Astrochemistry of Acetonitrile Ices

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Outline

Astrochemistry of Nitriles

- The importance of nitriles
- CN-bearing species

Laboratory Astrochemistry

- Instrumentations
- Surface structure
- RAIRS Studies
- Energetic Processing

Summary

Why we study nitriles?

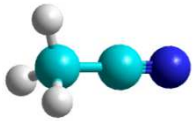
- Nitriles represent large class of organic molecules in the ISM

- Nitriles are thought to be the parents of many of the amino acids

- Understanding their chemistry is important to determine their abundance in the interstellar environments

CN-bearing molecules

Molecule	Titan's Atmosphere	Comets	ISM
CH_3CN	✓	✓	✓
CH_3CH_2CN	-	-	✓
$(CH_3)_2CHCN$	-	-	-
$(CH_3)_3CCN$	-	-	-
CH_2CHCN	-	-	✓
HCCCN	✓	✓	✓
C_2N_2	✓	-	-

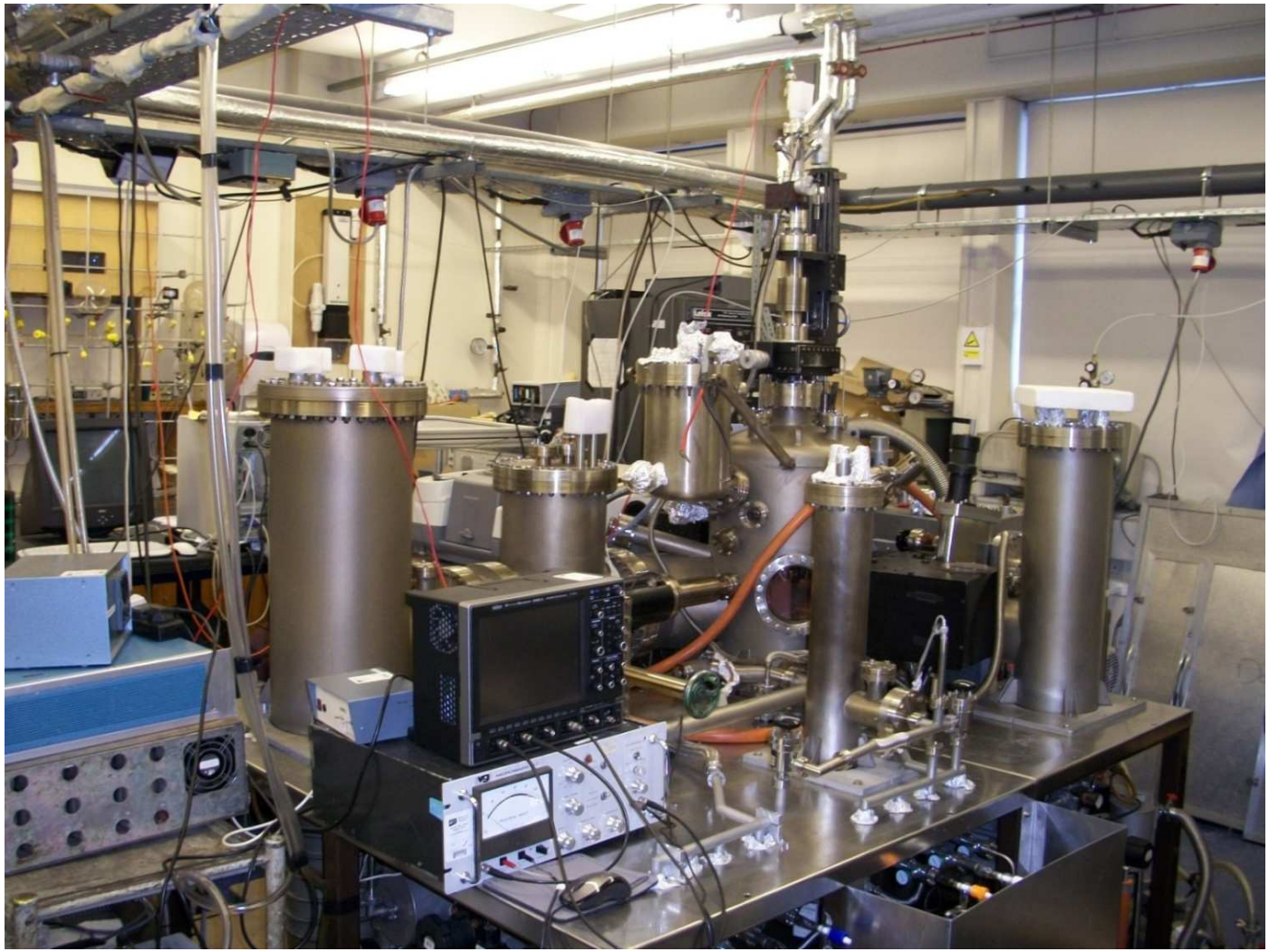


Environment	Abundance
Titan's atmosphere	0.003[a]
Cometary coma (Hale-Bopp)	0.02[b]
Cold molecular cloud (L134N)	<0.01[b]
Hot cores Sgr B_2(N)	0.3[b]

Hudson et al, Icarus, 2004, **171**, 466.
Kelly Beatty et al, The New Solar System, 4th ed, 1999. pp 280
Charnley et al., *Adv. Space Res.*, 2002, **30**, 1419.

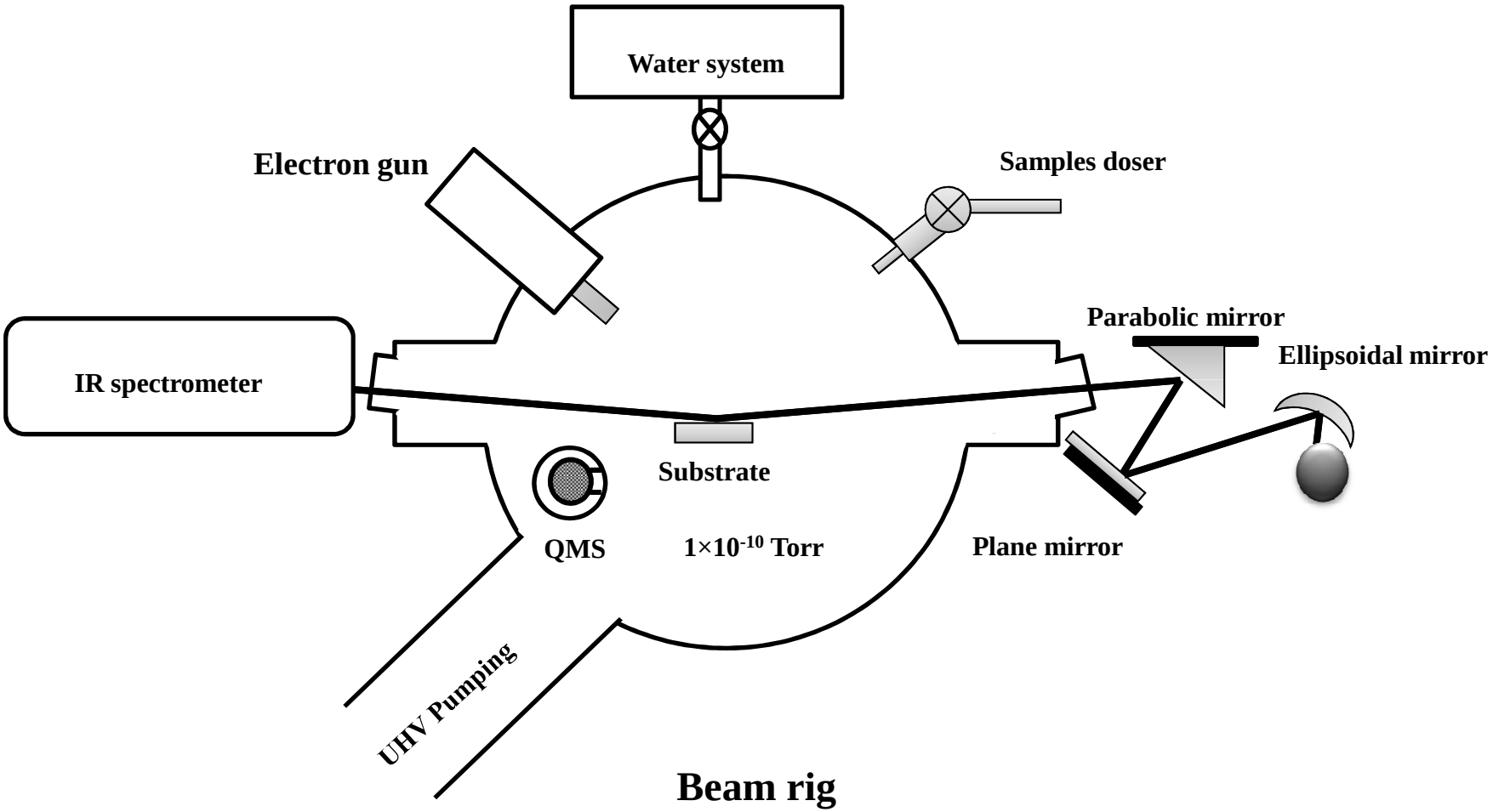
[a] Fractional abundance in ppm
[b] Fractional abundance relative to water

Laboratory Astrochemistry at HWU



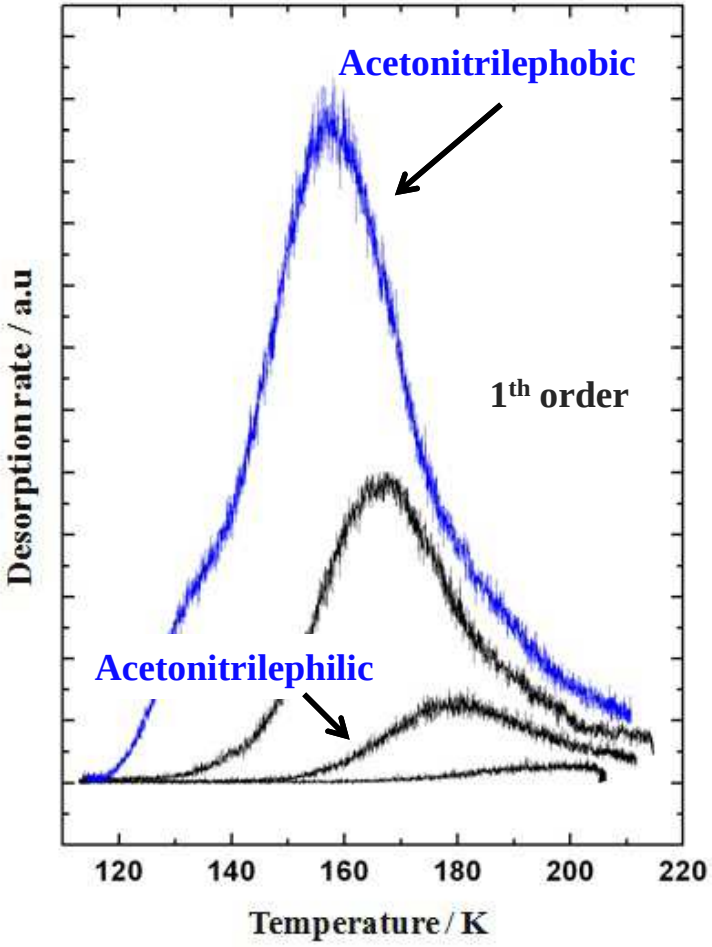
Beam Rig

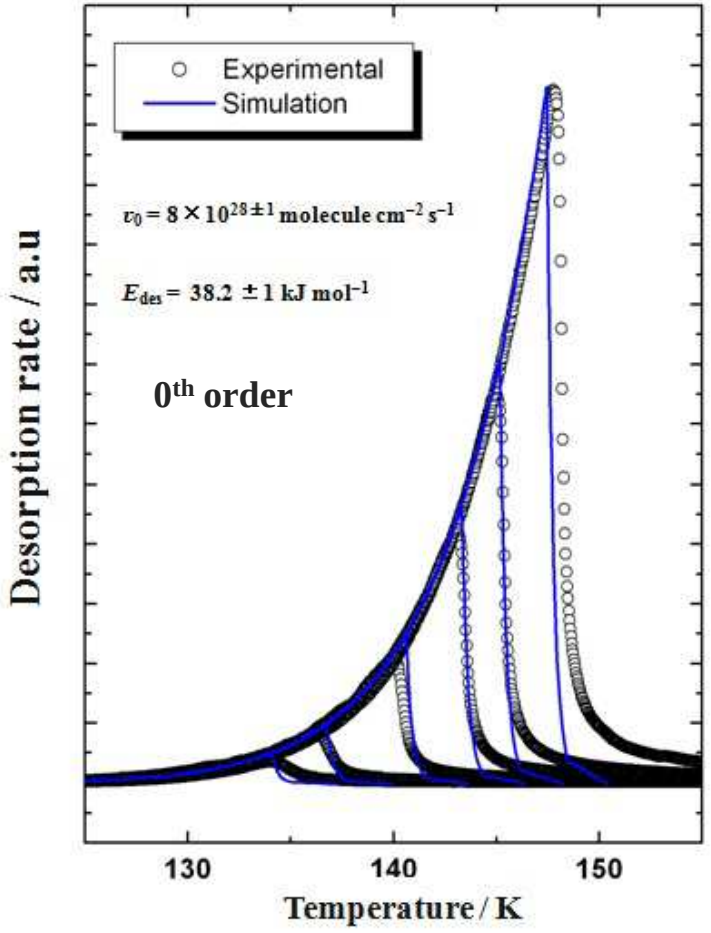
Laboratory Astrochemistry at HWU



Beam rig

Surface Structure





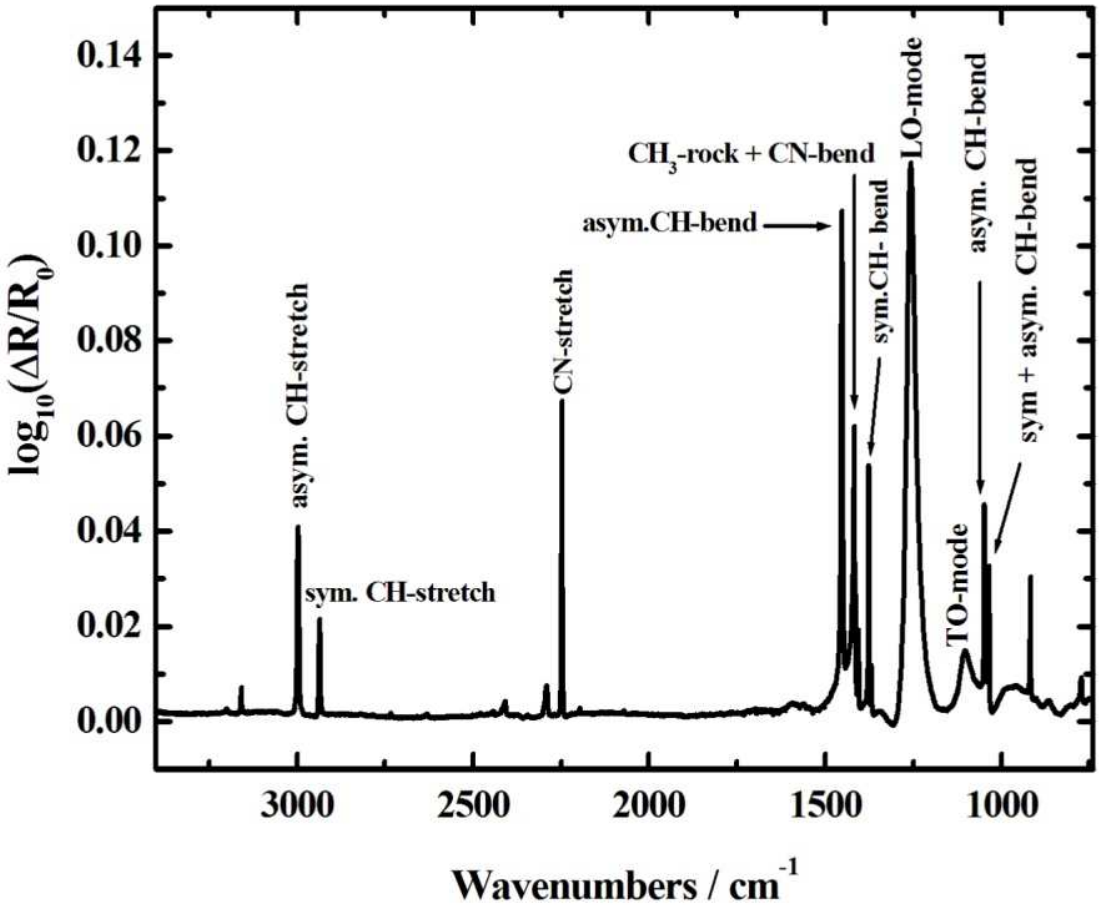
Sub- and monolayer coverages

Multilayer coverages

Acetonitrilephobic: clustering and islanding (E_{des} < 40 kJ mol^{-1})

Acetonitrilephilic: isolated adsorbate (E_{des}> 40 kJ mol^{-1})

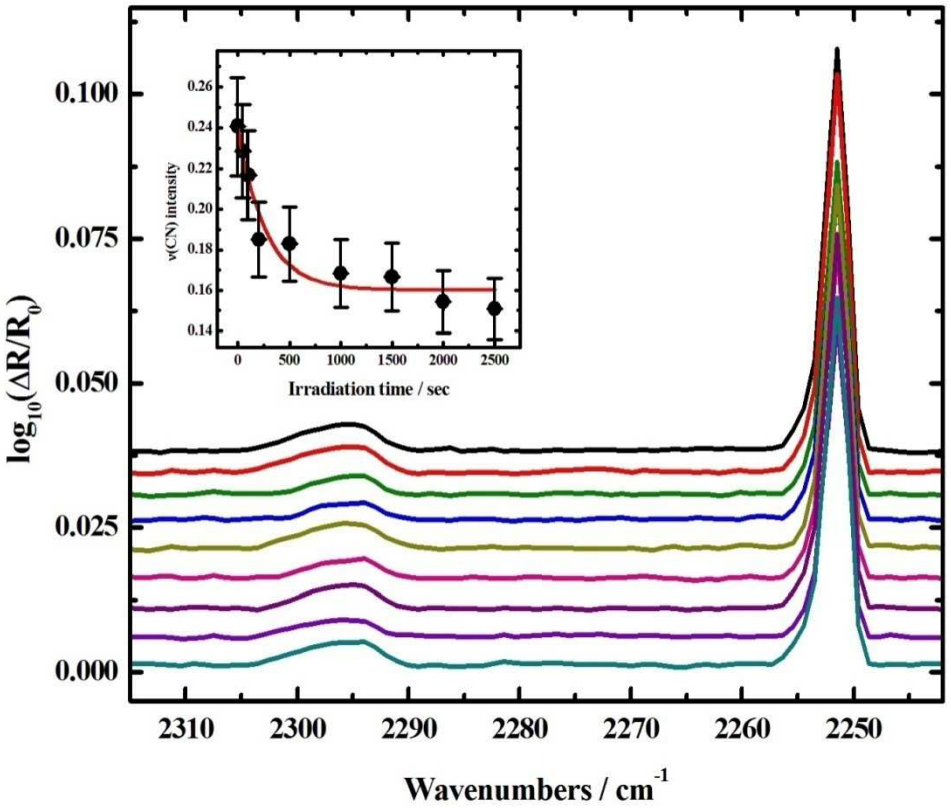
RAIRS Studies



70 nm CH_3CN on SiO_2

Energetic Processing

Low energy electron-induced processing



RAIRS spectra of 28 nm unirradiated (black line) and Irradiated (colourful lines) CH_3CN ice

Electron Energy (eV)	Desorption Cross-section (cm^2)
250	1.9 (± 0.08) ×10^{-17}
300	4.2 (± 0.01) ×10^{-17}
350	1.1 (± 0.004) ×10^{-17}
400	1.1 (± 0.002) ×10^{-17}

Laboratory Astrophysics at Catania

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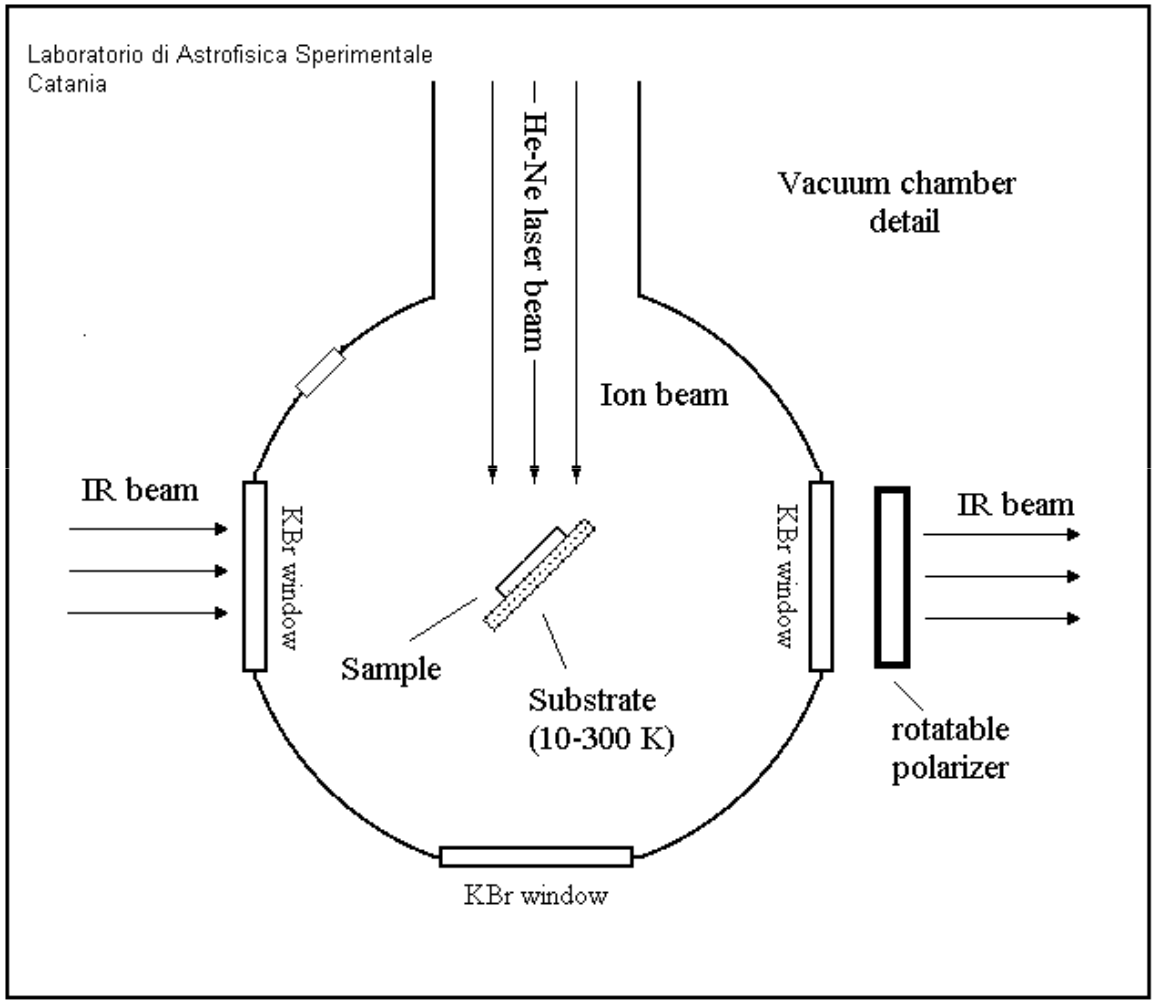
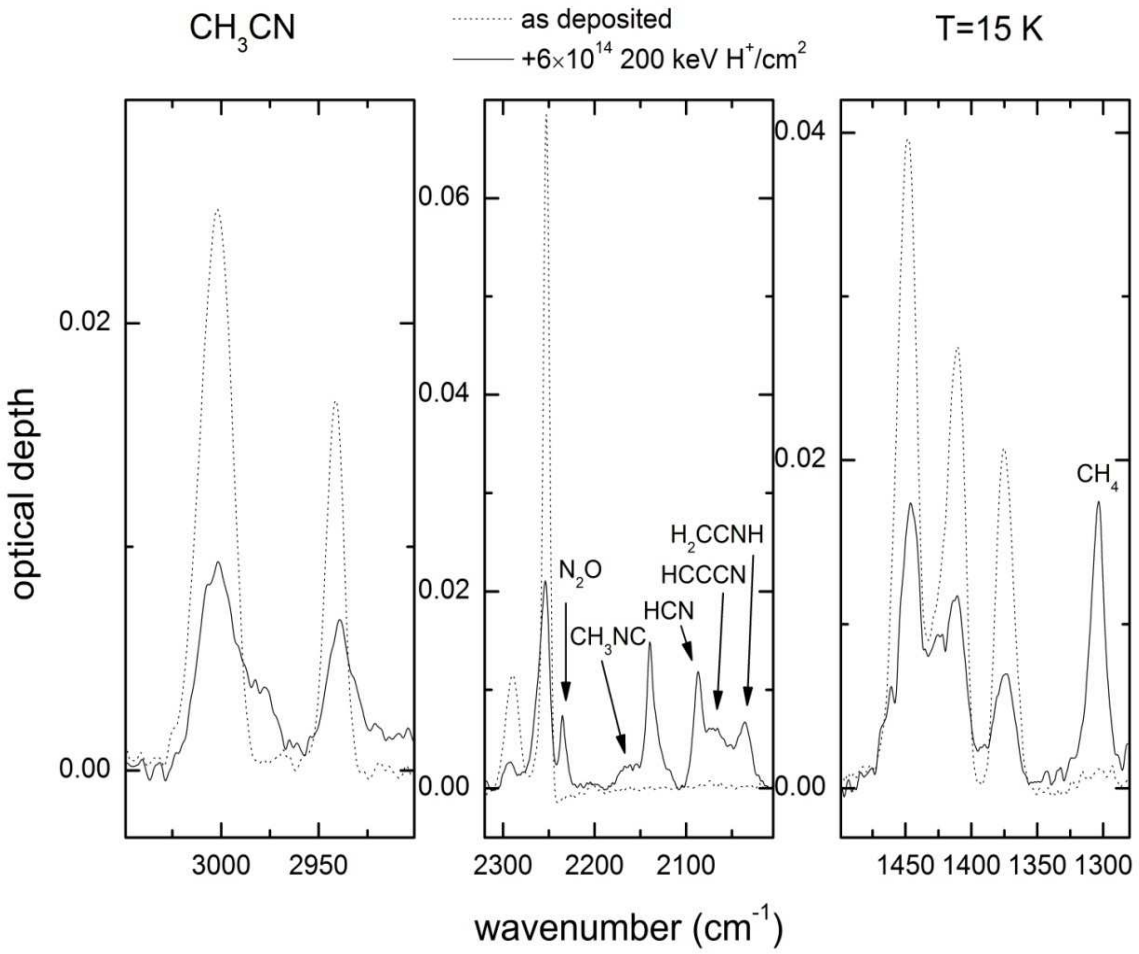


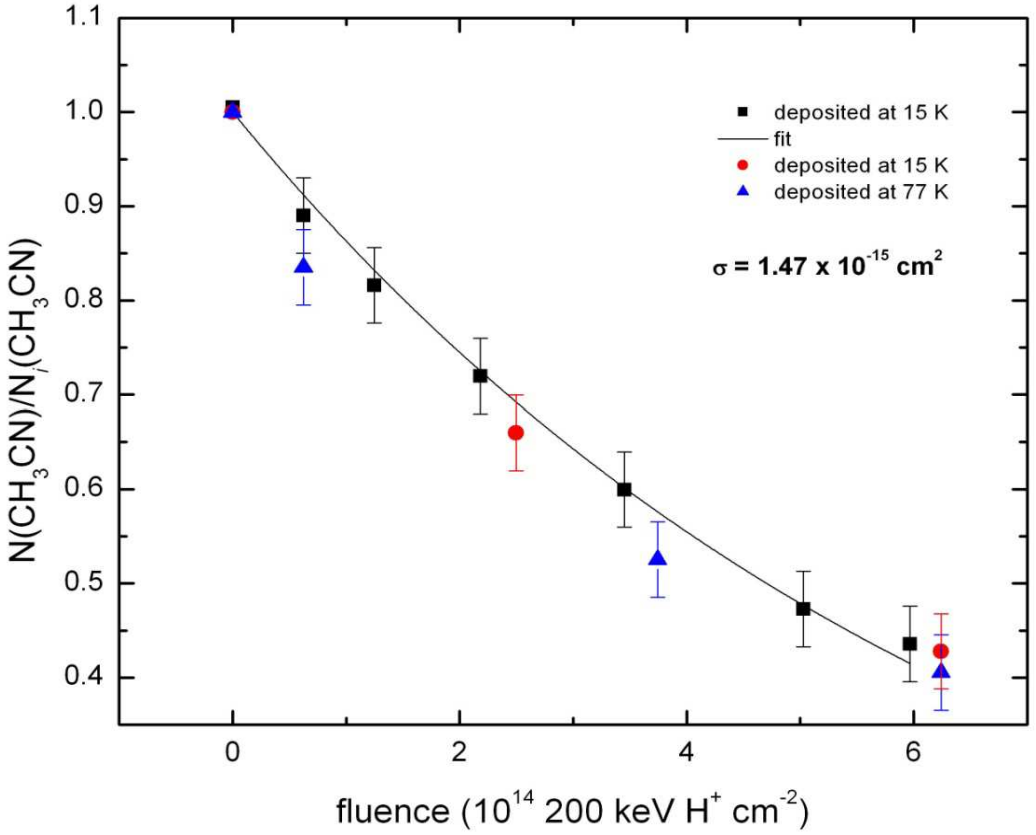
Energetic Processing

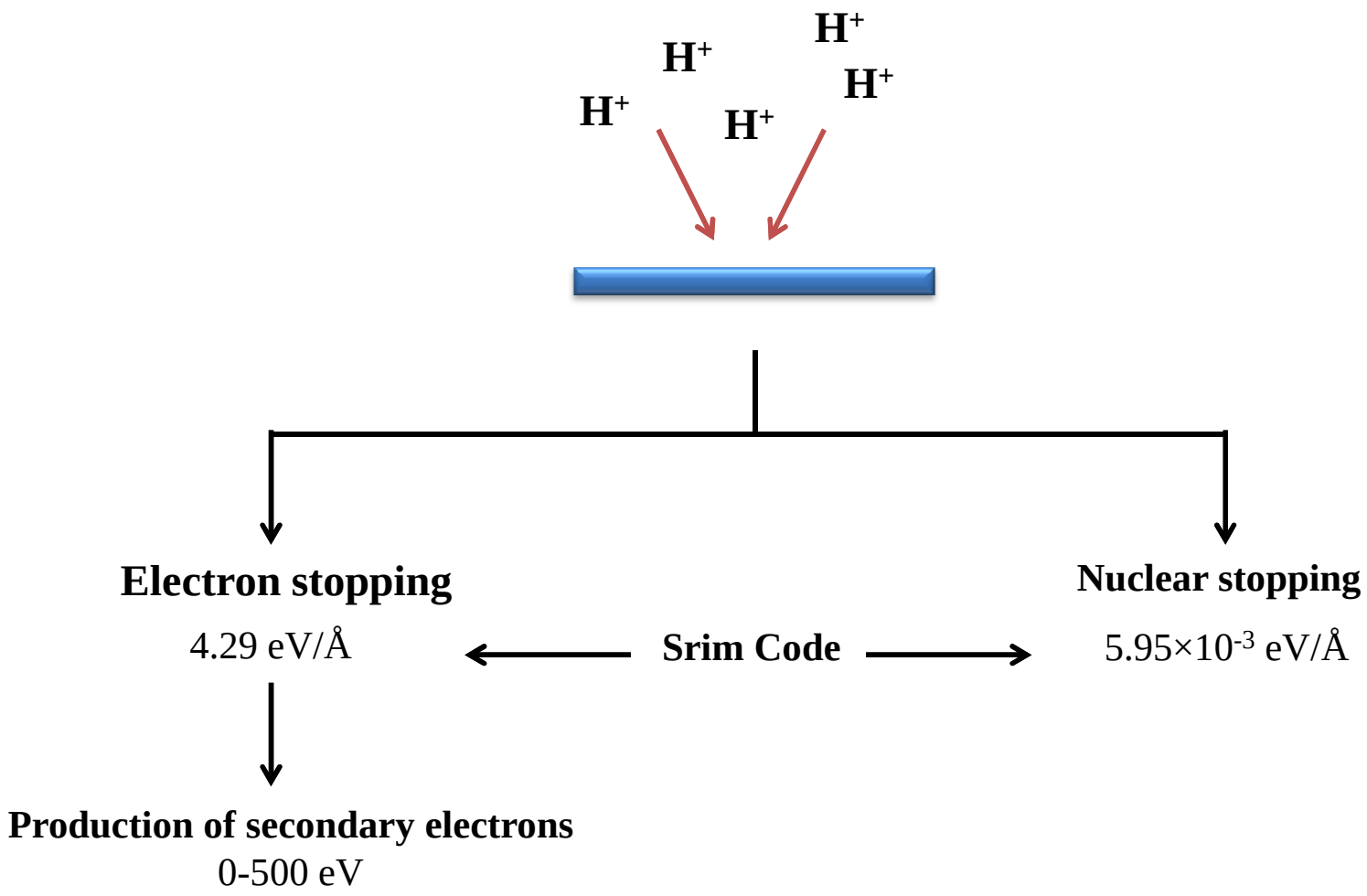
Ion-induced processing



Energetic Processing

Ion-induced processing




H+
H+
H+
H+
H+
Electron stopping
4.29 eV/Å
Srim Code
Nuclear stopping
5.95×10-3 eV/Å
Production of secondary electrons
0-500 eV

Summary

Heriot-Watt University

1. Surface structure:

1) < 0.28 nm sub-monolayer growth is favoured with strong E_{des} to the surface.
2) At 0.28-1.4 nm, completion of the monolayer (clustering and islanding) at 35 kJ mol^{-1} resulting in 1st order desorption regime.
3) At high films thickness up to 70 nm of CH_3CN (island formation), 0th order desorption regime is resulted.

2. RAIRS:

Negligible shifts in IR peaks of CH_3CN because it does not interact strongly with silica surface (Van der Waals forces).

3. Energetic Processing (Low energy electron processing):

- For CH_3CN/ silica regime and within any film thickness, the interaction is electron-promoted desorption with *k* value of 1.18×10^{-5} s^{-1} .

Summary

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Energetic Processing (Ion processing):

- Ion irradiation resulted in the formation of new absorption bands indicating the presence of many new species such as H_2CCNH, HCCCN, HCN and CH_3NC.
- the rate constant for chemical transformation of the CH_3CN determined in the proton irradiation (1.47×10^{-3} s^{-1}) is higher than the rate constant for electron-promoted desorption performed at the HWU.

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Thank you for your attention