Chemistry in the CSM: Unveiling the Dust Formation Zone

T. J. Millar,

School of Mathematics and Physics, Queen's University Belfast

LTE chemistry

Shock-driven chemistry – dust growth & molecule formation

Photochemistry – molecular shells, hydrocarbons, anions, dust as a source of molecules

Metallic species as probes of inner structure

Molecules as tracers of the AGB – PPN - PN transition

Evolved carbon-rich stars IRC+10216 (CW Leo):

Brightest object in the sky at 2 microns – optically invisible

Has an extended (~ 1 lt yr) circumstellar envelope expanding at a velocity of 15 km s⁻¹

Very rich carbon chemistry – about 60 molecules detected, mostly linear hydrocarbons, including $C_{6}H^{-}$

LTE chemistry near photosphere makes simple molecules, CO, N_2 , HCN, C_2H_2

Carbonaceous dust (and PAHs) made in this type of object

Recent detections of H_2O , OH and H_2CO

Chemical Structure of AGB CSE



LTE Chemistry in AGB Stars

Effect of C/O Ratio on Fractional Abundances



CS

SO

Maser emission is an excellent probe of conditions near the photosphere, particularly if driven by IR pumping.

In IRC+10216, HCN detected up to v=4, SiS detected up to v=0, J=15-14 (Exposito et al. 2006)

Dust Formation in AGB Stars

Dust formation in AGB stars requires:

(i) a cooling flow

(ii) high collisional rates

(iii) time

Shocks caused by pulsations are critical – they give large density enhancements, strong post-shock cooling, and lift material slowly away from stellar surface

Spatial scale is less than 5 stellar radii

Probe with vibrationally excited/maser species (line-widths less than terminal velocity/IR pumped) – eg thermal v=1SiS emission (Exposito et al. 2006)

SMA J = 5-4 SiO observations (Schoier et al. 2006) show SiO much more abundant than LTE value in IRC+10216 at 3-8 stellar radii

but lower at larger radii – condensation on to dust grains?

Pulsations and Shock Waves

Density and temperature profiles as a function of phase following a 20 km/s shock at a radial distance of 1.2 stellar radii



Shock propagates outward with shock velocity decreasing with increasing radial distance

Shock Chemistry

Input – LTE abundances for IRC+10216 parameters



Each cycle breaks down into three zones:

- (ii) Immediate post-shock H2 and other LTE molecules destroyed
- (ii) Post-shock H2 and other molecules form
- (ii) Dynamical time less than chemical time freeze-out of abundances
- (iv) No significant water formed in shock

Abundances at the end of the pulsation zone can be very different from LTESiO enhanced, HCN, CS destroyed in C-stars (Willacy & Cherchneff 1998)

Shock Chemistry

Formation of PAH Particles



PAH chemistry from Frenklach & Fiegelson

- (ii) Molecules with several benzene rings, An, form in one cycle
- (iii) Most abundant ring is A7, ie rings grow efficiently
- (iii) Dimers, DAn, grow in abundance during cycle
- (iv) Yields are too low to explain abundance of C-dust but may explain nano-crystalline cores in pre-solar grains

(Cau 2002)

Shock Chemistry

Formation of Molecules in O-rich and S-type Stars

Form carbon-bearing molecules in O-rich stars – C/O < 1: (ii) HCN increased by 6 orders of magnitude above LTE value (iii) CO_2 increased by 3 orders of magnitude (iv) CS increased by 3 orders of magnitude (Duari, Cherchneff & Willacy 1999)

For S-type stars (Chi Cygni) – C/O ~1:

HCN in inner envelope increased by 4 orders of magnitude (vibrationally excited HCN detected here – IR pumping within 33 stellar radii)

(Duari & Hatchell 2000)

Photochemistry in CSEs

Destruction of Parents by IS UV Radiation Field

Self-Shielding

H2 - very reactive, daughter (H atoms) unreactive

CO – very unreactive, daughters (C, C+) very reactive

Cosmic ray ionisation

f(H3+) varies as r^2

 $N(H3+) \sim 1e12 \text{ cm}^{-2}$ for CRI rate of 1e-17 s^-1, an order of magnitude less than that detected in the interstellar medium

Photodissociation and photoionisation

Acetylene is the species which determines the complexity of the hydrocarbon chemistry

Photochemistry in CSEs

Shell distributions – the photodestruction of acetylene



IRC+10216

Acetylene has a relatively large photoionisation cross-section

Ions and radicals form in outer CSE where both density and UV field are relatively large

(Millar, Herbst & Bettens 2000)

Hydrocarbon formation

Shell distributions – rapid formation of hydrocarbons

IRC+10216



C2H and C2H2+ are both very reactive with acetylene and derivative species

Peak abundances occur at slightly larger radii as size increases

Degradation of grains may give inverse behaviour

(Millar, Herbst & Bettens 2000)

Cyanopolyyne formation

Shell distributions – rapid formation of hydrocarbons

IRC+10216

Neutral chemistry important in forming cyanopolyynes and other molecules (Agundez talk)



(Guelin et al. 2000)



4×10¹⁶

16 6×10¹ Radius (cm) HC₅N

8×10¹⁶

1×10¹⁷

5.0×10-

2×10¹⁶



Anion formation

Anion column densities ~ 0.1 - 0.2 neutral column densities

IRC+10216



High electron fraction and high density allow formation of abundant anions

C6H- recently detected in IRC+10216 by McCarthy et al. ApJL, in press

(Millar, Herbst & Bettens 2000)

Metal species in IRC+10216

LTE calculations predict metal halides (Tsuji)

NaCI, KCI, AICI, AIF – observed centrally peaked, spatial scales few arcsec

fractional abundance (AIF, AICI/H2) ~ 1e-7 for 5 arcsec source (Highberger et al 2001, Guelin et al. 1997) – large fraction of metal NOT in dust

ALMA will be important to test LTE models, formation of clumps/dust formation, chemistry driven by shock pulsations

MgCN, MgNC, AINC, SiCN, SiNC – shell distribution, spatial scales ~15 arcsec

ALMA will test fraction of metallic elements either NEVER incorporated into dust grains or RELEASED from dust in outer CSE

Metal compound formation

MgNC formation – N(MgNC) ~ 2e13 cm-2 ~observed

IRC+10216



Are outer shell species formed in shock chemistry and transported outward, or by photochemistry ?

MgNC formed by radiative association of Mg+ with cyanopolyynes

(Dunbar & Petrie 2002)

Structures in the outer CSE

Enhanced density rings/arcs in IRC+10216



Several narrow shells/arcs detected by Mauron & Huggins:

density enhanced by 2-3

thin, 0.5-3 arcsec

correlated with molecular distributions

Chemical models:

Rings provide additional extinction and decrease collisional time-scales

Not all rings contribute

Steepen and narrow molecular distributions

(Brown & Millar 2003)

Formation of Water (and other molecules)



(Willacy 2004)

In C-rich source (IRC+10216),

 $f(H_2O) \sim 0.4-2.4 \ 10^{-6}$ and

 $f(OH) \sim 4 \ 10^{-8}$.

Possibility – evaporation of comets

(formed in O-rich material in the neighbourhood – presence of HDO?)

Shock chemistry ? No

Formation of water by Fischer-Tropsch catalysis

 $CO + 3H_2 \rightarrow CH_4 + H_2O$

on iron grains

Need few percent of Fe in iron or F-Ni alloy.

The Future with ALMA

Increase the sample of stars in which we can get spatial information on molecules – no longer reliant only on IRC+10216

Probe isotopic ratios as a function of radial distance to probe nucleosynthesis as a function of time

Study structures, velocity fields, in inner regions – pre-dust and dust-forming zones

Importance of pulsational shocks

Origin of asymmetry in post-AGB objects?

Probe the dust-forming zones of O-rich stars – what are the precursors to dust?

The importance of dust as a sink/source molecules in both the inner/outer envelope

If important as a source, carbonaceous dust may provide significant molecules to the ISM

Astrophysical Chemistry Group

Dust, Gas and Chemistry in the Interstellar Medium Belfast, January 4-5 2007

Invited Speakers:

Student travel bursaries available

www.astrochemistry.org.uk