The Thermal Reaction of Acrylonitrile and Oxygen Radicals on Analogues of Interstellar Dust Grains.

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Oxygen and Acrylonitrile in the Interstellar Medium

•Oxygen is the third most abundant element in the ISM.[1]
•There is significant interest in the relatively low abundance (the so-called *depletion*) of oxygen in the gas-phase in the interstellar medium.[2-4]
•It has been proposed that interstellar grains could act as a sink for oxygen atoms
•It has recently been confirmed that O atoms have sufficient mobility on interstellar dust grains for reactions to occur at appreciable rates.[5]

•Acrylonitrile (CH_2CHCN) contains a C-N triple bond. The C-N bond is often considered the most important bond in nature due to its presence in amino acids and therefore proteins.
•Acrylonitrile was the first double bond containing molecule to be observed in the ISM.[6]
•It has been observed in Sgr B2, TMC-1, Orion A and IRC+ 10216. Acrylonitrile has a column density of 37.2×10^{-13} cm^{-2} in Sgr B2(N).
•Although acrylonitrile has not yet been observed as an ice it can be inferred that it exists within interstellar ices given its measured gas-phase column densities and its adsorption energy.

Experimental and Modelling Results

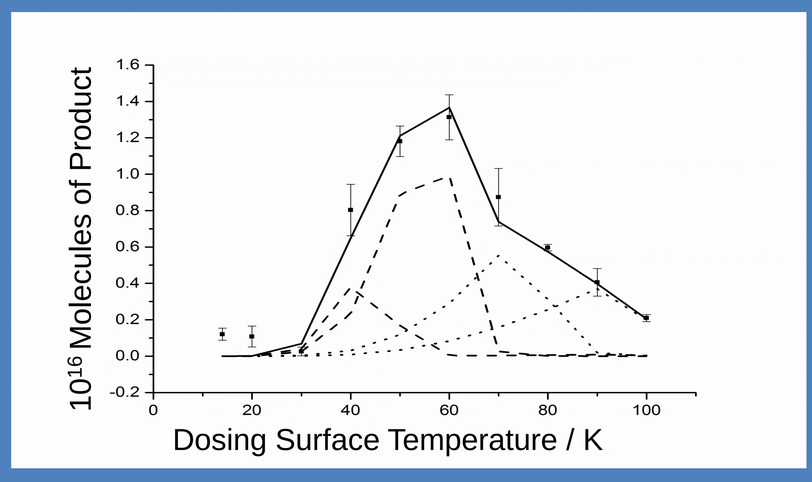
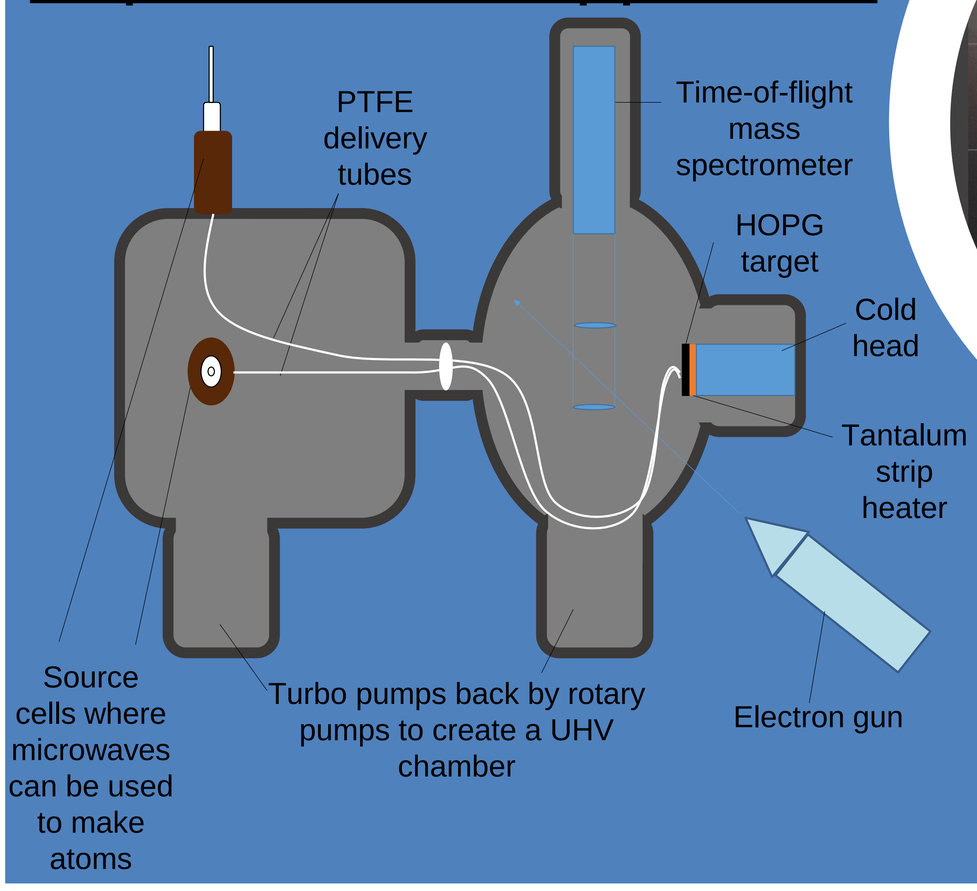
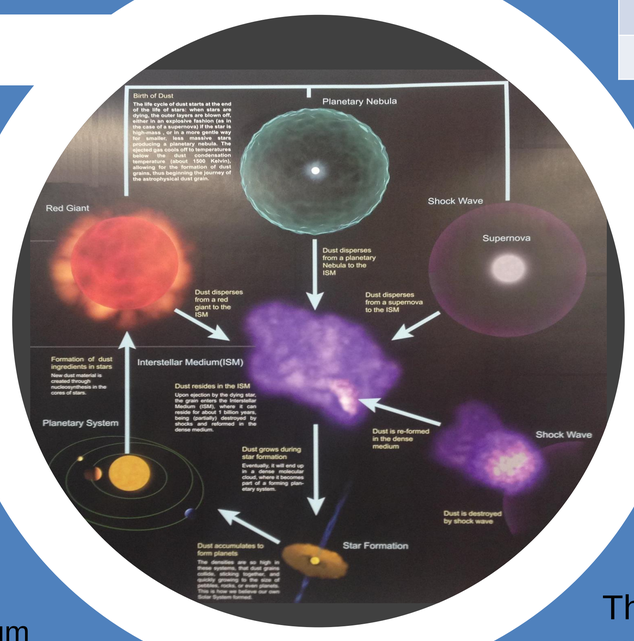


Figure 3: reaction temperature profile and model fitting

Parameter	Lower limit for desorption	Upper limit for desorption
A_{des,C_2H_3CN}	2.42×10^{12} s^{-1} [7]	2.42×10^{12} s^{-1} [7]
E_{des,C_2H_3CN}	19.2 ± 0.1 kJ mol^{-1}	24.1 ± 0.1 kJ mol^{-1}
$A_{des,O}$	3.10×10^{12} s^{-1} [8]	3.10×10^{12} s^{-1} [8]
$E_{des,O}$	12.0 ± 0.1 kJ mol^{-1}	15.0 ± 0.1 kJ mol^{-1}
A_{LH}	5.5×10^{-16} cm^2 $molecule^{-1}$ s^{-1}	9.0×10^{-16} cm^2 $molecule^{-1}$ s^{-1}
E_{LH}	270 ± 50 K	270 ± 50 K
A_{ER}	7.0×10^{-15} cm^2 $molecule^{-1}$ s^{-1}	2.0×10^{-16} cm^2 $molecule^{-1}$ s^{-1}
E_{ER}	270 ± 50 K	270 ± 50 K

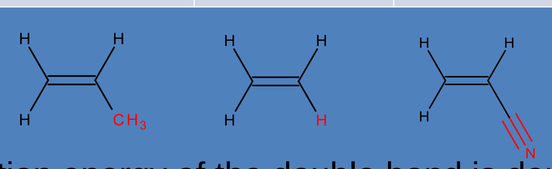
Experimental Apparatus





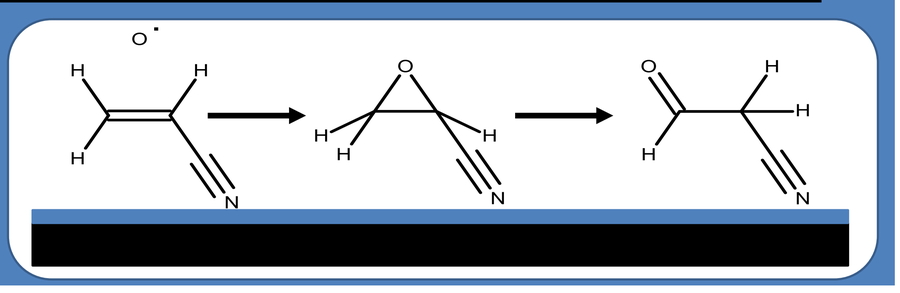
C=C Reactivity with O˙

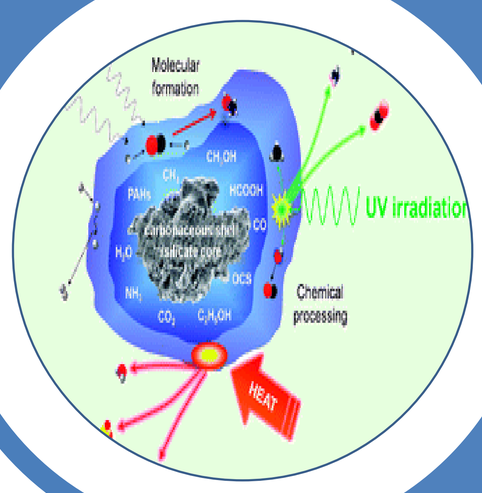
Propene	Ethene	Acrylonitrile
145 ± 10 K [9]	190 ± 45 K [9]	270 ± 50 K



The activation energy of the double bond is dependent on the R group. When the R group is electron withdrawing as in Acrylonitrile the activation energy of the double bond is larger.

Proposed reaction mechanism





Raw Data

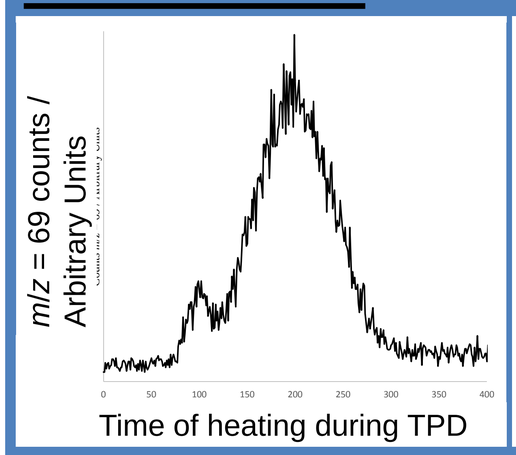


Figure 1: the TPD profile for *m*/*z* = 69

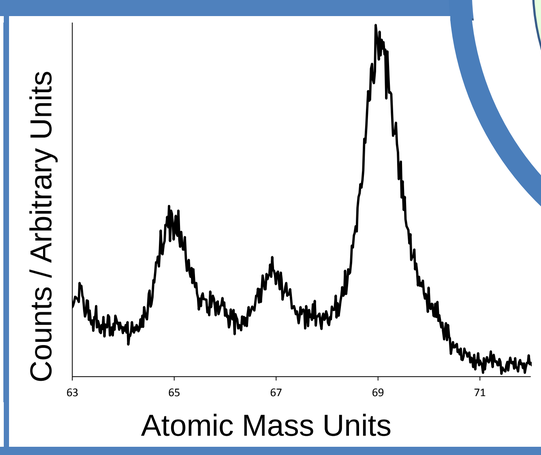


Figure 2: mass spectra to show the product peak at *m*/*z* = 69

Further Work

•To improve the apparatus to measure desorption temperatures of these reactants
•To develop the model to gain understanding about the increased rate below 30K

1. S. I. B. Cartledge, J. T. Lauroesch, D. M. Meyer and U. J. Sofia, *Astrophys. J.*, 2004, **613**, 1037-1048.
2. U. Hincelin, V. Wakelam, F. Hersant, S. Guilloteau, J. C. Loison, P. Honvault and J. Troe, *Astronomy & Astrophysics*, 2011, **530**.
3. D. C. B. Whittet, *Astrophysical Journal*, 2010, **710**, 1009-1016.
4. E. B. Jenkins, *Astrophysical Journal*, 2009, **700**, 1299-1348.
5. M. Minissale, E. Congiu, S. Baouche, H. Chaabouni, A. Moudens, F. Dulieu, M. Accolla, S. Cazaux, G. Manico and V. Pirronello, *Physical Review Letters*, 2013, **111**
6. F. F. Gardner and G. Winnewisser, *Astrophysical Journal*, 1975, **195**, L127-L130
7. H. Bergeron, N. Rougeau, V. Sidis, M. Sizun, D. Teillet-Billy and F. Aguillon, *J. Phys. Chem. A*, 2008, **112**, 11921-11930.
8. M. Rubes, J. Kysilka, P. Nachtigall and O. Bludsky, *Phys. Chem. Chem. Phys.*, 2010, **12**, 6438-6444.
9. M. D. Ward and S. D. Price, *Astrophysical Journal*, 2011, **741**.