Working with Observational and Laboratory Databases

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Scope

- Lecture 1 (Monday): What you need to know when planning, reducing, or analyzing infrared spectroscopic observations of dust and ices.

- Lecture 2 (Tuesday): Basic physical and chemical information derived from interstellar ice observations. *Not discussed:* laboratory techniques (see Palumbo lectures) and surface chemistry (see Cuppen lectures).

- Lecture 3 (Tuesday): Infrared spectroscopic databases. What's in them and how (not) to use them.

- Drylabs (Tuesday): Using databases of interstellar infrared spectra and of laboratory ices. Deriving ice abundances and analyzing ice band profiles.

NOTE: Please download all presentations and drylab tar file:

spider.ipac.caltech.edu/~aboogert/Cuijk/

Observational Infrared Databases Overview

Infrared photometric and spectroscopic databases can be accessed from:

irsa.ipac.caltech.edu

Supported missions: see left column main page

IRSA site contains 'search' capability that will give overview of all data available for a given target, separated in catalogs, photometric data, and spectroscopic data and allows download of those data.

More complex search can be done with full 'Gator' interface. See 'Information' button on main IRSA page for Gator tutorials.

Similar information can be obtained from Simbad, VO tools.

Observational Infrared Databases Overview

Note that search is always done by coordinates, although many sites allow source name to be entered. Be careful that source name corresponds to intended coordinates. Check literature using (don't automatically use SIMBAD coordinates)

simbad.u-strasbg.fr/simbad/

Observational Infrared Databases: Photometry

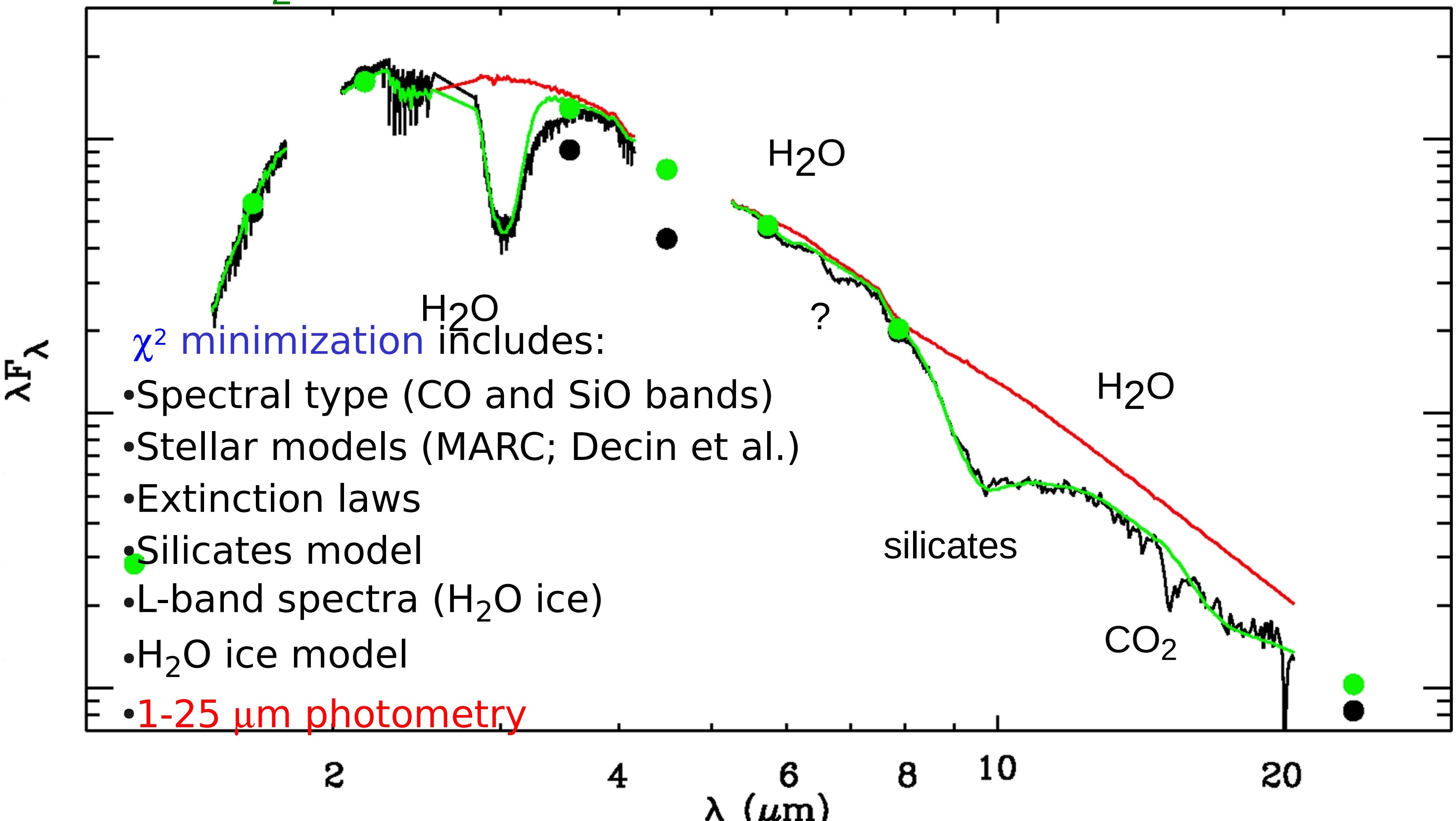
Flux calibration of spectra taken with slit not very accurate (pointing errors lead to photometric errors). Broadband photometric fluxes much more accurate. Does analysis spectra of dust and ices need infrared photometry?

- Usually not for analysis of single absorption features (because τ=-ln(Flux/Continuum))
- Yes, to tie together spectra taken with different facilities or different settings of same instrument
- Yes, to calibrate emission features
- Yes, to get a larger baseline for continuum determination.
- Yes, to get additional physical information, e.g., extinction

Observational Infrared Databases: Photometry

Red: M1 III model and featureless extinction curve at A_K=1.5 magn

Green: H_2O ice and silicate model added



χ² minimization includes:

- Spectral type (CO and SiO bands)
- Stellar models (MARC; Decin et al.)
- Extinction laws
- Silicates model
- L-band spectra (H_2O ice)
- H_2O ice model
- 1-25 μm photometry

Observational Infrared Databases: Photometry

Infrared photometric databases tend to be well documented, complete (all sky or large clouds, galactic plane), and often read to use for science (not always though, e.g., c2d IRAC saturation). Examples, relevant for ice/dust studies.

- **2MASS**: all sky J, H, K-band
- **Spitzer c2d project**: deep 3, 6, 8, 12, 25, 80 um photometry (combined with 2MASS J,H,K) of selected clouds and cores
- **Spitzer GLIMPSE project**: deep 3, 6, 8, 12, 25, 80 um photometry (combined with 2MASS J,H,K) of Galactic Plane
- **IRAS**: all sky 12, 25, 60, 100 um (not sensitive, large beam)
- **WISE**: all sky 3.4, 4.6, 12, 22 um

When using photometric data, be careful with source blending and saturation. Information usually stored in flags, but not always (c2d does not flag saturation!)

Observational Infrared Databases: Spectroscopy

Spectra from infrared spectroscopic databases tend to be of less homogeneous quality and less ready for analysis than data from photometric databases. *Great care must be taken in using these spectra directly for science.*

Spectral databases relevant for ice and dust studies:

- **Spitzer c2d project:** highly processed 5-20 or 5-34 um spectra of low mass YSOs and some background stars in selected clouds and cores. Accessible from IRSA only, in .tbl (ascii) format.
- **Spitzer/IRS enhanced products:** best-effort pipeline processed, no individual enhancements. Accessible from IRSA only, in .tbl (ascii) format.
- **Spitzer/IRS Heritage Archive:** allows enhanced products, highly processed products, and intermediate pipeline products to be accessed. sha.ipac.caltech.edu/applications/Spitzer/SHA

Observational Infrared Databases: Spectroscopy

Spectral databases relevant for ice and dust studies (continued):

- **ISO SWS/LWS**, using
  - Official ESA ISO archive
    - 'official' ISO IDL format (swaa fits files)
    - Highly processed data Frieswijk et al. (swaa fits files)
    - Highly process data Sloan et al. (standard fits files)
  - VOSpec (VO format only, cannot read other formats)
  - simbad.u-strasbg.fr/simbad/ CDS portal (SWAA files, need IDL+OSIA)
  - IRSA: .tbl (ascii) files of standard ('_sws.tbl') and improved ('_pws.tbl') spectra (Sloan et al.)

- **Ground based >3 um spectra:** go to observatory pages (ESO, Keck [KOA at IPAC])...but less ready for science analysis than satellite spectra. E.g., wavelength calibration, sky absorption line correction.

Observational Infrared Databases: Spectroscopy

Note on Virtual Observatory tools. VO tools are sometimes OK to vizualize spectra from public databases, but they are not developed and flexible enough for analysis and comparing to laboratory spectra:

- **Topcat**: star.bris.ac.uk/~mbt/topcat/ good with VO format files, some IPAC .tbl files, some ascii files (laboratory spectra), but has limited analysis capabilities (no polynomial fitting)

- **VOSpec**: esavo.esac.esa.int/vospec/ has poynomial fit capabilities, but insufficient .tbl and ascii file import (works best with VO format files). Access to many databases, but only the VO compatible ones, so not Spitzer/IRS and laboratory ices.

More flexible tools such as IDL and GDL are needed for analysis.

Observational Infrared Databases: Spectroscopy

Spectra from observational databases often suffer from artifacts. Be careful with interpretation of ice and dust features:

- For 'highly processed' ISO and Spitzer spectra, consult the accompanying documentation
- Slit spectroscopy and pointing offsets may give unreliable photometric calibration (Spitzer). Correctable with Spitzer photometry.
- Large aperture may include more than main source (ISO).
- Different apertures/slit widths for different detector bands for a single instrument may cause jumps (ISO and Spitzer)

Observational Infrared Databases: Spectroscopy

Spectral artifacts (continued):

- ISO-SWS issues strongly band dependent: band 2 dark current residuals (wrong zero level), band 3 standing waves, band 4 cosmic ray dominated
- Spitzer/IRS: extraction issues, crowded regions, background residuals, standing waves, hot pixels (LH)
- Akari: source confusion/overlap
- Ground-based instruments: standing waves, atmospheric residuals, wavelength calibration (sky lines best). E.g., VLT/ISAAC pipeline only uses lamp lines, ignoring grating drifts and offset...need to use atmospheric lines.

Databases of Laboratory Ices

No central database of laboratory ices available:

- Laboratories post spectra on their own web sites (but not always!)
- Spectra published as online ascii files accompanying ApJ and A&A papers.
- Some publish only transmission spectra, some transmission+optical constants, and some only optical constants.

Available 'databases':

- **Catania Astrophysical Observatory, Italy**
  - ct.astro.it/lasp/
  - optical constants of pure CO and CO2
  - irradiated CH4 spectra
  - CO2 formed by irradiation experiments

Databases of Laboratory Ices

Available 'databases' (continued):

- **Sackler Laboratory (Leiden, NL):**
  - strw.leidenuniv.nl/lab/databases/databases 2007.htm
  - CO and CO2 ices, pure or mixed with H2O, O2, or N2. Transmission, optical constants, calculated spectra for different particle shapes (Ehrenfreund et al. 1996 A&A 315, 341; 1997 A&A 328, 649)
  - CO2 mixed with H2O and/or CH3OH at different T. No optical constants.
  - Mixed and layered CO/CO2 ices
  - CO over or under or mixed with a number of other species (Fraser et al. AdSpR 2004)
  - UV irradiated mixtures of H2O, NH3, CH4, CO, H2CO, CH3OH, O2, N2, and CO2 at different UV doses and T. Absorbance (optical depth/ln10) spectra, no optical constants.
  - H2O:CO2 ices in various ratios: effect on H2O profile and integrated strength (Oberg et al. 2007, A&A 462, 1187)
  - Pure HCOOH and binary and tertiary mixtures as function of T (Bisschop et al. 2007, A&A 470, 749)

Databases of Laboratory Ices

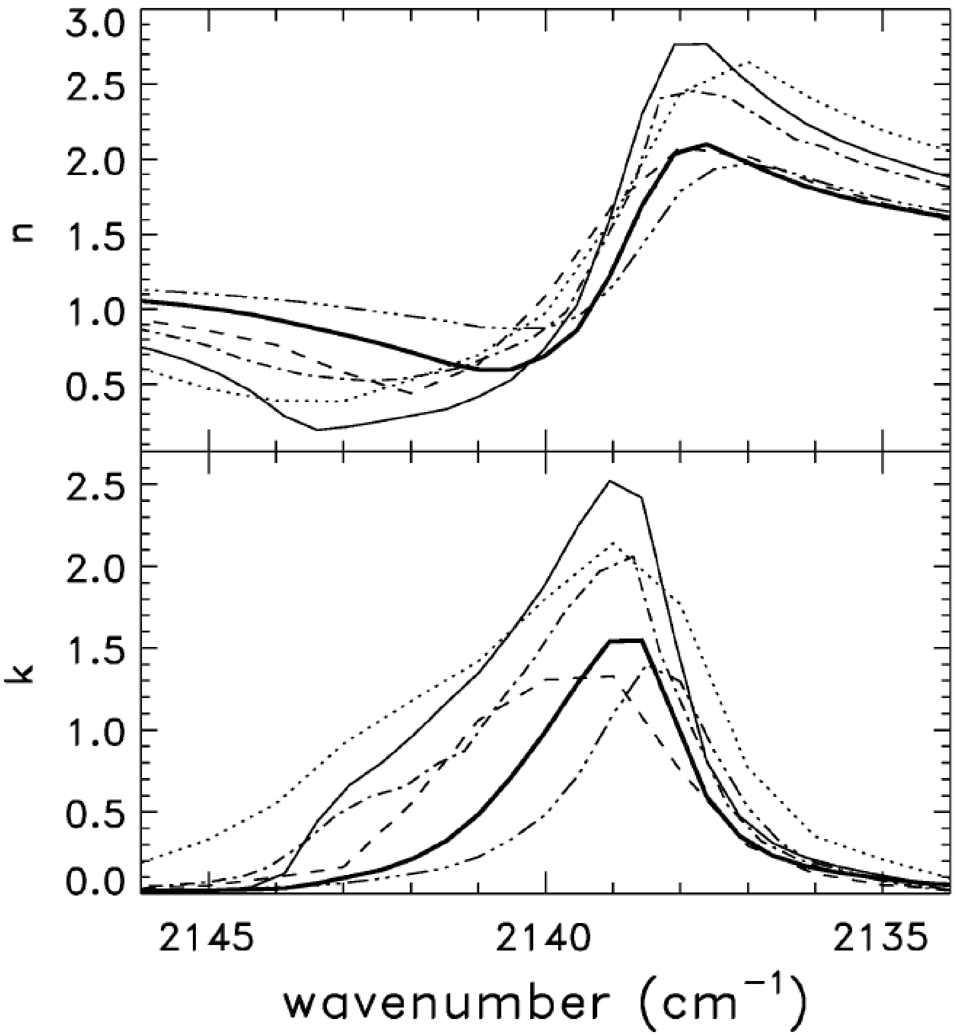
Available 'databases' (continued):

- **NASA Ames (Mountain View, USA):**
  - astrochem.org/db.php
  - Hudgins et al. (1993, ApJS 86, 713) basic transmission spectra and optical constants of H2O, CH3OH, CO2, OCS, CH4, CO2+CH4, CO2+OCS, CO+CH4, CO+OCS, O2+CH4, O2+OCS, N2+CH4, N2+OCS, H2O+CH4, H2O+OCS, H2O+CH3OH+CO+NH3. Range 2.5-20 um, but some 2.5-200 um (!). Also available through online tables ADS/Simbad/Vizier.
  - Optical constants CO ice+mixtures (Elsila et al. 1997, ApJ 479, 818)

- Exhaustive **list of references** (not actual data) of laboratory experiments of simple species:
  - astro.uni-jena.de/Laboratory/Database/jpdoc/2-ices.html
  - astro.uni-jena.de/Laboratory/Database/jpdoc/2-organ.html

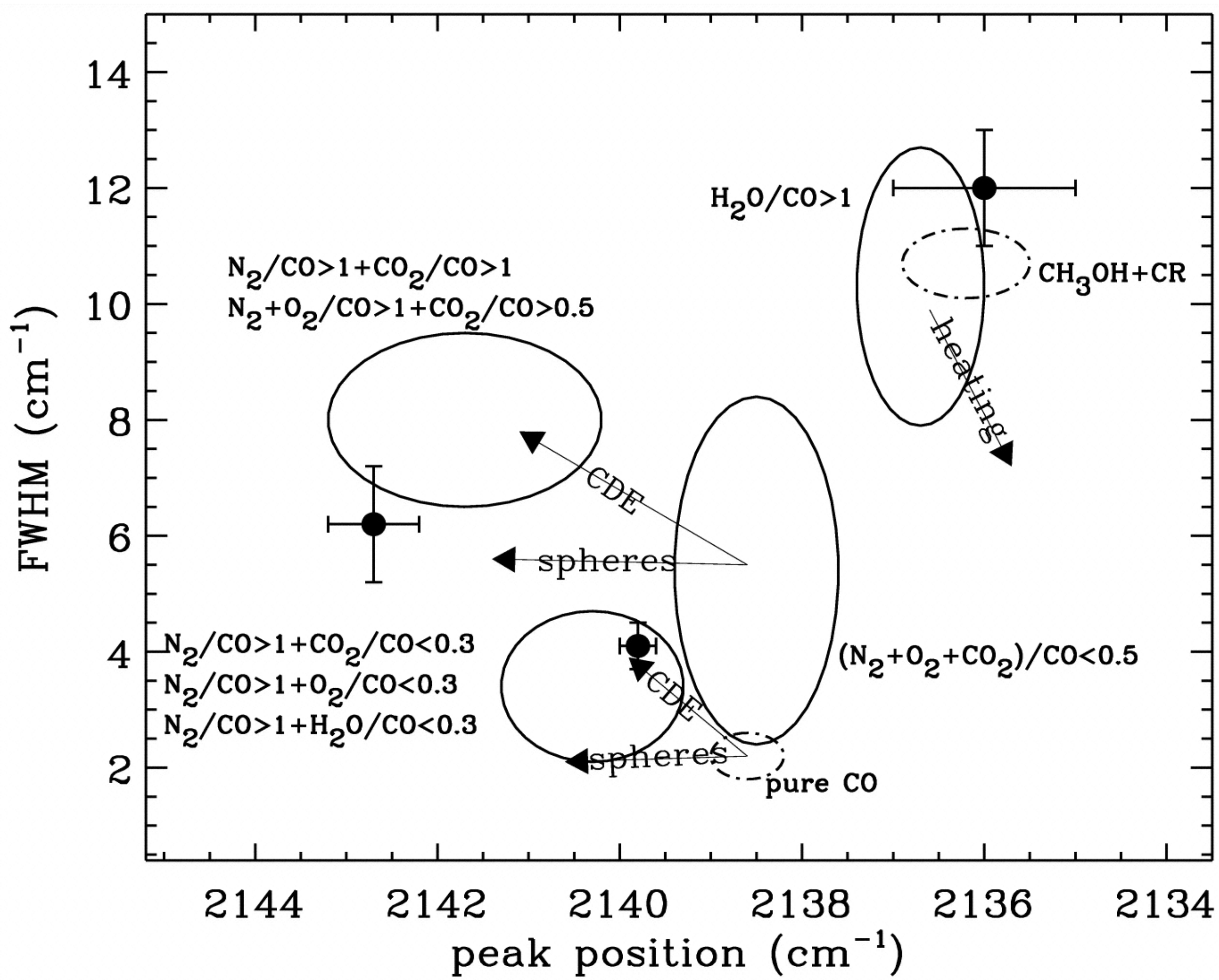
- Online tables accompanying **ApJ and A&A papers.** Example: H2O2/H2O experiments Smith et al. 2011, ApJ 743, 131.

Databases of Laboratory Ices



Warning 1: there are differences in ice preparation, exact composition, data acquisition between different laboratories that limit interpretation of interstellar spectra somewhat. If you can...use spectra from different laboratories for comparison. Example: pure CO (Ehrenfreund et al. 2007)

Databases of Laboratory Ices



Warning 2: many factors influence peak position and shape of ice absorption bands. Do not over-interpret the data. Peak positions versus widths already give much information.