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## NEW INSIGHTS IN THE PHOTOCHEMISTRY OF GRAIN MANTLES:

THE IDENTIFICATION OF THE 4.62 AND 6.87  $\mu\text{m}$  BANDS

by

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The mid-IR spectral region of molecular clouds is known to show the fingerprints of molecules frozen in the icy mantles of the interstellar grains. So far, only a few molecules have been positively identified:  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{OCS}$ ,  $\text{H}_2\text{S}$  and  $\text{CH}_3\text{OH}$ . With the recent identification of the 4.62  $\mu\text{m}$  absorption band in W33A with the  $\text{OCN}^-$  ion (Grim and Greenberg 1987) a new field of potential candidates became available. To study in more detail the complex chemical and physical interactions going on in the ice mantles accreted on grains in molecular clouds we performed numerous experiments involving UV irradiation and diffusion experiments. We present here some new ideas about the photochemistry of molecular ices, whereas the diffusion will be addressed in the paper by Schmitt *et al.*.

Although our ultimate aim was to study irradiated astrophysically relevant molecular ices for comparison with interstellar spectra, we have started our research with the irradiation of binary ices. Using isotopic labelling on  $\text{NH}_3/\text{CO}$  and  $\text{NH}_3/\text{O}_2$  ices we have identified numerous compounds, of which the  $\text{OCN}^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ , and  $\text{NH}_4^+$  ions are the most interesting ones since they reveal a new type of chemical reactions. It appeared that these compounds were formed by proton transfer reactions induced by the interaction between an acid ( $\text{HNCO}$ ,  $\text{HNO}_2$ ,  $\text{HNO}_3$ ) and a base ( $\text{NH}_3$ ) through a hydrogen bond. This mechanism has been confirmed by a study of photolyzed diluted argon mixtures ( $\text{Ar}/\text{NH}_3/\text{CO}$  and  $\text{Ar}/\text{NH}_3/\text{O}_2$ ) that were allowed to anneal slowly, permitting the transfer reactions to occur. Using the collected data of these two particularly studies, we reached a better understanding of the effects of UV irradiation of such complex mixtures as  $\text{H}_2\text{O}/\text{NH}_3/\text{CO}/\text{O}_2 = 10/1/1/1$ .

The main astrophysically relevant results from the overall study are presented. Firstly, the 4.62  $\mu\text{m}$  band in W33A can be reproduced with  $\text{NH}_3/\text{CO}$  containing irradiated ices and has been identified with  $\text{OCN}^-$  (Grim and Greenberg 1987). The 6.87  $\mu\text{m}$  band in W33A and other protostellar objects is reproduced with  $\text{NH}_3/\text{O}_2$  containing ices (Figure 1a) and is identified with  $\text{NH}_4^+$ .

For W33A the following column densities relative to  $\text{H}_2\text{O}$  have been calculated:  $[\text{OCN}^-]/[\text{H}_2\text{O}] \sim 1\%$  and  $[\text{NH}_4^+]/[\text{H}_2\text{O}] \sim 2\%$ . The 5-8  $\mu\text{m}$  spectrum of W33A shows significant line of sight effects. The 6.0  $\mu\text{m}$   $\text{H}_2\text{O}$  band is carried by grains that have a relatively low temperature, but the position of the 6.87  $\mu\text{m}$  indicated grains that are heated to higher temperatures. The more complex 5-8  $\mu\text{m}$  spectrum of Mon R2/IRS 2 shows three interesting regions (Figure 1b): (i) an absorption excess from 5.2 to 5.8  $\mu\text{m}$  which is not understood yet, (ii) a very steep rise at 6.1  $\mu\text{m}$  that constrains the maximum contribution of  $\text{H}_2\text{O}$  and requires the presence of other compounds to account for the observed 6.0  $\mu\text{m}$  band, and (iii) the broad 6.87  $\mu\text{m}$  band can not be explained solely by  $\text{NH}_4^+$ , but ammonium salts might explain the observed broadening.

References:

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Tielens, A.G.G.M., and Allamandola, L.J., 1987, in *Physical processes in interstellar clouds*, eds. Morfill, G., and Sciles, M.

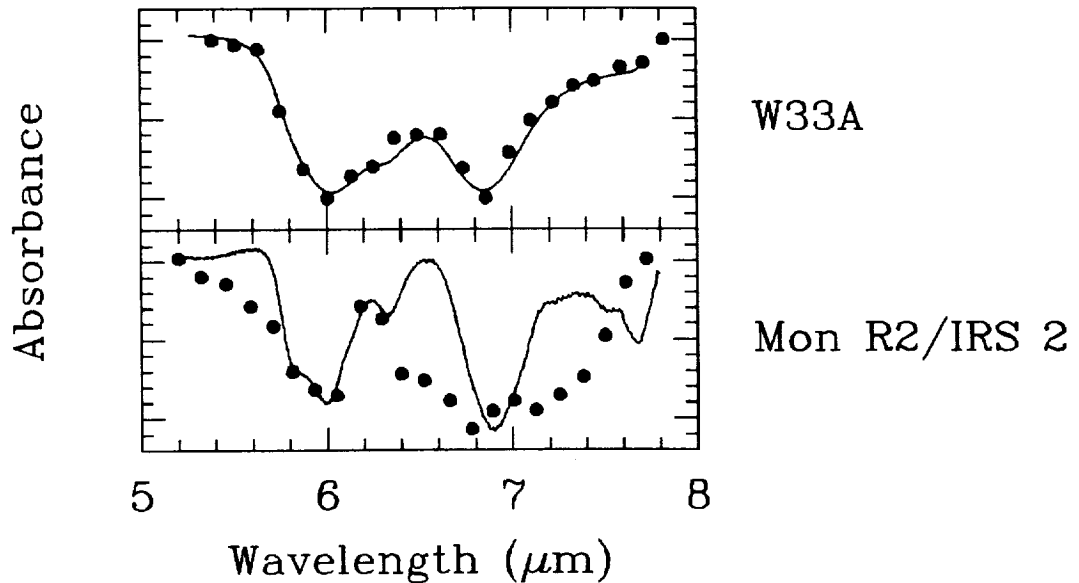


Figure 1: The 5-8  $\mu\text{m}$  spectrum of W33A compared with  $\text{H}_2\text{O}/\text{NH}_3/\text{CO}/\text{O}_2 = 10/1/1/1$  after UV irradiation and annealing to 176 K (a), and the 5-8  $\mu\text{m}$  spectrum of Mon R2/IRS 2 compared with the same mixture but after sufficient time at 176 K to sublimate all  $\text{H}_2\text{O}$  (b). The observational data are taken from Tielens and Allamandola (1987).