COMPLEX NON-EQUILIBRIUM CHEMISTRY IN THE SHOCK ACCELERATED OUTFLOW OF THE PRE-PLANETARY NEBULA 0H231.8+4.2

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ABSTRACT

- Evolved stars are:

- Primarily responsible for ISM (InterStellar Medium) enrichment
- Efficient factories of molecules

- We present preliminary results on the chemistry study towards OH231.8+4.2 an Oxygen rich envelope/star

- Observations:
 - IRAM 30 meters antenna and its new generation EMIR receivers
 - Milimeter survey from 79 GHz to 350 GHz

- OH231.8+4.2 shows a particularly rich chemistry (probably strongly affected by Shock

induced chemistry)

EVOLVED SUN-TYPE STARS

- Stars ranging from: 0.8 8 $\rm M_{\odot}$
- AGB (Asimpthotic Giant Branch) phase:
 - Mass loss: $dM/dt \sim 10^{-8} 10^{-4} M_{\odot}$
 - Expanding spherical symmetric envelope:

 $v_{exp} \sim 5 - 30$ km/s

- Post-AGB phase:
 - Mass loss stops
 - Detached & expanding envelope
 - High-velocity winds: v ~ 100 1000 km/s
 - Spherical symmetry break up
- In both cases molecular gas is the predominant component



TYPICAL STRUCTURE OF AGB ENVELOPES



- C-Rich stars: [C]/[O] > 1
- O-Rich stars: [C]/[O] < 1
- Carbon & Oxigen react to form all CO as possible, and Oxygen remains to form new compounds in case of O-rich stars
- So far today Carbon rich stars and their envelopes are the most studied: IRC+10216 (Cernicharo et al., 2010), CRL618 (J.R.Pardo et al., 2007)
- Typical molecular content in C-rich: HCN, HNC, CS, SiS, HC₃N (Bujarrabal et al., 1994)
- Typical molecular conten in O-rich: SiO, SO, SO, (Bujarrabal et al., 1994)



OH231.8 + 4.2. GENERAL OVERVIEW

- Bipolar nebula + QX Pup (AGB Mira, M9III) + A0V companion

- Some properties of the molecular envelope:

Plateau de Bure Interferometer Map (IRAM)

dM/dt ~ 10⁻⁴ M_{$_{\odot}$} , T = 20 K, n ~ 10³ – 10⁵ cm⁻³ , M_{envelope} ~ 1 M_{$_{\odot}$}

20 sec. North Offset (arc 20 40 ¹²CO 20 -20East Offset (arc sec.) (Alcolea et al., 2001)

Hubble Space Telescope image

Blue. Shock excited Ha emission

Yellow: Reflection nebula

(Sánchez Contreras et al., 2004)

OH231.8 + 4.2. VELOCITY GRADIENT

- High-velocity gradient range:

Velocity-position map (PdBI IRAM)





(Alcolea et al., 2001)



OH231.8 + 4.2. CHEMISTRY

- Rich and peculiar chemistry

- HNC, HCN, CS, NH₃, HCO+, OCS, SiO, SO, SO₂

(Morris et al., 1987)

- Shocks are maybe important to explain chemistry



(Sánchez Contreras et al., 2000)



HCO+

J=1-0

OBSERVATIONS

- On-going observations (3 runs in 2009, 2010, 2011) with the 30 meters antenna of IRAM (Institute de Radioastonomie Milimétrique) in Pico de Veleta, Granada (Spain)

- EMIR "state of the art" single pixel heterodyne receivers (Carter et al., 2012)

- Covering 8 GHz simultaneously

Frequency (GHz)	HPBW(arcsec)	Feff(%)	Beff(%)
86	29	95	81
145	16	93	74
210	11	94	63
260	9	88	53
340	7.5	81	35

- Backends and resolutions:

[Backends	Channel width
	4 MHz	4 MHz
ĺ	WILMA	2 MHz
	FTS	$195,50 \ \rm kHz$
	VESPA	3.3 kHz-1.25MHz

Typical widths: 2 MHz ~ 1.5 – 7.5 km/s OH231 lines ~ 50 – 100 km/s

OBSERVATIONS: BEAM SIZE



Including the dense central parts and partially covers the fast bipolar outflows

RED: Beam at 90 GHz GREEN: Beam at 150 GHz BLUE: Beam at 250 GHz YELLOW: Beam at 340 GHz

- Summary of the observational results:

Source	Band	Fobs (GHz)	№ Setups	Texp (s)	RMS (mK)	Opacity
IKTau	E090/3mm	79.2-115.7	5	118300	1-2	0.09-0.21
IKTau	E150/2mm	128.3-167.6	14	162230	1-4	0.04-0.26
IKTau	E330/0mm	258.3-348.9*	17	77100	7-16	0.24-0.79
OH231.8+4.2	E090/3mm	79.2-115.7	5	105500	1-2	0.07-0.21
OH231.8+4.2	E150/2mm	128.3-167.6	13	142960	1-4	0.03-0.24
OH231.8+4.2	E330/0mm	258.3-348.9**	15	61250	9-20	0.17-0.76

- We have:

33 spectra (36 for IKTau) 131 GHz of total width (138 GHz for IKTau) > 400 lines ~ 3 lines / GHz 3mm & 2mm fully covered 0mm 50% covered 1mm not covered (yet)

OBSERVATIONAL RESULTS: THE SURVEY



OBSERVATIONAL RESULTS: THE SURVEY



OBSERVATIONAL RESULTS: THE SURVEY



Frequency (MHz)

LINE IDENTIFICATION: THE PROCEDURE

- Line identification procedure:

- 1) Establishing frequency of the line within a $\Delta v \sim 4$ MHz
- 2) Search in catalogues: CDMS, JPL, J. Cernicharo personal catalogue
- 3) Select a candidate within following criteria:
 - Previously detected
 - Upper level energy of the transition
 - Einstein coefficient
 - Species complexity
- 4) Compare with synthetic spectra

Confirm species, identifying several transitions for the same molecule for firm confirmation

LINE IDENTIFICATION: SYNTHETIC SPECTRA

- Using MODSOURCE task from CLASS software (http://iram.fr/IRAMFR/GILDAS/)

HNCO model sample:



LINE IDENTIFICATION: SYNTHETIC SPECTRA

HNCO model sample:







- Population diagrams or Rotational diagrams give rotational temperature and column density for a specific molecular specie and allow to constraint input values for the sinthetic spectra creation

- Under Local Thermodynamic Equilibrium (LTE) -> Collisional excitation

rot

- Equation (Goldsmith & Langer, 1991):

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} exp(-\frac{h\nu_o}{kT})$$
With: $T = T_{ex} \rightarrow \text{Under LTE: } T_{ex} = T_{rot}$

$$\log \frac{3kW}{8\pi^3 \nu S_{ul} \mu^2} = \log \frac{N}{Z_{rot}} - \frac{\log e}{kT_{rot}} E_u$$
T - N from fitting

ANALYSIS: ROTATIONAL DIAGRAMS

- Rotational diagram for SO₂ towards OH231.8 + 4.2:



OH231.8+4.2:

- 69% lines identified
- Thermal lines: CO, CS, SiO, SO, SO₂, HCN, HNC, HCO+, OCS, NS, SiS, H₂CO,
- H₂S, HNCO, PS, NO, N₂H+, HC₃N....
- Maser lines: SiO
- Tentative detections: PO, C3H, SO+, CN ...
- Many Uis (UnIdentified lines) **>** ¿Complex molecules: CH₃OH, CH₃OCHO?

IKTAU:

- 54% lines identified
- Thermal lines: CO, SiO, SiS, SO, SO₂, HCN, HNC, HCO+, CS, CN, NaCl, H₂CO,

PS, PN...

- Maser lines: SiO and H_2O
- Tentative detections: KCN, NaCN ...











- Broad profiles of ion lines:



PRELIMINARY ANALYSIS: ABUNDANCES

- 1st order characteristics abundances based on simple LTE calculations
- We assume this:

$$X(^{13}CO) \sim 2 \times 10^{-5}$$
 $T_{rot, OH231} \sim 20 \text{ K}$ $T_{rot, IKTAU} \sim 20 \text{ K}$

Molecule	OH231 Abundance	IKTau Abundance	
SO ₂	3 x 10 ⁻⁶	4 x 10 ⁻⁷	
SO	2 x 10 ⁻⁶	4 x 10 ⁻⁷	
H ₂ S	1.7 x 10 ⁻⁶	***	
HCN	3.4 x 10 ⁻⁸	1.3 x 10 ⁻⁷	
HNCO	3.1 x 10 ⁻⁸	< 4 x 10 ⁻⁹	
HCO+	1.6 x 10 ⁻⁸	4 x 10 ⁻⁹	
HNC	1.5 x 10 ⁻⁸	4 x 10 ⁻⁹	
HC ₃ N	3 x 10 ⁻⁹	< 4 x 10 ⁻⁹	
N ₂ H+	2 x 10 ⁻⁹	< 1 x 10 ⁻⁹	

QUALITATIVE ANALYSIS

- OH231.8 + 4.2 shows:

Less abundant SiO lines (compared with IKTau) No NaCl or H₂O lines

Probably low density at the inner parts of the envelope

More abundant ions lines

Shock induced chemistry

SUMMARY

- OH231.8+4.2 is a peculiar object: AGB central star + A0V companion + post-AGB-like envelope

- Fast winds & shocks
- Chemistry predominantly affected by shocks

FUTURE WORK:

- Complete the survey
- Complete identification
- Derive X(r) from non-LTE radiative transfer model using more realistic structure of the envelope
- Comparison with predictions from chemical models