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ON THE POSSIBLE DETECTION OF SOLID O_2 AND O_3 INTERSTELLAR GRAINS WITH ISO

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ABSTRACT

In various models of interstellar grain chemistry, solid O_2 is formed by accretion as well as by surface reactions on grains. In dense molecular cloud models, at a later stage of the evolution, the O_2 molecule may become a substantial grain mantle constituent. Since IR dipole vibrational transitions for the homonuclear diatomic molecule O_2 are forbidden, the abundance of this potentially important grain mantle component can not be determined. However, embedded in a dirty ice matrix, the fundamental vibration of O_2 at ~ 1550 cm^{-1} becomes observable at 10 K, due to interactions with surrounding molecules, which break the symmetry of molecular oxygen. This process might be applicable for the dust mantle environment of interstellar grains. We have studied the role of solid O_2 and O_3 in astrophysically relevant ice mixtures and discuss the possible detection of solid O_2 and its major photolysis product O_3 in interstellar grains, in dense molecular clouds. Both molecules represent a specific target to be observed by the ISO satellite in the near future.

INTRODUCTION

Infrared observations provide an important tool to study interstellar chemistry. Many interstellar dust molecules have been already identified by comparing laboratory data with interstellar spectra /1,2/. These molecules reside on interstellar dust grain, which consist of a silicate core and an organic refractory mantle. In dense clouds at very low temperatures a dirty ice mantle is accreted /3,4/. Energetic UV photoprocessing of these dirty ice mantles (mostly UV photolysis) creates new molecules and radicals on the grain surface which are potential targets for astronomical observations /5/. There is even evidence that very complex molecules reside on interstellar grains /6/.

Oxygen, the most cosmic abundant element after H and He plays an important role in interstellar chemistry. In various models of interstellar grain chemistry, solid O_2 is formed by accretion as well as by surface reactions on grains. In dense molecular cloud models, at a later stage of evolution, the O_2 molecule may become a *substantial* grain mantle constituent, at the expense of the water ice abundance /4,7,8/.

Gas phase models about the form in which oxygen occurs are still contradicting. Either O_2 is the major species and atomic oxygen and H_2O depleted or most of the oxygen is still in atomic form and O_2 and H_2O are reduced /9/. Ground based observations are not able to solve this problem. Only satellite observations are able to measure correct abundances.

A diatomic homonuclear molecule like O_2 shows no transitions in the infrared (IR). Therefore no direct estimates of the abundance can be obtained. But the fundamental vibration of solid O_2 was however detected in the mid-IR, in laboratory experiments in various matrices /10,11,12/.

In this paper we discuss the possibility to detect solid O_2 and its photolysis product O_3 on interstellar grains outside the Earth's atmosphere with the ISO satellite.

METHODS

Laboratory spectra have been obtained with matrix isolation spectroscopic techniques. The interstellar icy grain mantle is simulated by condensing pure gases or gas mixtures on a 12 K polished aluminum substrate, situated in a vacuum chamber. Samples were exposed to irradiation from a vacuum UV hydrogen discharge lamp, which provides a very constant flux of 10^{15} photons s^{-1} cm^{-2}. IR spectra were obtained using an FTS IR Digilab spectrometer between 4000 - 500 cm^{-1} in reflection at a resolution of 4 cm^{-1}. The integrated cross section A_m ($cm.mol^{-1}$) in various matrices was calculated according to /13/.

RESULTS

By depositing a mixture of $CO_2 : O_2$ (10 : 1) onto the 10 K Al substrate we detected a weak absorption band at 1559 cm^{-1} corresponding to the predicted fundamental transition of molecular oxygen (**Fig. 1**) /12/. The result could be confirmed by measuring the isotopic shift of 90 cm^{-1}, using isotopically labelled $^{18}O_2$ under the same experimental conditions. The experimentally determined frequency for $^{18}O_2$ falls at 1470 cm^{-1} in the diluted CO_2 matrix. The integrated cross section for molecular oxygen diluted in CO_2 (1 : 10) has been calculated to be A_m ($cm.mol^{-1}$) = 3 ± 1x 10^{-18}, using the integrated absorbance A_m of the bending mode of CO_2 at 15.2 μm /14,15/.

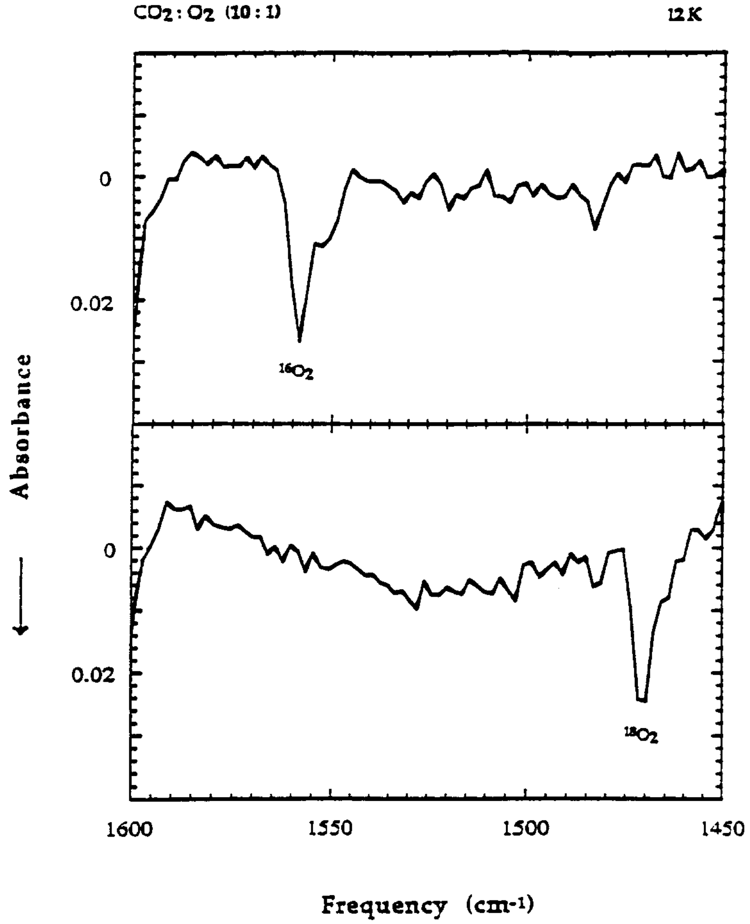

Fig. 1 Fundamental vibration of solid $^{16}O_2$ and $^{18}O_2$ in a CO_2 matrix ($CO_2 : O_2$/ 10:1) at 10 K

The behaviour of solid oxygen in astrophysically relevant ice mixtures was investigated by depositing a typical interstellar gas mixtures containing H_2O, CO, and CO_2 together with $^{16}O_2$. The O-H bending mode of the water ice band falls at ~ 1650 cm^{-1} and is characterized by an asymmetric wing at the long wavelength side, where the band of molecular oxygen is observed. Therefore the oxygen band was not detected or blended in experiments with a high amount of water ice. This result indicates that an environment where solid H_2O is highly abundant, will not be favourable for the detection of this weak O_2 transition.

The fundamental band of molecular oxygen is clearly visible at 1551 cm^{-1} with a half width of 8 cm^{-1} and is not blended by the water ice band in a gas mixture containing $H_2O : CO : O_2 : CO_2$ 2 : 2 : 1 : 0.5 /12/. This gas mixture corresponds to the calculated fractional abundances of grain mantle species evolving from a starting gas phase cosmic gas phase O/C ratio of ~ 3 in a dense molecular cloud at 10^7 years /8/.

Further experiments indicated the variation of the cross section of molecular oxygen in

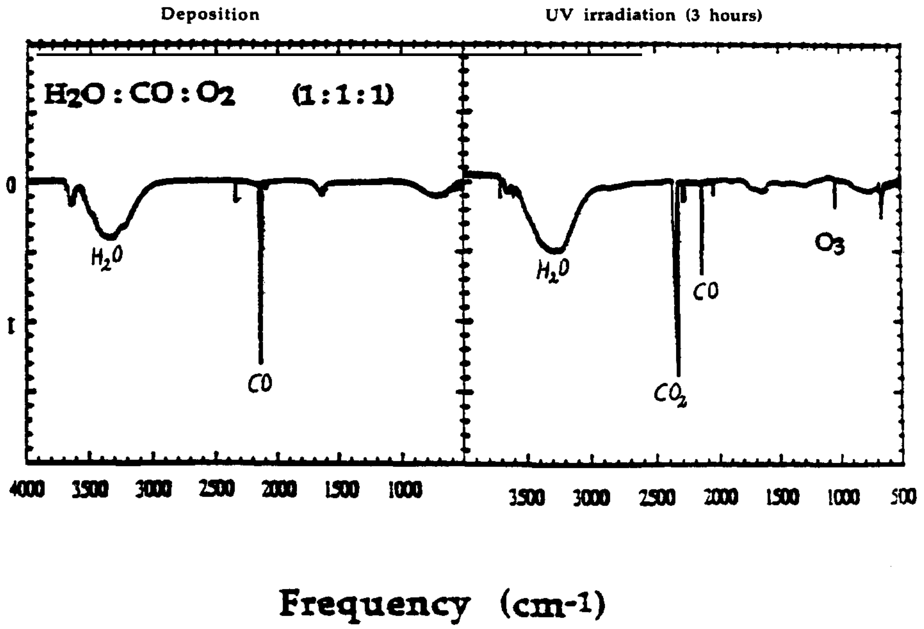

Fig. 2 IR spectrum of "dirty" ice mixture H_2O : CO : O_2 (1: 1: 1) before and after UV irradiation. The ν_3 band of O_3 at 1038 cm^{-1} as well as newly appearing bands,

e.g. to CO_2 can be observed

different ice mixtures. To have an correct estimation of O_2 abundances it will be therefore necessary to measure also the abundances of H_20, CO_2 and CO on grain mantles in the observed regions. The non-polar molecule CO_2 is responsible for the enhancement of the weak vibrational transition of O_2 in laboratory matrices, a process which may be applicable for interstellar grain mantles.

Laboratory experiments of irradiated ice mixtures containing solid O_2 show a strong, sharp band appearing at 9.6 µm (1038 cm^{-1}) with a FWHM of 9 cm^{-1}. This absorption at 1038 cm^{-1} is assigned to the ν_3 band of O_3 /16,12/. Its is assumed, that ozone is easily produced by the photodissociation of O_2 in the interstellar medium and the ν_3 strongest vibrational transition at 1038 cm^{-1} (9.6 µm) can be observed. Though this band can be obscured by the strong absorption band of silicates at 10 µm, it could still be detectable and show a narrow peak within the broad silicate feature. In **Fig. 2** we show an irradiated ice mixture and the appearance of a strong feature of ozone and CO_2 after UV irradiation. In **Fig. 3** we show the band of solid ozone in comparison with the measured telluric absorption. The correct removal of the numerous ozone bands of the Earth's atmosphere will complicate the possible detection of cosmic solid ozone by ground based observations.

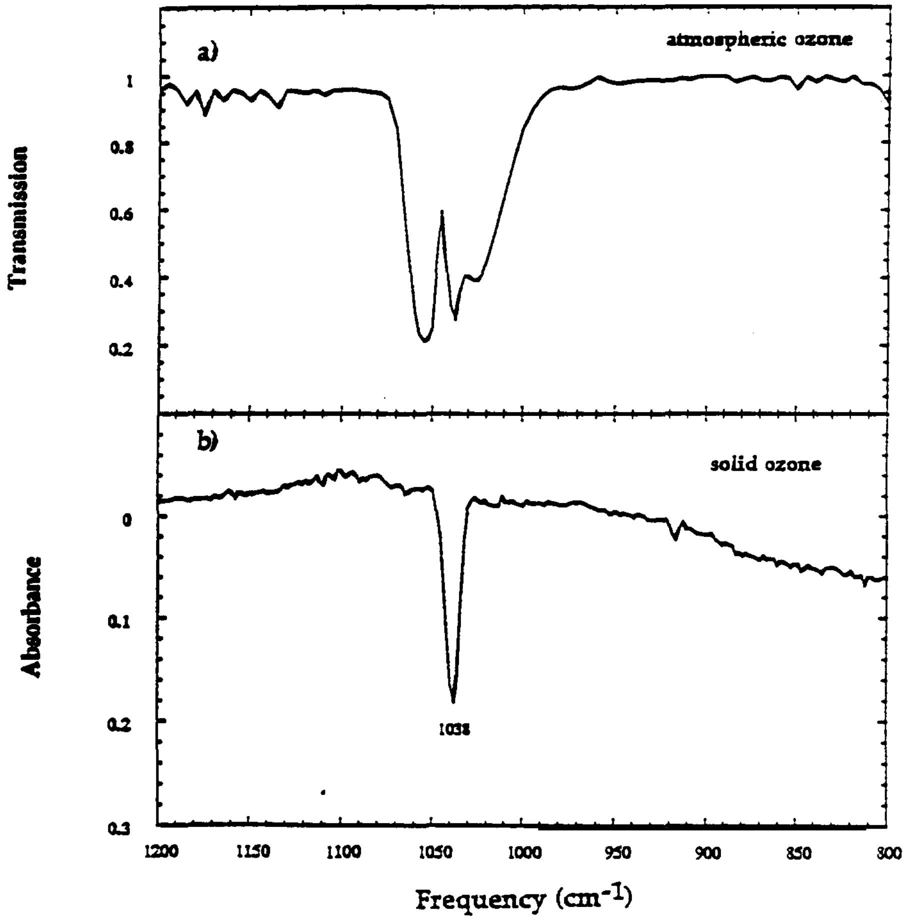

Fig. 3 a) atmospheric transmission expected at an altitude of 4000 m /19/
b) IR spectrum of the ν_3 band of ozone trapped in a molecular ice at 10 K

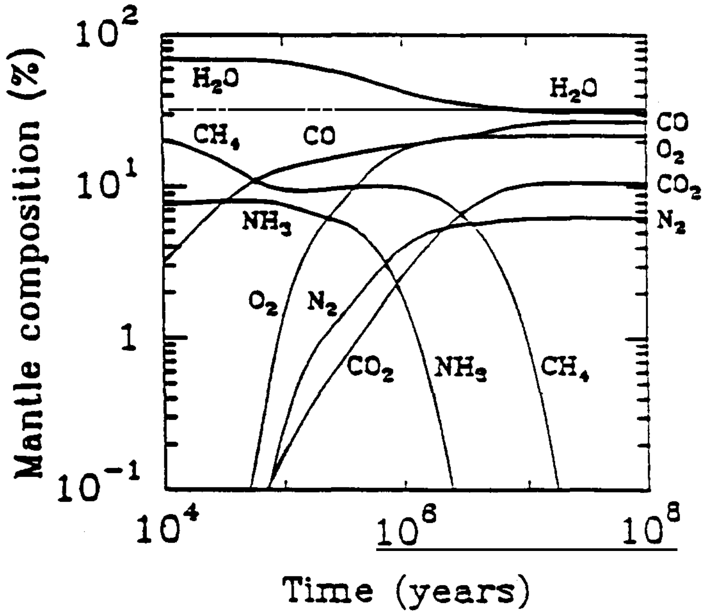

Fig. 4 Time evolution of the grain mantle composition for a dark cloud (taken from Breukers, 1991).

DISCUSSION

A time evolution of the grain mantle composition for a dark cloud has been calculated by /8/. **Fig. 4** shows the time evolution of the grain mantle composition for a dark cloud. Calculations for dense molecular clouds show that C and H are rapidly converted into CO and H_2 respectively at a very short timescale of a few times 10^5 years. As H is depleted, the production of solid H_2O decreases, resulting in a lower grain mantle fraction of solid H_2O. Other species such as O_2, N_2 and CO_2, may then constitute a major fraction of the grain mantle.

The best targets for the search for the fundamental transition of O_2 and O_3 are dense molecular clouds with high extinction. In the case of solid ozone astronomical sources with a non-saturated silicate feature have to be selected in order to observe the sharp band of ozone at 9.6 µm. Tielens et al. /17/ have shown, that grain mantle components dominated by non-polar ice mixtures containing CO_2, N_2, O_2 and CO are present in protostar regions. These environments are particularly important to observe. Regions where other grain mantle constituents have already been identified can be helpful to probe the presence of molecular oxygen. The observed shape of the solid CO band in W3/IRS 5 and AFGL 490 are best fit by CO/O_2 mixtures and they represent therefore excellent observational targets for the search of O_2 /17/. Additionally, sources with large CO column densities like NGC 7538/IRS 9 and Elias 16 are a good choice in view of the volatility of O_2.
The abundances of solid CO in various sources has been derived by /17/. Column densities of molecular oxygen which show a clear appearance of the fundamental transition in the laboratory spectra (at 4 cm^{-1} resolution) are around 1.0 10^{18} /12/. From our laboratory experiments we expect an optical depth of about 10^{-2} in objects like NGC 7538/IRS9, if O_2 is a dominant species in grain mantles in the line of sight. Although this imposes a very high quality data requirement, such an observation is within the capabilities of ISO. If solid CO_2 is abundant in grain mantles, the detectability of O_2 may be greatly enhanced.

It follows from all that was said above that an observatory operating outside the Earth's atmosphere is needed to detect unambiguously molecular oxygene and ozone in the interstellar medium, because only there all telluric absorption is eliminated and the infrared background emission is sufficiently small. A unique opportunity for the kind of observations proposed in this paper will be provided by the Infrared Space Observatory (ISO) satellite with its short wavelengths spectrometer (SWS). SWS has two grating spectrometers which cover the wavelength region 2.4 - 45 µm with spectral resolving powers between 1000 - 2000. It can detect a line flux of 3 10^{-16} W/m^2 at a signal to noise ratio of 20 within 900 s /18/. SWS grating spectra are composed of subspectra which are taken instanteneousely by arrays of 12 detectors, covering a spectral range of 8 resolution elements. Applying the sensitivity values given in the Scientific Capabilities Document to the case where one wants to make a grating line measurement at 6.5 µm (9.6) µm with an S/N ≥ 100 (taking the small optical depth into account) of a source with flux 30 Jy, one finds that the integration time for a subspectrum with width 0.04 µm is only 36 (72)s.

We expect the full bandwidth of the O_2 and the O_3 lines to be larger than the width of such a subspectrum, and therefore a partial wavelength range grating scan to be the optimum observation strategy. To cover the wavelength range 6.3 - 6.6 and 9.2 - 10.0 µm with this observing mode takes in our example around 2300 s all overheads included.

The detection of solid oxygen and ozone and the estimation of the abundances of these molecules represents an exciting tool in infrared astronomy and can be used to reveal the important role of oxygen in the interstellar medium.

We conclude that the comparison of laboratory spectra and astronomical observations and in particular, observations with the ISO satellite represent an important task to derive the abundance of various constituents of the interstellar grain mantles.

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