# THE INFLUENCE OF PARTICLE SHAPES AND SIZES IN THE CO ICE BAND PROFILE THE INFLUENCE

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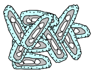
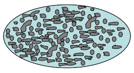
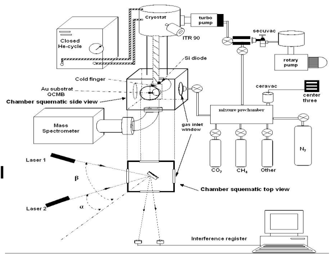
**Dust particles play a key role in the balance of thermal control in different astrophysical environments such as interstellar and circumstellar media and cometary dust tails. The grain morphology can change from one astrophysical environment to another. However, ices such as $H_2O$, CO and $CO_2$ are typical constituents. They form a mantle covering the small core grains. The coagulation could lead to the formation of heterogeneous mixtures (ice/silicates/carbonaceous material) in a volume or an aggregate. Light is scattered and absorbed by these dust particles and emitted in the infrared (IR) range. Absorption and emission spectra and extinction curves give information about the constituents. The peak profiles and their position are influenced by different factors, such as molecular environment [1, 2], temperature [3, 4, 5], irradiation history [6, 7] and particle shape and size [8, 9].**

**Our knowledge of chemical and physical properties of ices in astrophysical environments is mainly based on the comparison between observations and laboratory measurements.**

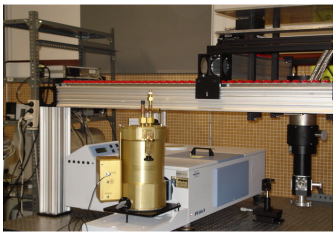
**The laboratory measurements of IR ice spectra of astrophysical interest are obtained from films formed by deposition at low temperature on a flat substrate. However, in the astrophysical environments grains grow and ices are mixed in a volume or aggregate.**







Scheme of the experimental setup



The spectrometer Bruker IFS 66v/S, the movable cold finger and the bolometer

**Regarding the observations, there are two independent solid CO components which are observed along most lines of sight (one narrow band generally centered at about 2140 $cm^{-1}$ and a broader one at 2136 $cm^{-1}$). Laboratory studies with astrophysical relevant mixtures of CO and $CO_2$ ices have shown that the narrow CO band at 2140 $cm^{-1}$ occurs in mixtures dominated by non-polar molecules ($CO_2$, $O_2$, $N_2$), and the broad feature is due to mixtures with polar molecules such as $H_2O$ ice as have been shown by some authors [2, 10, 11, 12].**

**These authors also carried out calculations with scattering codes trying to understand the possible influence of the physical characteristics of the grains on these features profiles. Therefore, it is of great interest to study how the grain morphology (shape and size) could affect the CO and $CO_2$ ice band profiles.**

## CALCULATIONS:

**We have calculated the extinction factors of some CO and $CO_2$ ice bands using Mie and Discrete Dipole Approximation codes. Shapes such as spheres, spheroids of axis ratio 5, the so-called compact irregular particle (DW1996) and aggregates of spheres randomly generated with a size monomer of 0.17 µm have been considered. The aggregates have been generated by For the generation of the aggregates we performed a Fortran implementation of both a particle-cluster aggregation (PCA) and a cluster-cluster aggregation (CCA) method. PCA process starts with a single sphere in a fix position. mechanism. Initially, the calculations have been carried out by considering only ice as constituent. The results are the followings:**

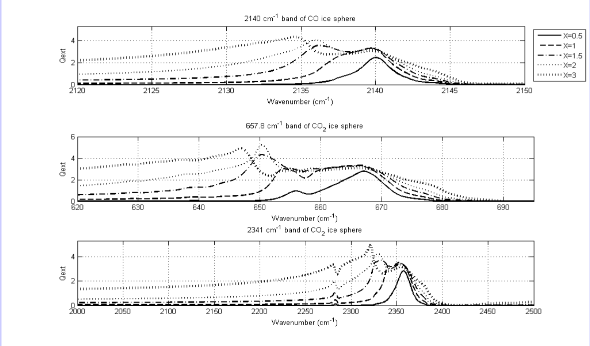


**Fig.1:** The extinction factors of the 2140 $cm^{-1}$ band of CO ice sphere (up) and 657.8 and 2341 $cm^{-1}$ bands of $CO_2$ ice sphere (center and bottom) versus the wavenumber for values of size parameter of 0.5, 1, 2 and 3.

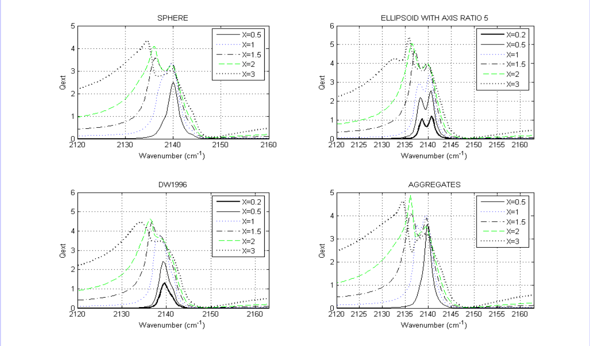


**Fig.2:** Comparison of the extinction factors of the 2140 $cm^{-1}$ band of CO ice for shapes: sphere (top left), ellipsoid (top right), DW1996 (bottom left) and aggregate randomly generated with a size monomer of the 0.17 µm (bottom right) from values of the size parameter from 0.5 to 4. These aggregates are shown in the next figure.

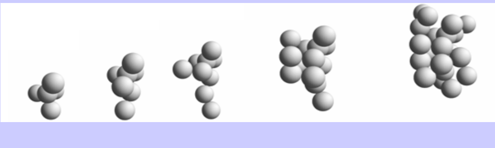


**Fig. 3:** An image of five aggregates randomly generated with a radius monomer of 0.17 µm. The size parameters of each aggregate are 0.5, 1, 1.5, 2 and 2.5, respectively (from left to right).

**We have tested the influence of including silicate as constituent. In order to do this we have randomly changed the refractive index of 25% of the dipoles. A comparison between the extinction factors obtained for a mixture of ice (75%) and silicate (25%) and the extinction factors previously calculated with only CO ice as a constituent for the aggregates showed in Fig. 3 and for size parameters of 0.5, 1, 1.5 and 2 is shown in the next figure.**

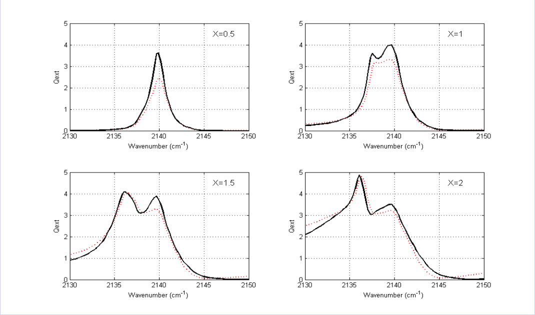
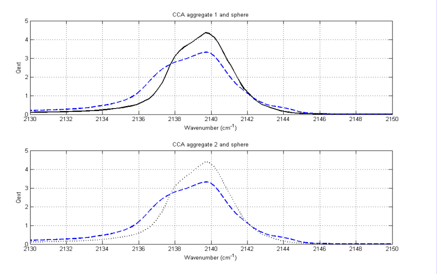


**Fig.4:** The extinction factors corresponding to aggregates of CO ice with silicate (dotted line) with the shapes shown in Fig. 3. The radius of the monomers is set to 0.1 microns and the size parameter to 0.5 (up-left), 1 (up-right), 1.5 (bottom-left) and 2 (bottom-right) compared with the results previously obtained to these aggregates without silicate (solid line).

**For the generation of the aggregates we performed a Fortran implementation of both a particle-cluster aggregation (PCA) and a cluster-cluster aggregation (CCA) method. Fig. 5 shows an image of two new aggregates. We set the radius of the monomers of these aggregates to 0.1 µm and the size parameter of the whole particle to X=1. Both aggregates were generated with the CCA technique, which gives fluffier particles than PCA method. In Fig. 6 the extinction factors of the aggregates (with radius of the monomers 0.1µm) are compared to the extinction factors obtained for a sphere of X=1. As it is shown, the profiles of both of the aggregates are almost the same, and quite close to those corresponding to the sphere.**



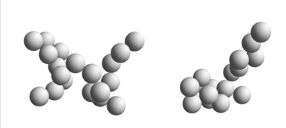


**Fig. 5:** An image of two aggregates 1 and 2 generated with PCA method. The radius of the monomer was set to 0.1 µm and the size parameter of the particles to X = 1.

**Fig. 6:** Comparison of the calculated extinction factors of the aggregate 1 (solid line) and aggregate 2 (dotted line) in Fig. 5 and the extinction factors obtained with a sphere (dashed line) of about X=1.

## RESULTS:

**1.- A broad scattering peak, slightly displaced towards red with respect to the absorption peak for size parameters larger than X=1, for all studied cases.**

**2.- Some particle shapes with size parameter smaller or equal 1 (the ellipsoid of axis ratio 5 and the aggregate with radius of the monomer 0.7 µm), the profile of the CO ice band appears as double peak structure due to the surface modes.**

**3.-The calculations including silicate have shown variations in the band strength but not significant changes in the feature of the profile. the random method used to add the silicate inclusions would be improved by changing the refractive index of not only of isolated dipoles if not of several dipoles surrounding every one.**

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