. A* **104,** 783-793 (2000).

Email contact person: B.P. Luo (luo@mpch-mainz.mog.de)
ftp://ftp.mpch-mainz.mpg.de/pub/nwg/

Files: **h2so4T*.niedziela**

Data: Real and imaginary indices of liquid H_2SO_4/H_2O at 8 temperatures (200 to 300K) from 825 to 4700 cm^{-1}.

Reference: Niedziela, R.F., M.L. Norman, C.L. deForest, R.E. Miller, and D.R. Worsnop, "A Temperature and Composition-Dependent Study of H_2SO_4 Aerosol Optical Constants Using Fourier Transform and Tunable Diode Laser Infrared Spectroscopy," *J.Phys.Chem. A* **103,** 8030-8040 (1999).

Email contact person: R.E. Miller (remiller@unc.edu)
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File: **SutherlandandKhanna.dat**

Data: Real and imaginary refractive indices of organic-based nonvolatile aerosols produced by burning vegetation from 525 to 5000 cm^{-1}. The mixed weed sample indices of Table 2 from the paper by Sutherland and Khanna are tabulated here.

Reference: Sutherland, R.A., and R.K. Khanna, "Optical Properties of Organic-based Aerosols Produced by Burning Vegetation," *Aerosol Science and Technology* **14,** 331-342 (1991).

File: **QuerryandTyler.dat**

Data: Real and imaginary indices of liquid HNO_3/H_2O at room temperature from 250 to 4987 cm^{-1} as a function of the HNO_3 concentration by weight. The concentrations of 3.1, 6.1, 11.8, 22.3, 40.3, and 70% HNO_3 correspond to the molar (M) concentrations of 0.5, 1.0, 2.0, 4.0, 8.0, and 15.7 cited in the Querry and Tyler paper.

Reference: Querry, M.R., and I.L. Tyler, "Reflectance and complex refractive indices in the infrared of aqueous solutions of nitric acid," *J.Chem.Phys.* **72,** 2495-2499 (1980).

File: **hno3t*.biermann**

Data: Real indices of liquid HNO_3/H_2O from 0 to 16382 cm^{-1} and imaginary indices from 432 to 5028 cm^{-1} at 7 tempertatures (213 to 293K) as a function of the HNO_3 concentration by weight.

Reference: Biermann, U.M., B.P. Luo, and Th. Peter, "Absorption Spectra and Optical Constants of Binary and Ternary Solutions of H_2SO_4, HNO_3, and H_2O in the Mid Infrared at Atmospheric Temperatures," *J.Phys.Chem. A* **104,** 783-793 (2000).

Email contact person: B.P. Luo (luo@mpch-mainz.mog.de)
ftp://ftp.mpch-mainz.mpg.de/pub/nwg/

File: **nad*.niedziela**

Data: Real and imaginary indices of nitric acid dyhydrate (NAD) at 3 temperatures (160 to 190 K) from 700 to 4700 cm^{-1}.

Reference: Niedziela, R.F., R.E. Miller, and D.R. Worsnop, "Temperature and Frequency-Dependent Optical Constants for Nitric Acid Dihydrate from Aerosol Spectroscopy," *J.Phys.Chem. A* **102,** 6477-6484 (1998).

Email contact person: R.E. Miller (remiller@unc.edu)
ftp://frenchie.chem.unc.edu/ri/

File: **Richwine_etal.dat**

Data: Real and imaginary refractive indices of nitric acid trihydrate (NAT) at 160 K from 711 to 4004 cm^{-1}.

Reference: Richwine, L.J., M.L. Clapp, R.E. Miller, and D.R. Worsnop, "Complex refractive indices in the infrared of nitric acid trihydrate aerosols," *Geo.Res.Lett.* **22,** 2625-2628 (1995).

Email contact person: R.E. Miller (remiller@unc.edu)
ftp://frenchie.chem.unc.edu/ri/

File: **ice*.clapp**

Data: Real and imaginary indices of water ice at 9 temperatures (130 to 210 K) from 800 to 4004 cm^{-1}.

Reference: Clapp, M.L., R.E. Miller, and D.R. Worsnop, "Frequency-Dependent Optical Constants of Water Ice Obtained Directly from Aerosol Extinction Spectra," *J.Phys.Chem*. **99,** 6317-6326 (1995).

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ftp://frenchie.chem.unc.edu/ri/