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Models and Observations of astronomical calibration sources
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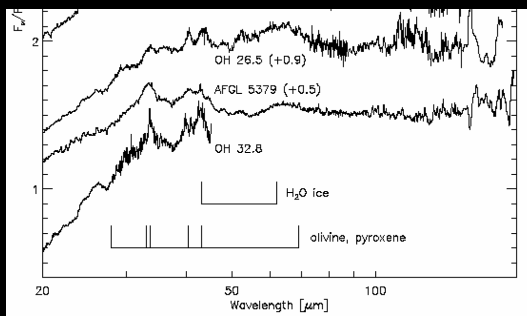
Solid State Features in the Far-Infrared

Franz Kerschbaum,
Thomas Posch (Vienna)
&
Harald Mutschke (Jena)

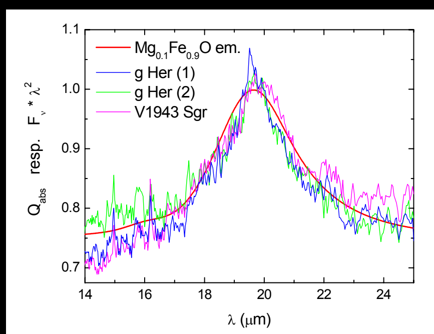
ISO's Astromineralogy Legacy

- ISO caused a revolution in the field of astromineralogy in all dusty environments from the earliest to the latest stages of stellar evolution (for an overview, see Henning 2003)
- But most of these findings were in the SWS- and not the LWS-range!
- Herschel-PACS operational in the 57-210μm range with unprece-dented sensitivity and spatial resolution - What can we expect?



Sylvester et al. (1999)

Posch et al. (2002)



Some basic physics

Principal mechanisms for emission in the 57µm+ range:

1. Lattice vibrations of heavy ions and/or ion groups with low bond energies

- Example KBr is highly transparent in the NIR and MIR (matrix material for transmission spectroscopy!) but opaque in the FIR (transverse optical mode at 86µm). NaCl and KCl are similar cases (61 and 69µm, respectively)
- This can be understood by a harm. oscillator law (e.g. Beran et al. 2004):

$$\lambda_{vib} \propto \sqrt{\frac{\mu}{k}}$$

with μ being the reduced mass and k the force constant.
- Limited range of mass numbers of dust forming elements

Some basic physics

Principal mechanisms for emission in the 57µm+ range:

2. Phonon-difference processes

- Phonon-difference processes mainly contribute to the continuum emissivity (e.g. Mitra & Nudelmam 1970)
- No well defined individual bands expected
- Nevertheless their contribution to the continuum may partly mask FIR bands

Comparison of grains (Jones 2004)

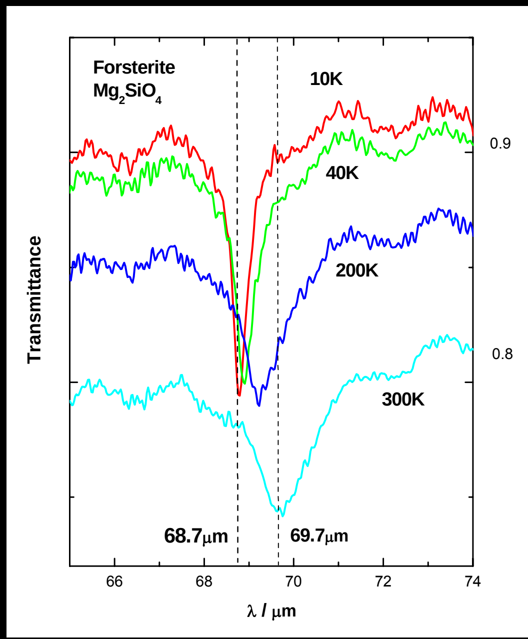
interstellar	circumstellar	pre-solar
aromatic hydrocarbons aliphatic hydrocarbons	aromatic hydrocarbons aliphatic hydrocarbons	[aromatic hydrocarbons]
	[nano]diamond	graphite Nanodiamond
amorphous silicates	amorphous silicates [aluminosilicate]	amorphous silicates (GEMS) **5 grains known**
	Mg-rich crystalline silicates (forsterite, Mg_2SiO_4 enstatite, $MgSiO_3$ diopside, $CaMgSi_2O_6$)	Mg-rich crystalline silicate (forsterite, Mg_2SiO_4 **only 1 grain!**) olivine (3 grains) pyroxene (4 grains)
[Mg & Fe oxides]	oxides ($Fe_{0.9}Mg_{0.1}O$, spinel, $MgAl_2O_4$ corundum, Al_2O_3)	crystalline oxides (spinel, $MgAl_2O_4$ hibonite, $CaAl_{12}O_{19}$, corundum, Al_2O_3)
	β-SiC	β-SiC
		TiC (as inclusions in graphite) Si_3N_4

Dust composition as a function of MLR

stellar mass loss rate [M_{Sun} yr $^{-1}$]	dust composition	after Waters (2004)
$\approx 10^{-7}$	**oxides ($Fe_{0.9}Mg_{0.1}O$, spinel, $MgAl_2O_4$ corundum, Al_2O_3),** amorphous silicates	a minor component
$\approx 10^{-6}$	amorphous silicates	observed in emission
$\approx 10^{-5}$	**amorphous silicates,** **crystalline silicates (olivine & pyroxene)**	**self-absorbed** **Fe-poor** **5-15 % of dust mass**
$> 10^{-5}$	**H_2O ice**	also observed
PNe (e.g. NGC 6302)	diopside ($CaMgSi_2O_6$), calcite ($CaCO_3$), dolomite ($CaMg(CO_3)_2$)	also in RL OH/IR stars Origin ??? < 1 % of cold dust mass

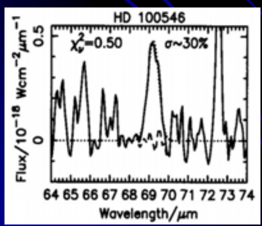
Forsterite

- Crystalline silicates initially identified by Waelkens et al. (1996) on basis of ISO-SWS observations and subsequently also in ISO-LWS spectra) with forsterite's 69μm band (Malfait et al. 1998)
- Bowey et al. (2002) showed that the 69μm band strongly sharpens at low temperatures in parallel to a shift in peak position (for 295, 77 and 3.5K)
- We complement these results by measurements at 300, 200, 40 and 10K
- Respective transmittance spectra show a shift of the band position from 69.7 to 68.7μm, consistent with Bowey et al.



Powder pellet, sample thickness 0.8mm

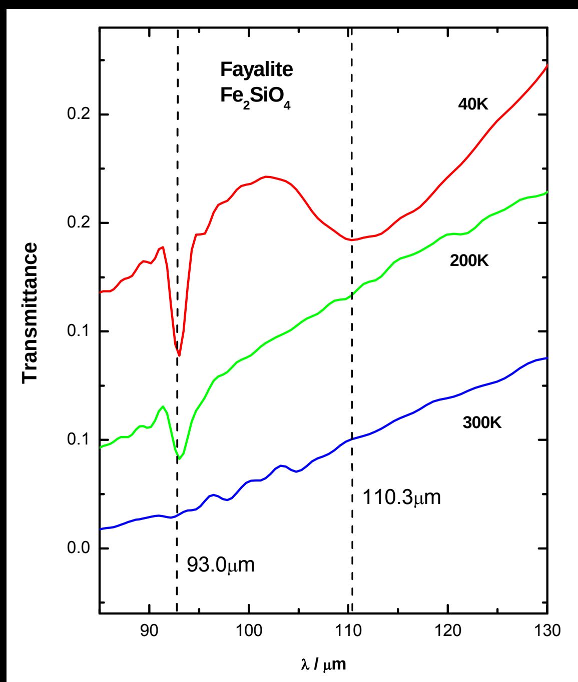
See also Koike et al. and Suto et al. (2004)



Bowey et al. (2002)

Fayalite

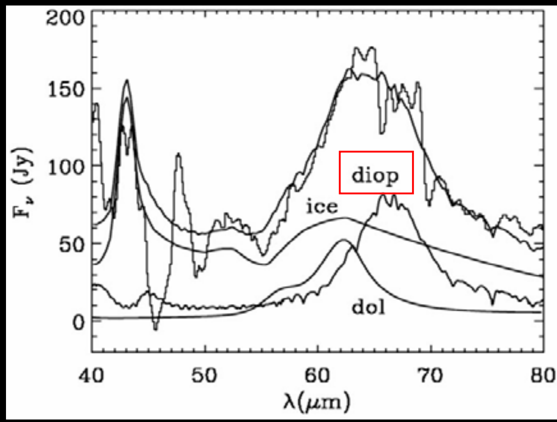
- Iron-rich endmember of olivine group
- Hofmeister (1997): at least two vib. bands in Herschel-PACS range centered at 94 and 110μm with the latter seen in powder transmission spectra only if sample thickness and S/N ratio are sufficient
- New measurements of both bands at low temperatures (T=200K for the 93-94 μm band, T=40K for the 110μm band needed).
- For the 93-94μm band: significant sharpening as sample cools down
- T-dependence of position: 93.0μm at 200K, 92.9μm at 40K and 92.6μm at 10K
- Mutschke et al. (2004) will present a detailed analysis of olivines at low T!



Powder pellet, sample thickness 0.8mm

Diopside

- Koike et al. (2000): crystalline diopside has a peak wavelength of lowest energy vib. band at 65-66µm. Peak not present in amorphous diopside!
- Compared to the 60+µm bands of crystalline orthoenstatite, clinoenstatite and orthopyroxene, its 65-66µm band is much stronger
- Found in planetary nebulae (Koike et al. 2000, Kemper et al. 2002)
- SF-regions such as the Carina Nebula and S171 also exhibit a 65-66µm emission feature attributable to crystalline $CaMgSi_2O_6$ (Onaka & Okada 2003)



NGC6302, Kemper et al. (2002)

Other Silicates

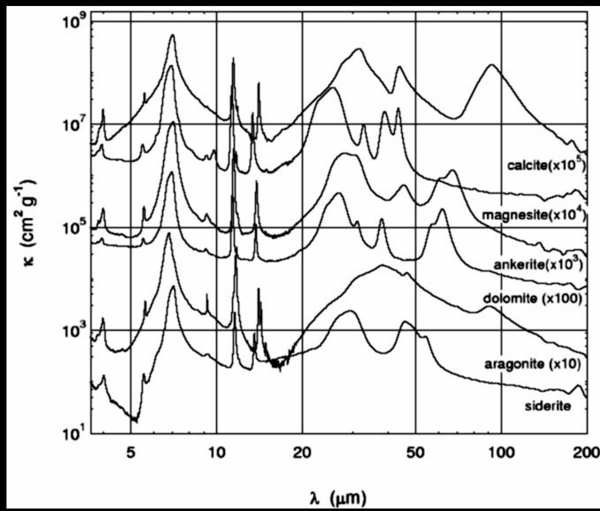
There do exist others silicate of astrophysical relevance with signatures in the 60+µm range:

- Malfait et al. (1999) consider montmorillonite - a hydrous silicate containing Ca, Na, Al, Mg and Fe - as carrier of a broad band centered at 100-110µm, detectable in the spectrum of the young star HD 142527!
- Gehlenite ($Ca_2Al_2SiO_7$): broad band at 66µm
- Fassaite ($(Ca,Na)(Mg,Fe,Al,Ti)(Si,Al)_2O_6$): band at 62µm

(Keller & Flynn 2003, LPI Conf. Abstr. 34, 1903)

Carbonates

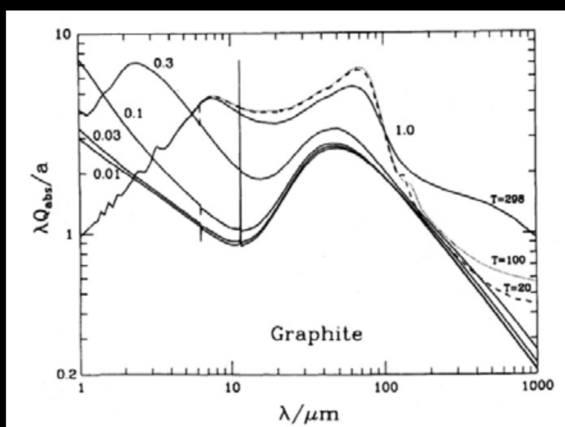
- Several carbonates have features of considerable strength in the 60+µm range (e.g. Kemper et al. 2002)
- These resonance features are not related to C-O stretching or bending modes, but to translations of metal cations (Ca, Mg, Fe) relative to the plane of the CO_3 anions following our earlier 'weak bond strength argument'
- Typical examples are: Calcite ($CaCO_3$) at 92µm Dolomite ($CaMg(CO_3)_2$) at 62µm



NGC6302, Kemper et al. (2002)

Graphite

- Hexagonal polymorph of carbon
- Sharp features in the MIR and a broad band at 50-70µm
- Draine & Lee (1984) pointed out that:
  - exact position of this broad band depends both on grain size and grain temperature
  - Grain sizes < 1µm: maximum of absorption efficiency at 50µm
  - Grain size of 1µm: maximum is shifted to 70µm
  - At low temperatures (100K), the width of the band is reduced from 100µm to 70µm!
  - Electronic origin of the feature (inter-band transition)
  - Even when broad and weak it may contribute to the uncertainty of the continuum!



Water ice

Frosty Leo in I,J, H
Roddier et al. (1993)

- Water ice has quite significant FIR-features!
  - The 44-46µm band is present both in amorphous and crystalline (hexagonal) water ice, the 62µm-band only in crystalline H_2O ice
  - At 120-130K: phase transition from the amorphous state (extremely low temperatures) to the crystalline state (at intermediate temperatures)
  - The 44-46µm band shifts in position at this transition (~46 → ~44µm), the 62µm band emerges

  → The 62µm band is an ideal diagnostic tool for the lattice structure of H_2O in cosmic dust (see e.g., Maldoni et al. 1999 and references therein)
  - The 62µm feature originates in the longit. acoustic mode of crystalline H_2O; the 44-46µm feature is the transverse optical mode

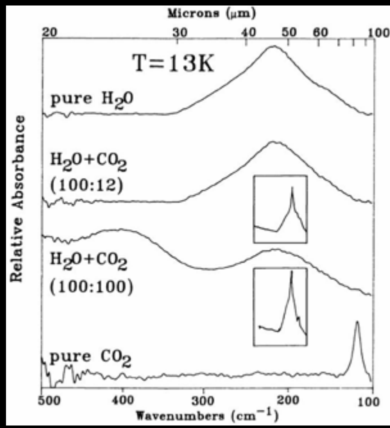
Water ice

Frosty Leo in I,J, H
Roddier et al. (1993)

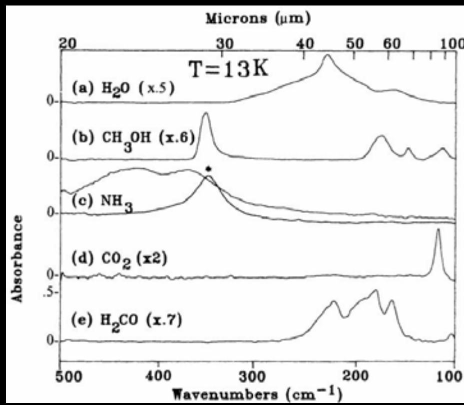
- Environments in which the 62µm water ice feature is detected:
  - Omont et al. (1990): IRAS 09371+1212 (Frosty Leo nebula), a post-AGB star with extremely cold dust (see Barlow et al. (1998) for more post-AGB stars)
  - Kemper et al. (2002) found water ice (1%) in the PN NGC 6302
  - Malfait et al. (1999) detected it in some Herbig Ae/Be stars
  - Molinari (1999) detected it in the Herbig-Haro object HH 7

Other ices

- Methanol ice (α-CH_3OH): according to Moore & Hudson (1994), amorphous form shows broad band 67.7µm (at 13K), while crystalline methanol ice has bands at 68.0 and 88.5µm
- Dry ice (CO_2): Amorphous phase shows a rather sharp feature located at 85.5µm (at 13K); the crystalline form has an even sharper ~85µm band with a quite strong T-dependence of the band position (40K and below: 88.5µm; 85K: 85.5µm) (Moore & Hudson 1994)
- Considering both the temperature dependences and the likelihood of mixtures of different ice species in space (formation of core-mantle-grains!), a lot of laboratory work remains to be done in this field!



Amorphous mixtures [+annealed]



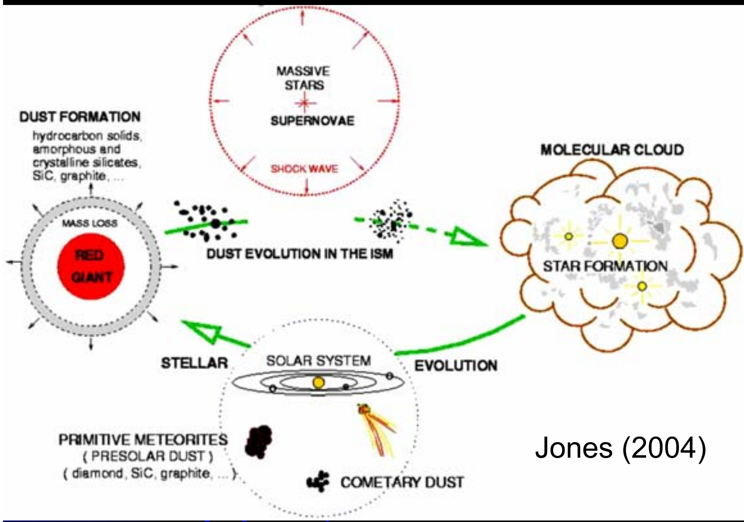
Crystalline forms

Selected dust and ice species with bands in the 60+µm range

Mineral	chemical formula	band positions [µm] (at λ > 60µm)	ref.
Forsterite	Mg_2SiO_4	69-70	[1]
Fayalite	Fe_2SiO_4	93-94, 110	[1]
Diopside	$CaMgSi_2O_6$	65-66	[2]
Calcite	$CaCO_3$	92	[3]
Dolomite	$CaMg(CO_3)_2$	62	[3]
Graphite	C	50-70	[4]
Water ice	H_2O	62	[5]
Methanol ice	α-CH_3OH	68, 88.5	[6]
Dry ice	CO_2	85	[6]

[1] Posch et al. (2004), [2] Koike et al. (2000), [3] Kemper et al. (2000), [4] Draine & Lee (1984), [5] Maldoni et al. (1999), [6] Moore & Hudson (1994)

Dust Evolution

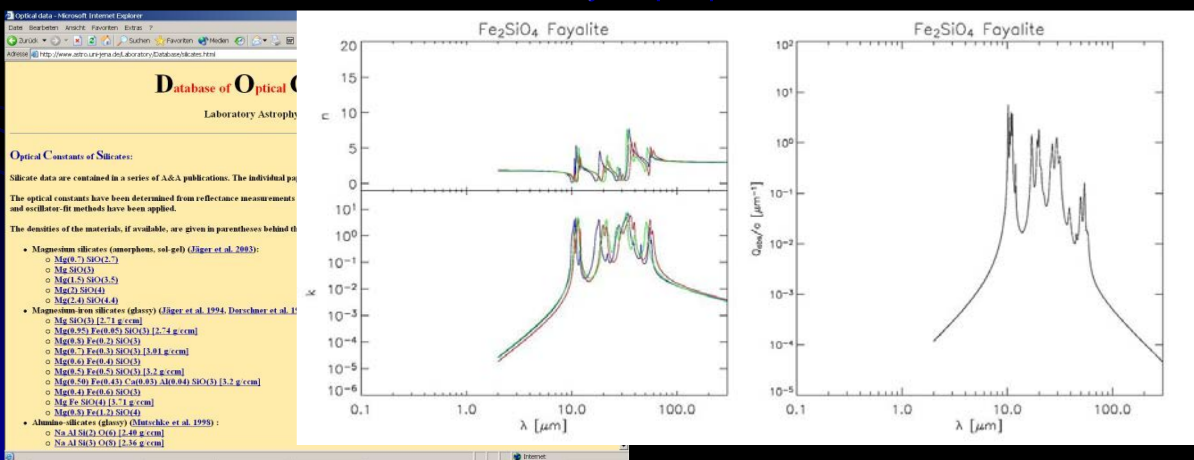


- Photo-processing
- Photo-destruction
- Amorphization (cosmic rays)
- Grain shattering/sputtering in supernovae shocks or turbulent clouds
- Grain coagulation
- …

Subsequent changes in optical properties need to be studied in the laboratory in much more detail!

Jena-Database of optical constants of astronomically relevant solids

- The Jena-database already provides the refractive index n(λ) and the absorption index k(λ) of a large number of silicates, oxides, sulfides and carbon materials from own laboratory measurements: *http://www.astro.uni-jena.de/Laboratory/Database/databases.html*
- A visualisation of n(λ), k(λ) and the absorption efficiency (Q_{abs}/a) linked to the database is currently in preparation



Some selected other databases

- St. Petersburg database: http://www.astro.spbu.ru/JPDOC
- B.T. Draine's page: http://www.astro.princeton.edu/~draine/dust/
- Astrobiology Group, Leiden: http://www.astrobiology.nl/isodb/index.html
- ASTER spectral library, JPL: http://speclib.jpl.nasa.gov/
- Crystran Ltd, Dorset, UK http://www.crystran.co.uk

Two printed classic atlases unfortunately only out to 25 µm:

- Salisbury J.W., Walter L.S., Vergo N, D'Aria D.M. (1991), *Infrared (2.1 – 25µm) Spectra of Minerals,* J.Hopkins University Press, Baltimore
- H. Moenke (1962), *Mineral Spektren,* I, Akademie-Verlag, Berlin

Summary

- In general the 57µm+ range is not as rich in vibrational bands as the MIR range is
- This is due to the typical masses and force constants of the relevant ions and group of ions in cosmically abundant solids
- The 57µm+ range contains some features that can serve as indicators of local physical/chemical conditions (e.g. 69µm forsterite or 62µm water ice)
- Further lab work should concentrate e.g. on the T-dependence of FIR spectra including very low temperatures