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A database of optical constants of cosmic dust analogs

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Abstract

We describe the current state and future of the WWW Jena-Petersburg database of optical constants (JPDOC) that also contains references to papers and links to internet resources related to measurements or calculations of the optical constants of materials of astronomical interest. The most important part of the JPDOC are data measured in broad wavelength ranges and partly at low temperatures in the Jena Laboratory. To demonstrate the use of these data, we show as examples infrared refractive indices of crystalline and amorphous magnesium silicates, spinel, and hydrogenated amorphous carbon and calculate the absorption cross-sections of small particles composed of these materials.

Keywords: Spectroscopy; Optical constants; Databases; Light scattering

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1. Introduction

Nanometer- and micrometer-sized solid particles are distributed in the interstellar medium and play an important role for astrophysical processes such as star and planet formation. These particles show a rich chemistry and mineralogy as has been revealed by spectroscopic astronomical observations in the last decades. Many new observational data have been measured in the last years, e.g. by the Infrared Space Observatory in 1995–1998, and the interpretation of these spectroscopic data is still in progress. This requires the comparison with data of "analog materials" delivered by spectroscopical laboratories.

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Various terrestrial analogs of cosmic solids have been studied in chemical and physical laboratories. However, many of these experiments neither took into account the specifics of cosmic dust materials (composition, lattice structure, processing, etc.), nor covered the wavelength intervals of the current astrophysical interests. Note also that these data are mainly in the form of graphics in papers, and free world wide web (WWW) resources on the optical constants are generally limited by several collections of refractive indices for a few materials.

Since 1992, the Astrophysical Institute and University Observatory (AIU) Jena operates a Chemical and Spectroscopical Laboratory with the goal to study optical properties of analog materials of cosmic dust in the wavelength range from the ultraviolet to the far infrared. During this period, a compilation of optical constants (i.e. the complex refractive index $m=n+ik$ or the complex dielectric function $\varepsilon=m^2$) of such materials has been created. In collaboration with the Astronomical Institute of St. Petersburg University, this collection was expanded into an internet database that has been made available for the public in 1998 at *http://www.astro.uni-jena.de/Users/database/entry.html* or *http://www.astro.spbu.ru/JPDOC/entry.html*.

In this paper, we describe the current state and future of the database and give several examples of the data it contains and their possible applications.

2. Electronic database

2.1. Current state

The Jena-Petersburg database of optical constants (JPDOC) provides access to *references* to the papers, *data* files and *links* to the internet resources related to measurements and calculations of optical constants in the wavelength interval from X-rays to the radio domain. The materials being considered are:

- amorphous/glassy/crystalline silicates of different kinds,
- silicon, SiO, crystalline/fused SiO_2,
- metals: Fe, Mg and others,
- oxides: FeO, Fe_2O_3, Fe_3O_4, MgO, Al_2O_3, $MgAl_2O_4$,
- sulfides: FeS, MgS, SiS_2,
- carbides: SiC, FeC, TiC,
- carbonaceous species: diamonds, graphite, coals, kerogens, HAC, glassy/amorphous carbon, PAHs and so on,
- organics: tholin, “organic refractory”, etc.,
- ices: H_2O, CO, CO_2, NH_3, HCN, etc., and their mixtures,
- FeSi, $CaCO_3$ and others.

The database contains more than 1000 references to the papers, reports, dissertations where the refractive index, reflectivity, transmittance, etc., were derived. It also gives references to useful books and reviews on the subject. Data accessible via the JPDOC are mainly those measured in the laboratory of the AIU Jena supplemented with data freely available in the internet. The database also provides links to internet collections of optical data files and personal WWW pages with relevant software.

The first version of the JPDOC was described in [1]. In the following years (1999–2001) only minor improvements were made. All the time the site was rather well visited—on average about five visitors a day and all together over 5000 visits for 3 years—and many visitors found the database helpful. That encouraged us to make essential updates in 2002. We increased by about 25% the number of references to papers (not only to the recent ones) in physical and astronomical journals as well as to books and reviews. Further, we opened access to more data from the Jena Laboratory, connected new pages presenting recently calculated low-temperature Rosseland and Planck mean opacities, included new materials (FeSi, $CaCO_3$, etc.), gave more links to other internet resources (incl. Ioffe Institute site, database of optical properties (DOP), etc.), and presented some more graphical illustrations and information about the physical properties of the materials.

2.2. *Future plans*

We intend to continue including new data and collecting references and links to resources on the subject. Collaboration is planned with the Physical Institute of the St. Petersburg University, Ioffe Physical Institute and the St. Petersburg Institute of Precise Mechanics and Optics. If it is successful, original data and bibliography for the materials—interesting not only for astronomical but some other applications—will be involved as well.

Some changes of the general design of the database are planned too, but main efforts will be directed at extension of the JPDOC. The next step will be the creation of the DOP of scatterer models which will include the JPDOC as a part.

2.3. *Database of optical properties*

In astrophysics, the optical constants are mainly used to calculate the optical properties of scatterers, i.e. cross-sections, scattering matrix, etc. For many applications, it is necessary to understand general trends in the data. This understanding can often be gained from consideration of results obtained by simplified scattering models. Optical properties derived from such models have been discussed in some books (see, e.g. [2,3]). In principle they can be calculated by using various light-scattering tools which are freely available via the internet [4]. Nevertheless, there is a definite necessity of a WWW database devoted to systematic consideration of the optical properties of various model scatterers and related topics. As of this writing, our database will include:

- original codes realizing various methods to calculate the optical properties of homogeneous and inhomogeneous, spherical and nonspherical particles;
- review(s) of exact and approximate methods of light scattering theory (including discussion of their applicability ranges);
- a review on the effective medium theory (EMT) and computer programs to mix the optical constants for composite particles according to different EMT rules;
- a database of several thousands references to papers on various aspects of light scattering theory and its applications;
- a graphics library illustrating light scattering by particles of different size/shape/structure (a part of the data will be in tabular form to serve as benchmarks);
- a special tool to calculate on-line selected optical characteristics of different scatterers (homogeneous and core-mantle spheres, infinite cylinders, spheroids, etc.);

- a self-training algorithm of determination of the optical properties of randomly oriented fractal-like clusters of spherical particles based on an artificial neural network (perceptron) (see [5] for more details);
- a collection of links to related internet resources.

The work on all the parts of the DOP is either in progress or has been finished. It is undertaken by several persons from different institutes of former Soviet Union countries under support of an INTAS grant. The DOP will be (partly) available via the Internet [6] upon its completion scheduled at the end of 2002. Because of the large volume due to the graphics library, the whole database may be available only on CDs.

3. Examples of data contained in the JPDOC

Most of the materials studied in Jena are synthetic compounds prepared especially for the purpose of spectroscopic investigation. They include silicates in both amorphous and crystalline state, oxides of magnesium, iron, and aluminum, sulfides, and carbon in different forms. Chemical and physical analytical methods were generally applied to confirm the homogeneity, composition, and crystal structure of the products prior to the spectroscopic measurements. Further, some natural crystals (oxides and silicates) have been included in the studies. If necessary, data have been determined for the different crystallographic axes. For part of the compounds, data are available at cryogenic temperatures. A summary of the data currently available is given in Table 1. In the following we give some examples of the data and their possible applications.

3.1. *Crystalline silicates*

Silicate minerals of the olivine and pyroxene classes have been shown to be present in outflows of evolved stars as well as in comets and protoplanetary disks. The positions of the infrared emission

Table 1
Summary of data measured in the Jena laboratory, which are currently available from the JPDOC

Compound	Composition	Cryst. state	Spectral range	Data sets	At 10 K
Silicates	$(Mg, Fe)SiO_3$, $(Mg, Fe)_2SiO_4$	Glassy	UV/VIS/IR	10	1
	$MgSiO_3$, $(Mg, Fe)_2SiO_4$	Cryst.	IR	2	1
	$MgSi_xO_y$	Amorph.	UV/VIS/IR	5	1
	$(Ca, Al, Mg, Fe)Si_xO_y$	Amorph.	IR	13	
Sulfides	$(Mg,Fe)S$	Cryst.	IR	5	1
	SiS_2	Cryst.	IR	1	
Oxides	$(Mg,Fe)O$	Cryst.	UV/VIS/IR	6	1
	Al_2O_3	Amorph.	IR	2	
	$(Mg, Al)O_x$	Cryst.	IR	8	
Carbon	a-C:H	Amorph.	UV/VIS/IR	6	

bands produced by these minerals are diagnostic for the crystal structure as well as for the chemical composition, especially the iron content. Comparison of the laboratory data with observed features can constrain the conditions in these environments which have led to the formation or processing of the dust grains.

We have used the infrared optical constants of forsterite contained in the database for calculating the absorption cross sections of spherical and nonspherical particles with sizes small compared to the wavelength (see Fig. 1). The calculations have been performed for prolate spheroidal shapes with the long spheroid axis corresponding to the crystallographic c direction. The spectra show resonances due to surface modes which shift very strongly as a function of the aspect ratio of the particles. This effect is probably very important for the identification of emission features in astronomical spectra [8,9]. Interstellar polarization measurements and laboratory experiments on the growth of silicate particles [10] support the presence of elongated grains in astrophysical environments. Information about the grain shape may provide constraints for the formation mechanism of crystalline silicate grains, i.e. the role of direct condensation vs. processing of previously amorphous material.

3.2. Amorphous magnesium silicate

About 85–90% of the dust condensing in the envelopes of oxygen-rich evolved stars consist of amorphous magnesium or magnesium–iron silicates [7]. Therefore, special attention is paid to the production and spectroscopic characterization of analog materials for this dust component. The comparison between differently produced magnesium silicates demonstrates that the amorphous state of any magnesium silicate is not unique. There exist different possibilities for the structural arrangement of subunits in the amorphous silicate network, similar to the varying structures of amorphous carbon.

Optical constants (n, k) of stoichiometric and nonstoichiometric magnesium silicates with Mg/Si ratios from 0.7 to 2.4 produced by the sol–gel method have been derived from reflection measurements by a combination of Kramers–Kronig analysis and Lorentz-oscillator fit method (see Fig. 2). The absorption cross sections calculated for particles small compared to the wavelength show that the Mg/Si ratio influences the position and the width of the 10 and 20 μm bands. With increasing MgO content the 10 μm band shifts to longer wavelengths whereas the 20 μm band becomes broadened and centered at shorter wavelengths.

The astrophysical relevance of these sol–gel silicates was tested by comparison of optically thin model spectra based on the new optical data with the dust emissivity derived from ISO-SWS spectra of AGB stars in the range between 8 and 30 μm. The emission spectrum of TY Dra, an evolved dust-forming star, can excellently be reproduced by the models, suggesting that the dust grains may indeed consist of pure amorphous Mg silicate [11].

3.3. Magnesium–aluminium oxide (spinel)

Magnesium–aluminium spinel ($MgAl_2O_4$) has been considered as a primary condensate in the outflows of oxygen-rich AGB stars and as a potential carrier of the 13 μm emission band observed in the spectra of these stars [12]. Therefore, in the Jena laboratory, a systematic study of the infrared properties of Mg–Al oxides of both synthetic and natural origin was performed in order to derive the

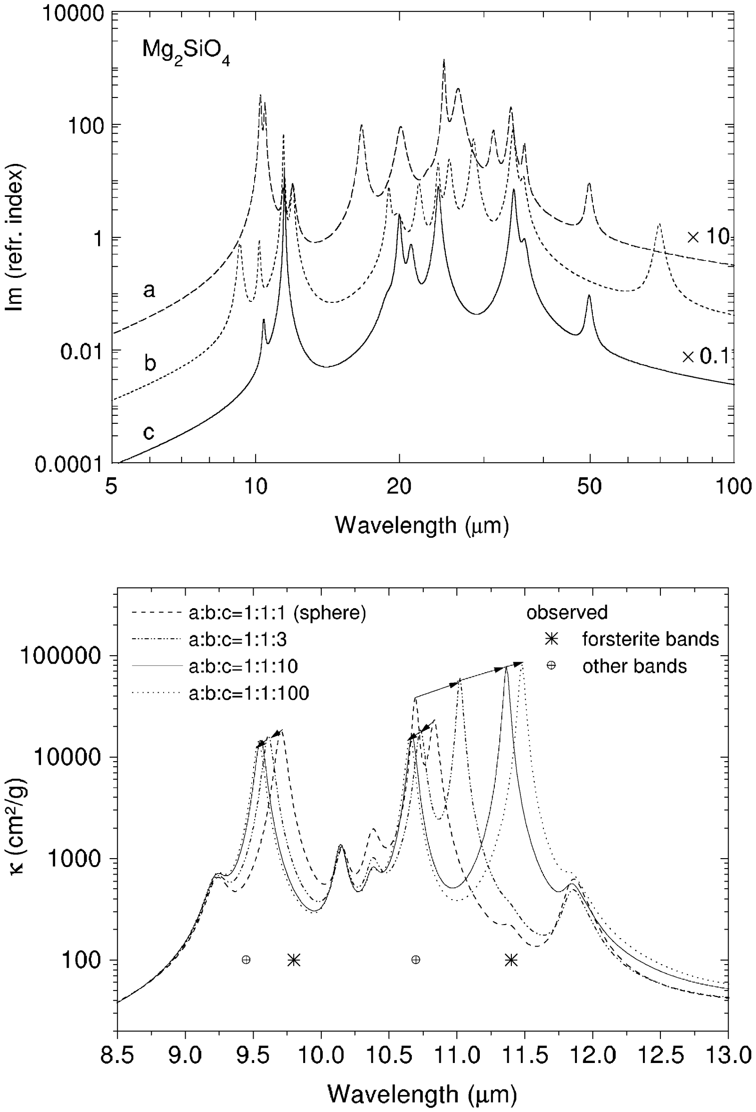

Fig. 1. Upper panel: Imaginary part of the refractive index for crystalline forsterite (Mg_2SiO_4) in the three different crystallographic directions. Lower panel: Mass-normalized absorption cross section of prolate spheroidal forsterite particles (averaged over all spatial orientations) with different axis ratios. The dots and asterisks below the spectra indicate positions of astronomically observed emission bands (after [7]).

optical constants of these materials. This led to the discovery of two accompanying features in the astronomical spectra at larger wavelengths, thereby strongly supporting the idea of spinel condensates in AGB star outflows (see Fig. 3, [13]). Recently, the experiments have been extended in the direction of Ca–Al oxide minerals [14] and condensation studies of oxide grains in low-pressure oxygen-rich atmospheres.

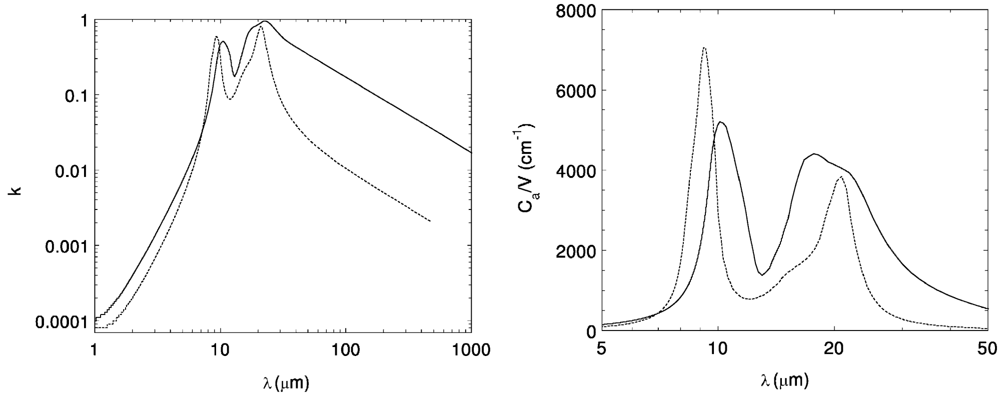

Fig. 2. Left panel: Imaginary part of the refractive index for amorphous Mg$_{0.7}$SiO$_{2.7}$ (dotted line) and Mg$_{2.4}$SiO$_{4.4}$ (solid line). Right panel: Absorption cross section normalized to particle volume calculated for a continuous distribution of ellipsoidal grain shapes (CDE [3], grain sizes small compared to the wavelength) composed of the same materials.

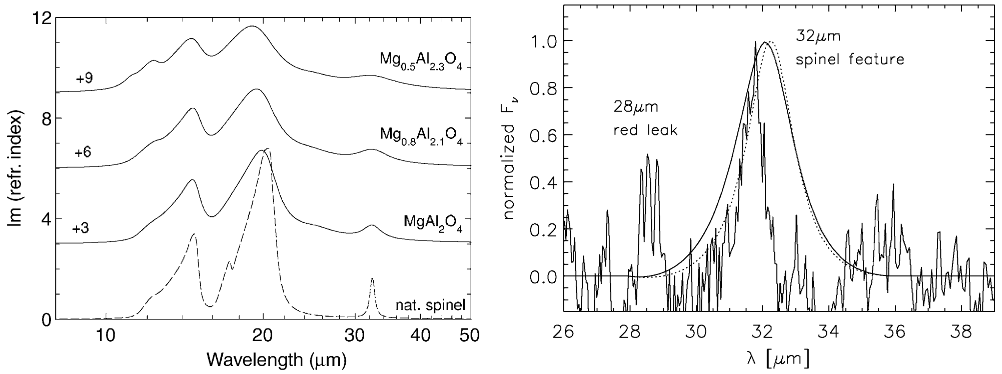

Fig. 3. Left panel: Imaginary part of the refractive index for synthetic and natural magnesium–aluminium spinels. Right panel: Calculated normalized absorption spectra for spherical particles small compared to the wavelength composed of natural spinel (smooth solid line) and synthetic MgAl$_2$O$_4$ (dotted line) in comparison to the band profile of the newly discovered 32 μm feature [13]. “Read leak” denotes an instrumental artifact in the astronomical spectrum.

3.4. Hydrogenated amorphous carbon

Amorphous carbonaceous materials can show a great diversity of optical properties due to the variability in their nanostructure. Especially in the infrared range, the optical constants can differ by orders of magnitude according to the conducting or insulating electrical behavior of the material. The amorphous-carbon data contained in the database cover a wide range of these properties as is illustrated by Fig. 4. The differently pyrolized celluloses are representative for a suit of carbonaceous material ranging from strongly disordered (mainly aliphatic, lower pyrolysis temperature) to graphitized (mainly aromatic, higher pyrolysis temperature) material.

Especially interesting for astronomy is the calculation of the absorption and scattering cross sections for particles small compared to the wavelength. Fig. 5 shows that particles composed of the

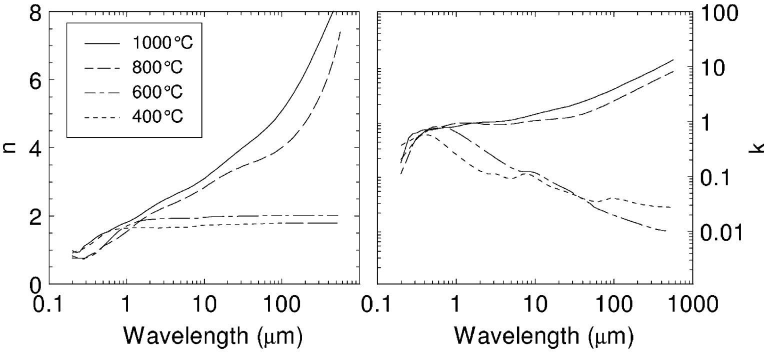

Fig. 4. Complex refractive index of hydrogenated amorphous carbon prepared by pyrolysis (annealing) of cellulose at different temperatures.

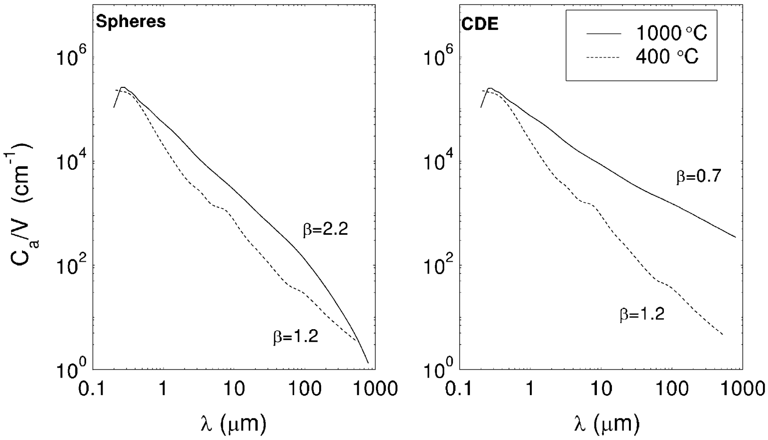

Fig. 5. Volume-normalized absorption cross section calculated for spherical grains small compared to the wavelength (left panel) and a continuous distribution of ellipsoidal grain shapes (CDE [3], right panel) from the optical data given in Fig. 4.

strongly disordered material (400°C) produce an absorption which is smaller by up to 3 orders of magnitude compared to particles formed from the graphitized material (1000°C). The absorption cross section of carbonaceous particles in the far infrared ($\lambda > 100$ μm) can be fitted by a power law ($C_{abs}/V \sim \lambda^{-\beta}$) depending strongly on the internal structure of the carbon materials and on the particle shape. In the case of spherical grains, the spectral index β is considerably lower for the highly disordered material than for the carbon material pyrolized at higher temperature. With increasing graphitization due to a higher pyrolysis temperature there is a gradual increase of β [15].

Our calculations for different particle shapes show that there is no morphological effect on the spectral index of the low-temperature samples in contrast to the more graphitic materials. For the latter materials we find a significantly lower index in the case of broad shape distributions (CDE) compared to spherical grain shapes. This is caused by percolation effects, present in the more graphitized samples which contain free charge carriers. We should note that the results of the CDE calculations serve as an illustrative example. For a more realistic calculation, one has to assume a special aggregate structure and/or shape distribution of the individual particles [16]. For extreme values of the refractive indices, however, computational methods for the calculation of the absorption by aggregates or elongated particles become numerically cumbersome and may even fail.

4. Summary and outlook

We have presented recent developments in the Jena-Petersburg database of optical constants (JPDOC) and have demonstrated examples for the application of optical constants contained for purposes of comparison with astronomical spectroscopic observations.

The database will be continued to be improved. This will include measurements on further analog materials of cosmic dust such as oxide and carbonaceous particles from gas condensation experiments, nanodiamonds, and others. An extensive database will give better possibilities to achieve uniqueness in the identification of astronomically observed bands and provide the possibility to study grain size, shape and agglomeration effects in a realistic way.

The authors will highly acknowledge any contribution to the database such as references, data files and links to be included in the database.

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