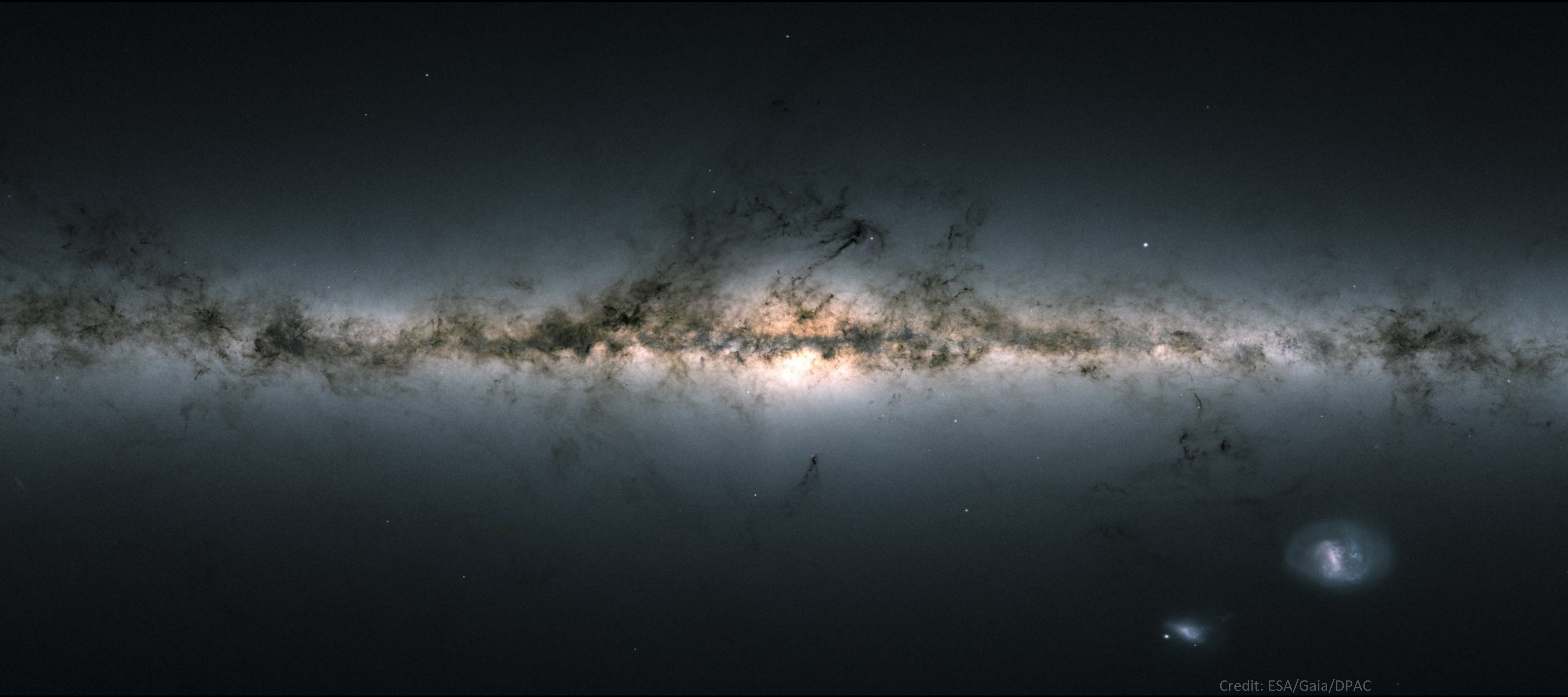
Unraveling molecular structures:

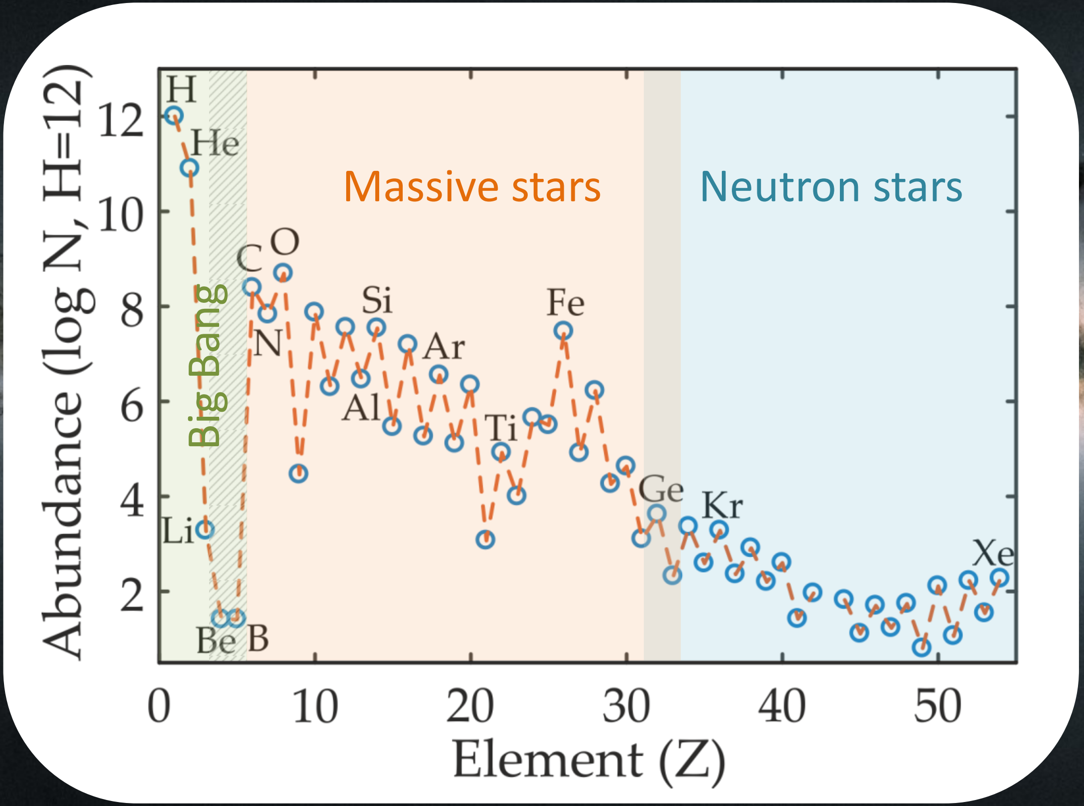
From (ultra)high-resolution spectroscopy to astrochemical insights

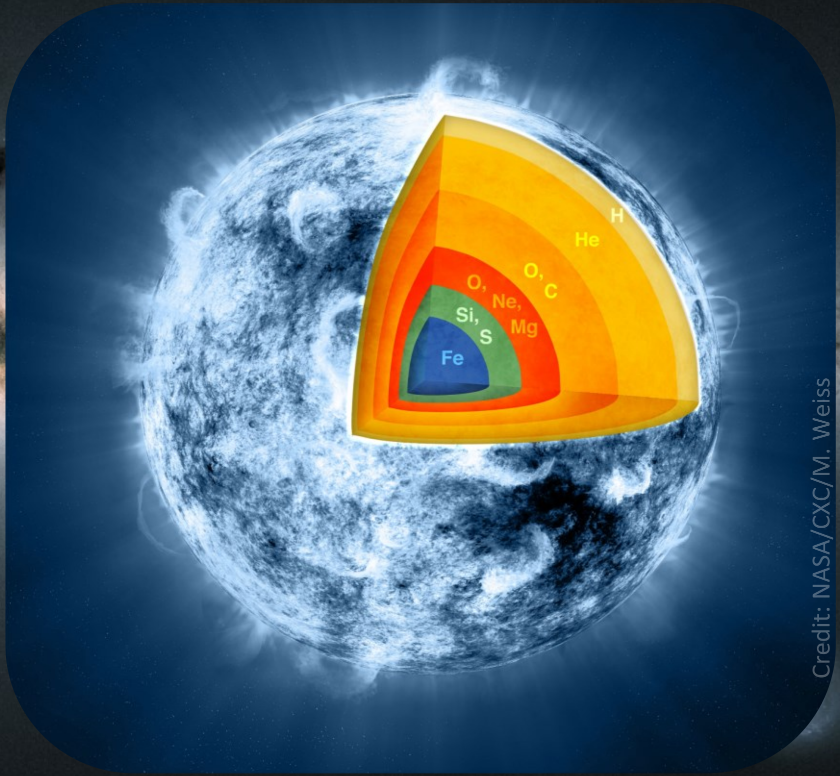
Alexander A. Breier

April 4th, 2024

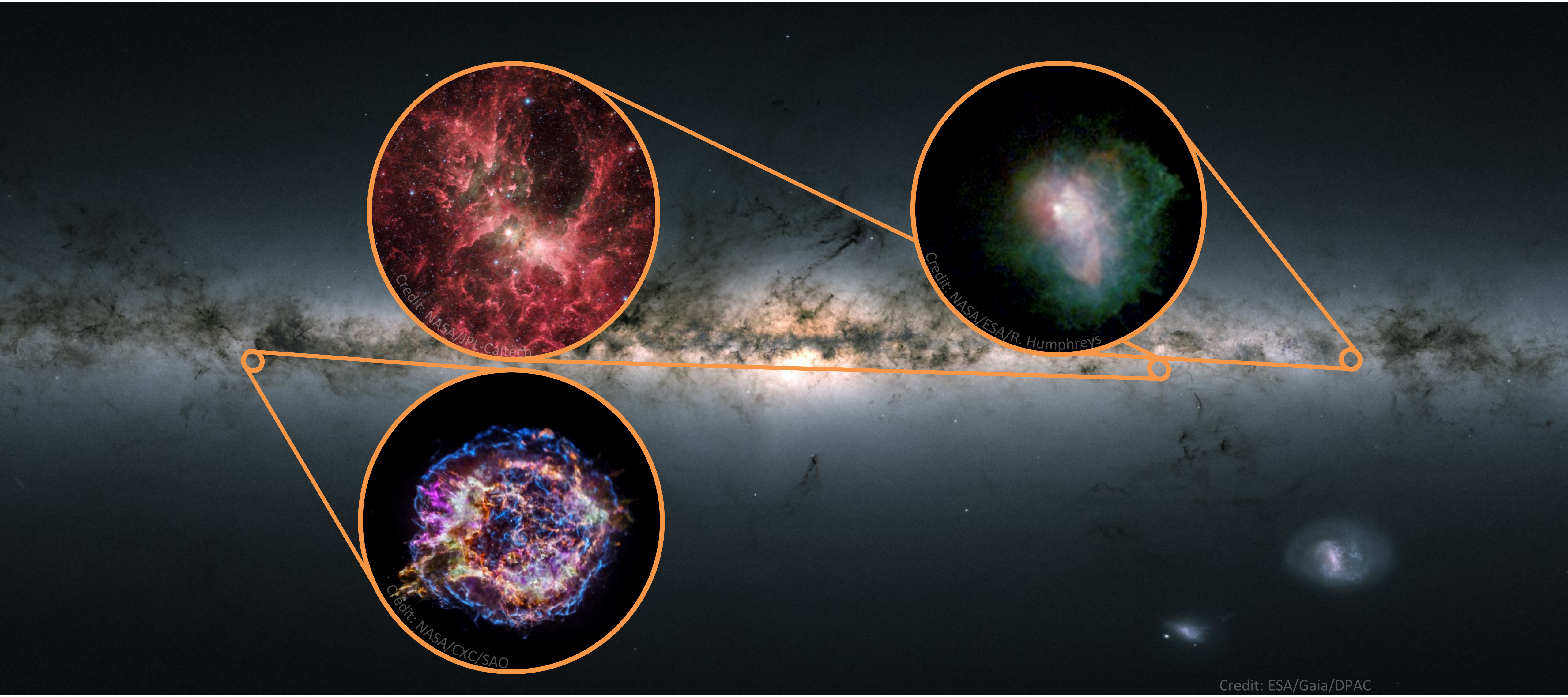
INT-24-1 Fundamental Physics with Radioactive Molecules

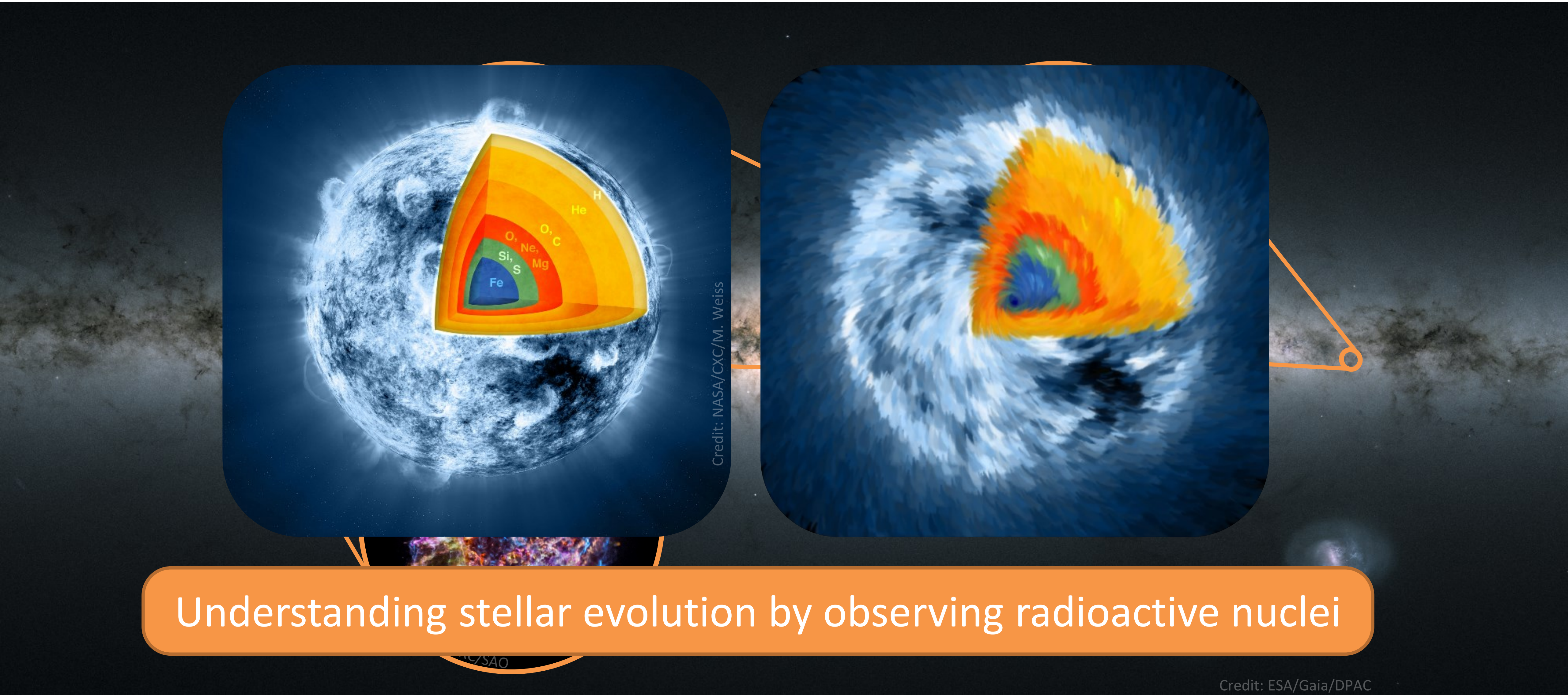

Credit: ESA/Gaia/DPAC





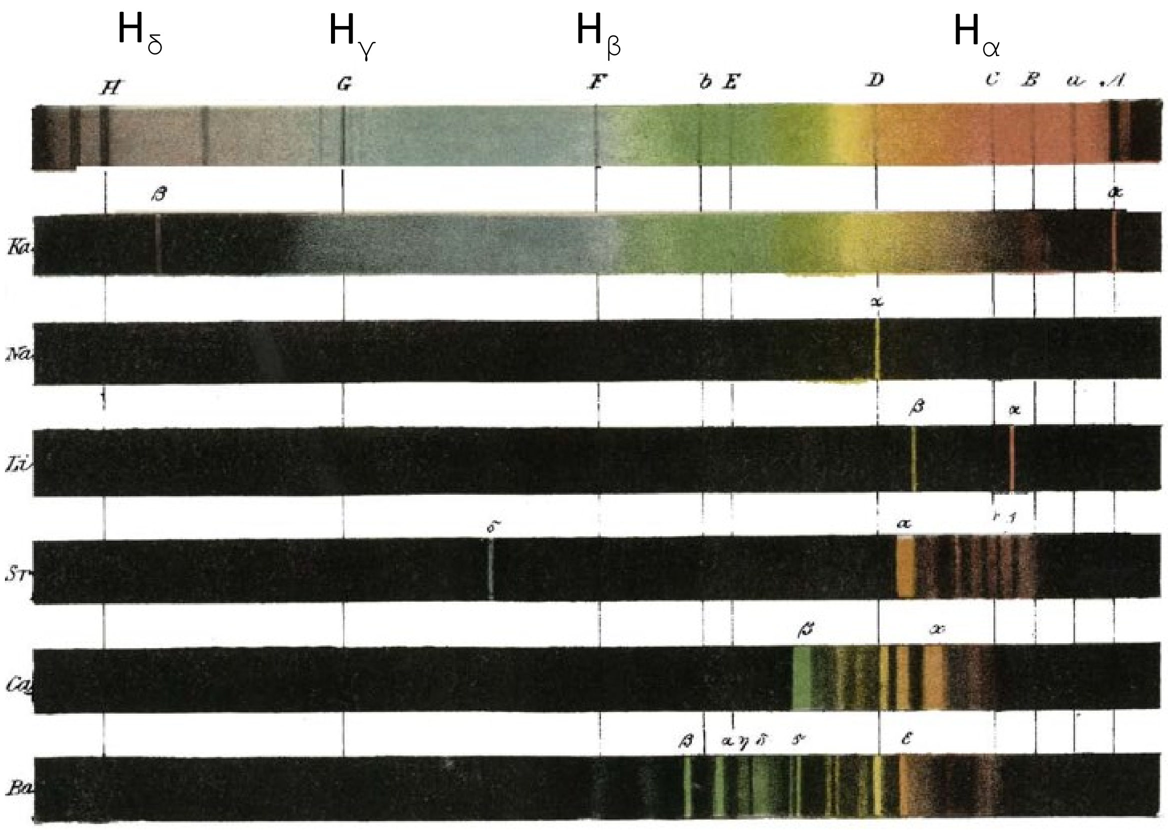
Credit: ESA/Gaia/DPAC


Credit: NASA/JPL-Caltech
Credit: NASA/ESA/R. Humphreys
Credit: NASA/CXC/SAO
Credit: ESA/Gaia/DPAC



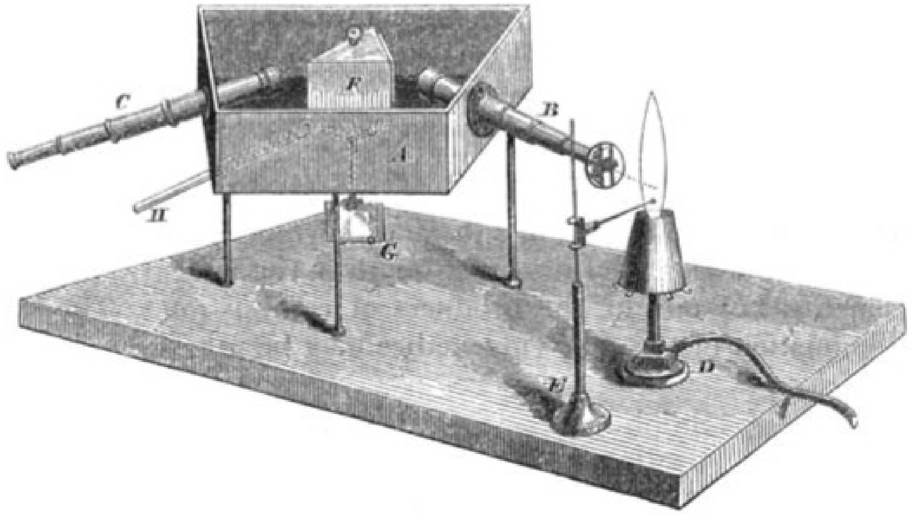
Understanding stellar evolution by observing radioactive nuclei

Observation of matter



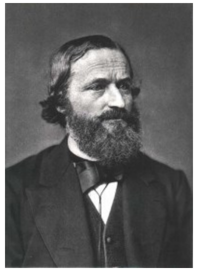
G.Kirchhoff, R.Bunsen, Ann.Phys.&Chem **110**.6, 162 (1860)

→dark features in the optical spectrum of the Sun



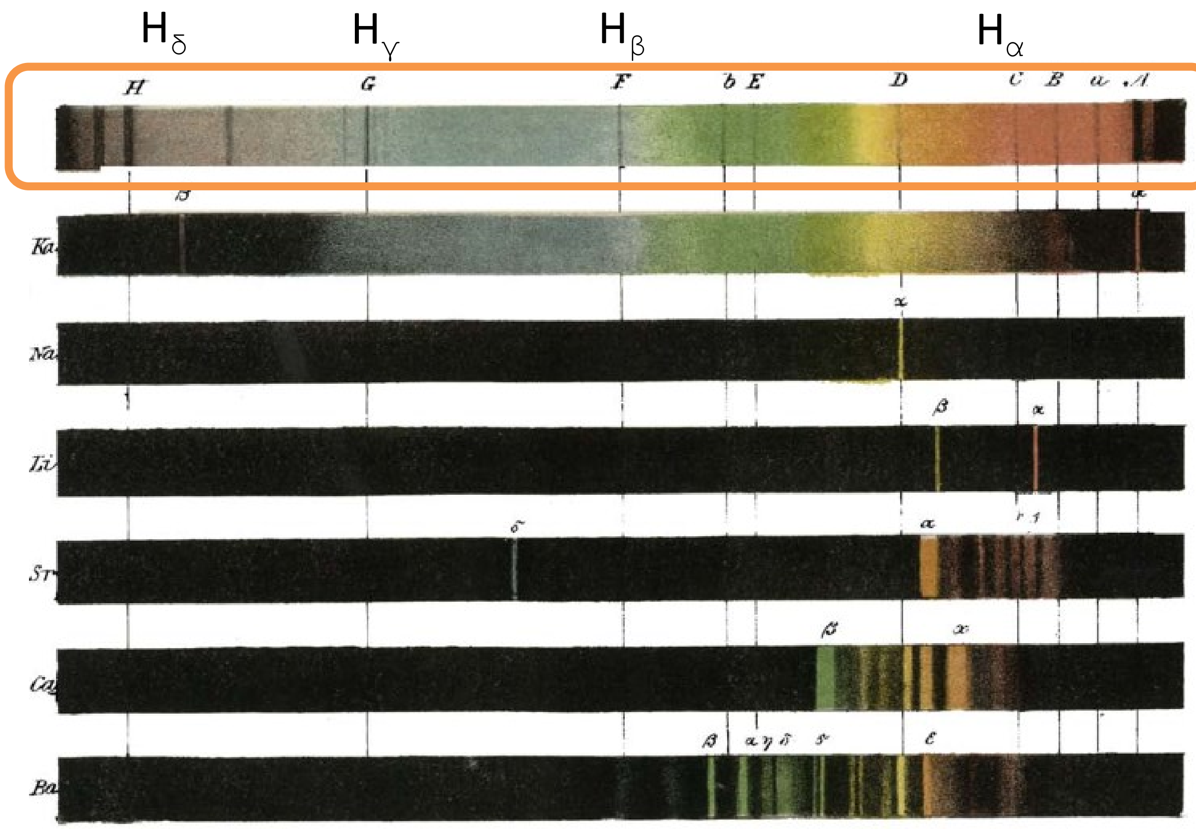
Fraunhofer

Kirchhoff



Bunsen

Observation of matter



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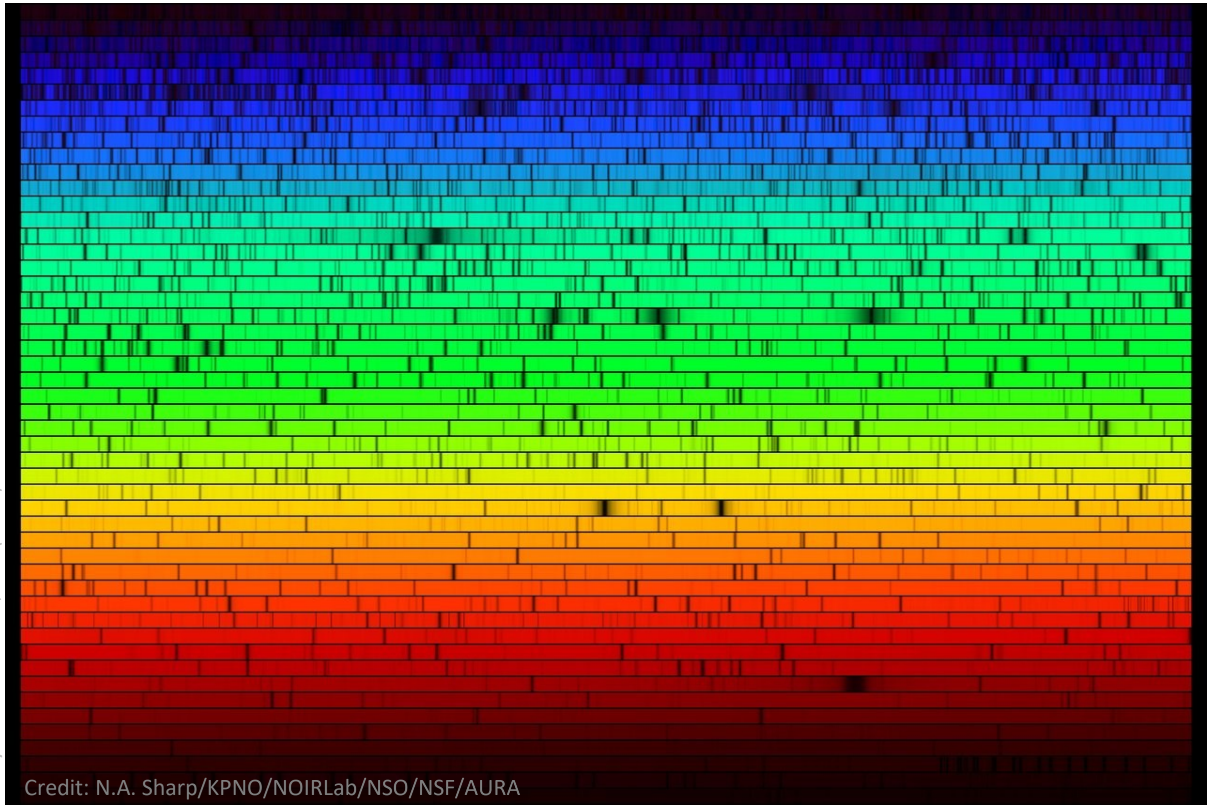
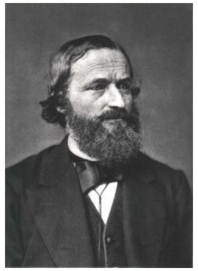


Fraunhofer

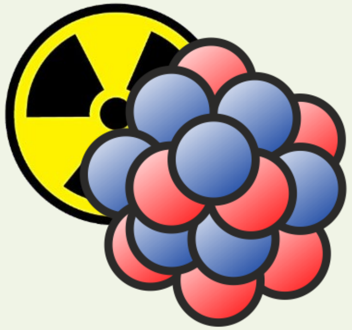
Kirchhoff



Bunsen

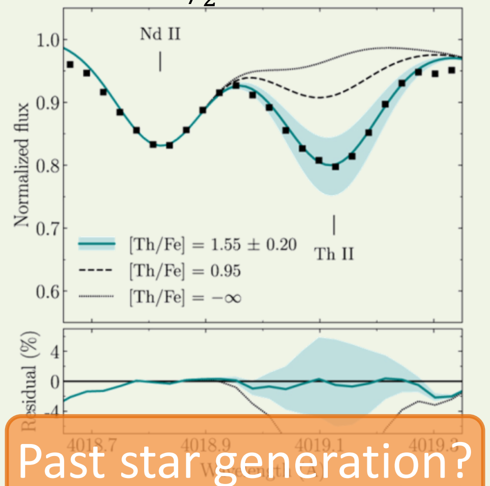
→dark features in the optical spectrum of the Sun

Radioactive nuclei: tracers of stellar dynamics



Radioactive nuclei

$^{232}\mathrm{Th}: \tau_{1/2} = 14.05\ \mathrm{Gyr}$



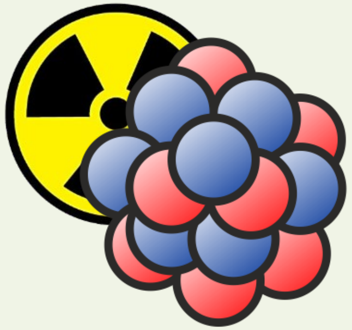
Past star generation?

E. M. Holmbeck *et al.* *ApJL* **859** L24 (2018)

2MASS J09544277+5246414 – giant star

Detection

Radioactive nuclei: tracers of stellar dynamics



Radioactive nuclei

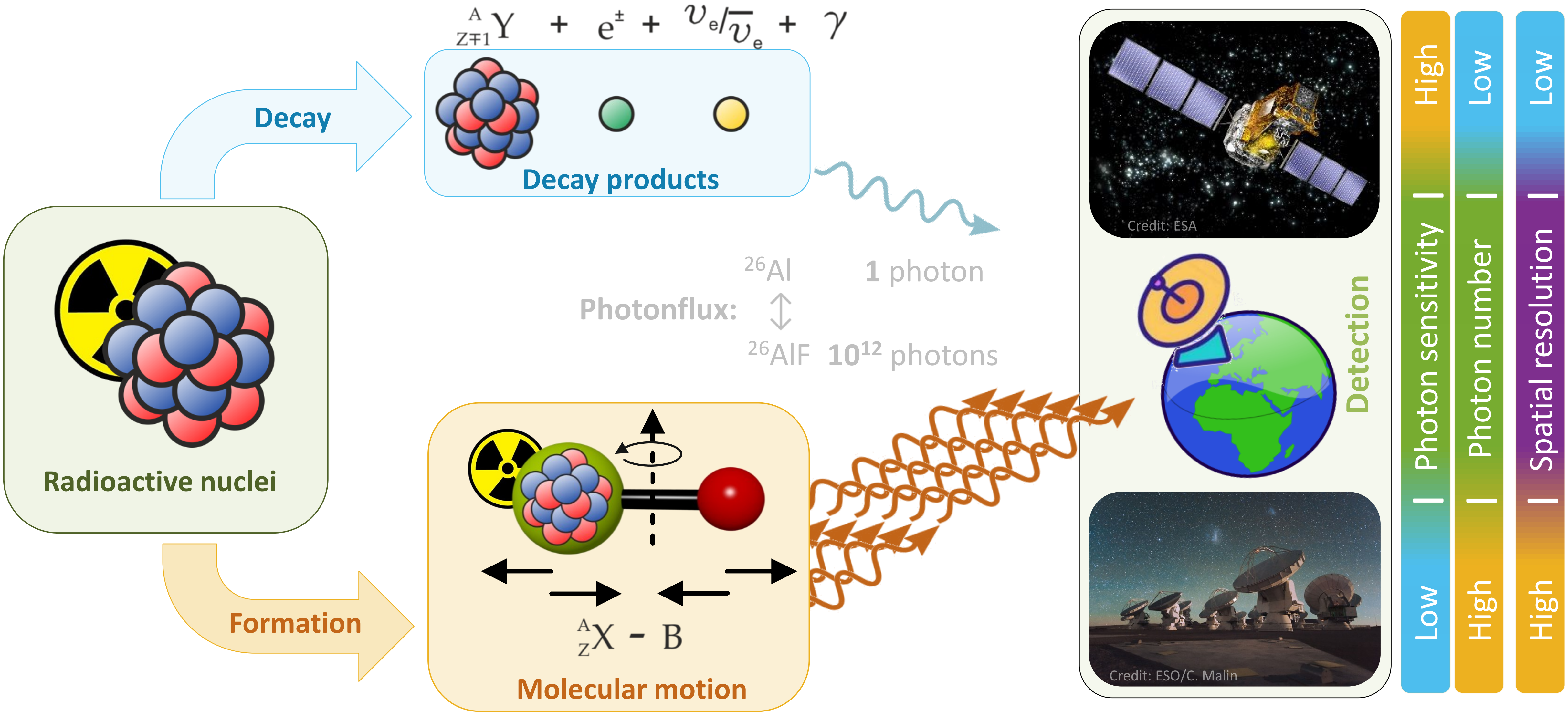
^{26}Al

^{44}Ti

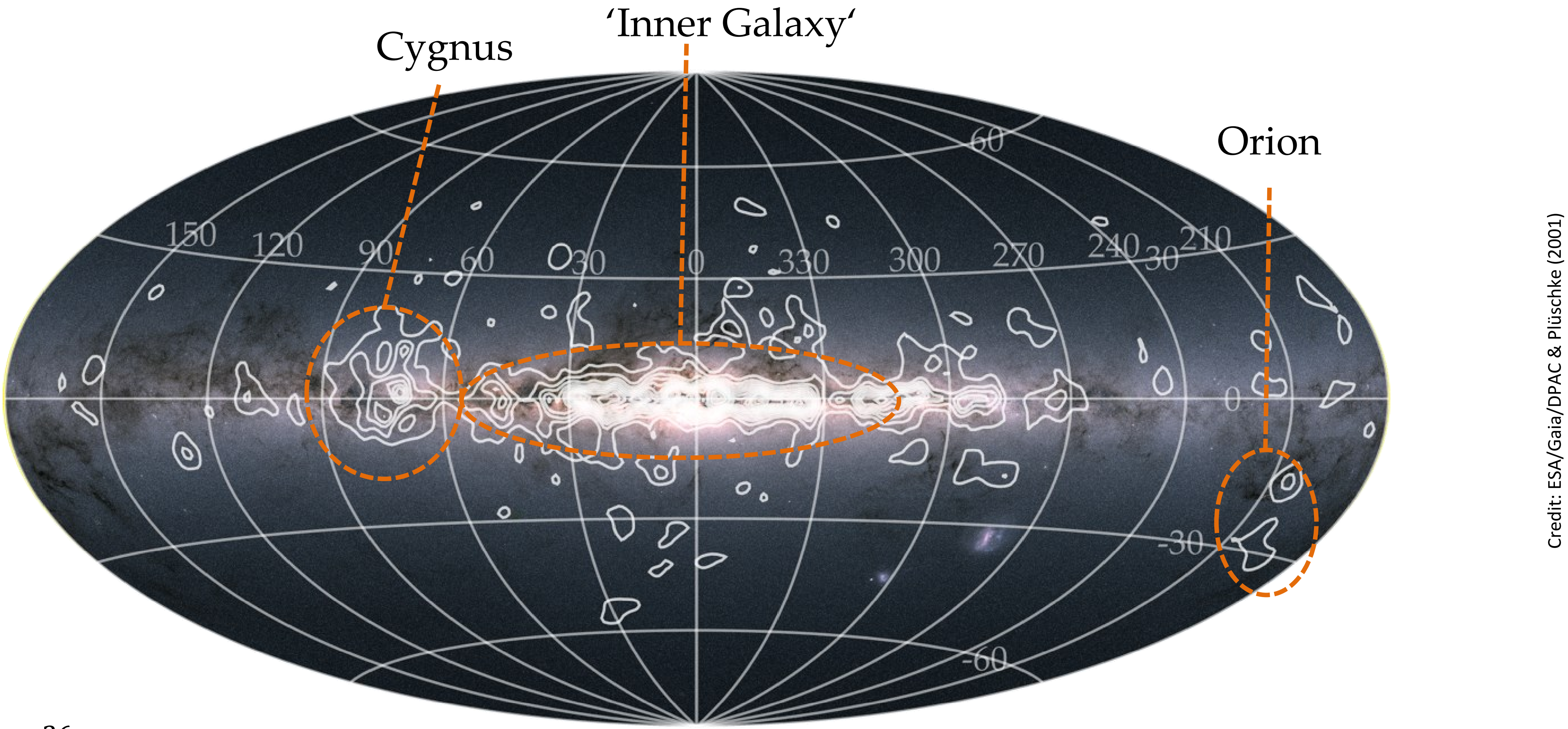
^{60}Fe

Detection

Radioactive nuclei: tracers of stellar dynamics



Galactic ^{26}Al distribution

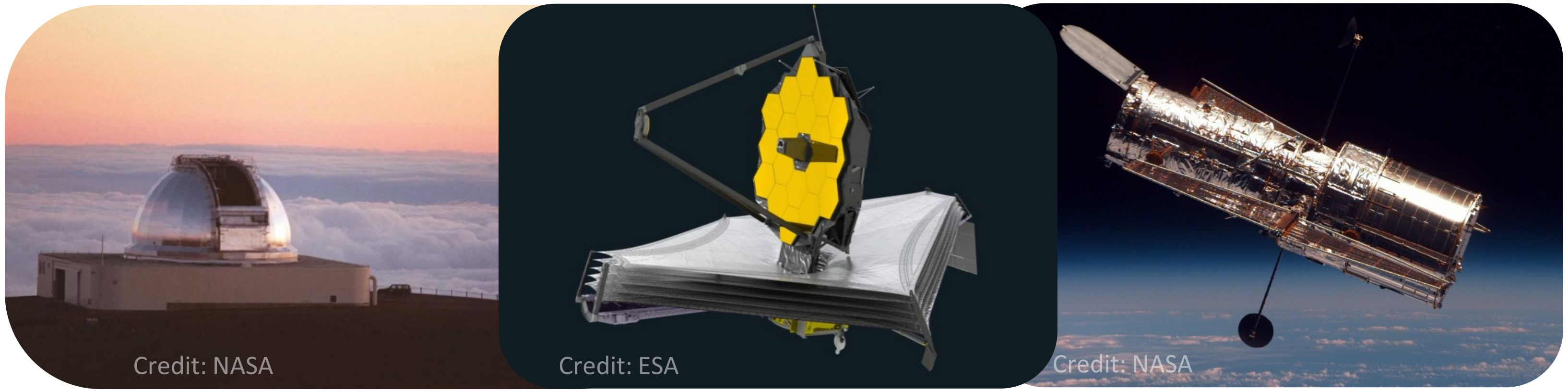


$$m_{total}^{26Al} = 2.8(8) \times M_{\odot}$$

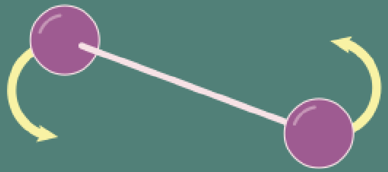
Diehl *et al.*, Nature **439**, 45 (2006)

Global structures as big as 100pc

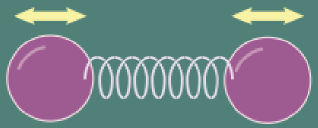
Pinpoint sources by molecular detection



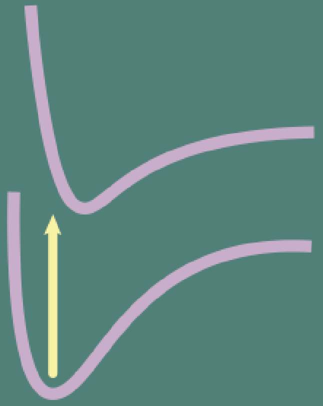
Rotational spectroscopy investigates the structure and dynamics of gas-phase molecules. Equilibrium structure determinations yield the equilibrium rotational constants.



Vibrational spectroscopy investigates the conformation and chemical linkages of molecules in gas and condensed phases. Accurate results require the inclusion of anharmonic contributions.



Electronic spectroscopy involves vibrational transitions between different electronic states. Vibrational signatures are defined by the overlaps between the vibrational wave functions of the initial and final electronic states.



Need: Transition information or molecular structure knowledge

Known Interstellar Molecules

2 Atoms
CH, CN, CH^+, OH, CO, H_2, SiO, CS, SO, SiS, NS, C_2, NO, HCl, NaCl, AlCl, KCl, AlF, PN, SiC, CP, NH, SiN, SO^+, CO^+, HF, N_2, CF^+, PO, O_2, AlO, CN^-, OH^+, SH^+, HCl^+, SH, TiO, ArH^+, NS^+, HeH^+, VO, PO^+, SiP, FeC

3 Atoms
H_2O, HCO^+, HCN, OCS, HNC, H_2S, N_2H^+, C_2H, SO_2, HCO, HNO, HCS^+, HOC^+, SiC_2, C_2S, C_3, CO_2, CH_2, C_2O, MgNC, NH_2, NaCN, N_2O, MgCN, H_3^+, SiCN, AlNC, SiNC, HCP, CCP, AlOH, H_2O^+, H_2Cl^+, KCN, FeCN, HO_2, TiO_2, CCN, SiCSi, S_2H, HCS, HSC, NCO, CaNC, NCS, MgC_2, HSO

4 Atoms
NH_3, H_2CO, HNCO, H_2CS, C_2H_2, C_3N, HNCS, $HOCO^+$, C_3O, *l*-C_3H, $HCNH^+$, H_3O^+, C_3S, *c*-C_3H, HC_2N, H_2CN, SiC_3, CH_3, C_3N^-, PH_3, HCNO, HOCN, HSCN, HOOH, *l*-C_3H^+, HMgNC, HCCO, CNCN, HONO, MgCCH, HCCS, HNCN, H_2NC, $HCCS^+$, CH_3^+

5 Atoms
HC_3N, HCOOH, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, *c*-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, HCCNC, HNCCC, H_2COH^+, C_4H^-, CNCHO, HNCNH, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, CHOSH, HCSCN, HC_3O, NaCCCN, MgC_3N^+

307 Molecules

Last Updated: 2 Feb 2024

6 Atoms
CH_3OH, CH_3CN, NH_2CHO, CH_3SH, C_2H_4, C_5H, CH_3NC, HC_2CHO, H_2C_4, C_5S, HC_3NH^+, C_5N, HC_4H, HC_4N, *c*-H_2C_3O, CH_2CNH, C_5N^-, HNCHCN, SiH_3CN, MgC_4H, CH_3CO^+, H_2CCCS, CH_2CCH, HCSCCH, C_5O, $HCCNCH^+$, C_5H^+, *c*-C_5H, HC_4S, HMgCCCN, MgC_4H^+, $H_2C_3H^+$, HOCOOH, H_2C_3N

7 Atoms
CH_3CHO, CH_3CCH, CH_3NH_2, CH_2CHCN, HC_5N, C_6H, *c*-C_2H_4O, CH_2CHOH, C_6H^-, CH_3NCO, HC_5O, $HOCH_2CN$, HC_4NC, HC_3HNH, *c*-C_3HCCH, MgC_5N, CH_2C_3N, *l*-H_2C_5, NC_4NH^+, MgC_5N^+

12 Atoms
C_6H_6, *n*-C_3H_7CN, *i*-C_3H_7CN, $C_2H_5OCH_3$, 1-C_5H_5CN, 2-C_5H_5CN, *n*-$CH_3CH_2CH_2OH$, *i*-$CH_3CH_2CH_2OH$, *i*-C_4H_8, 1-C_5H_4CCH, 2-C_5H_4CCH

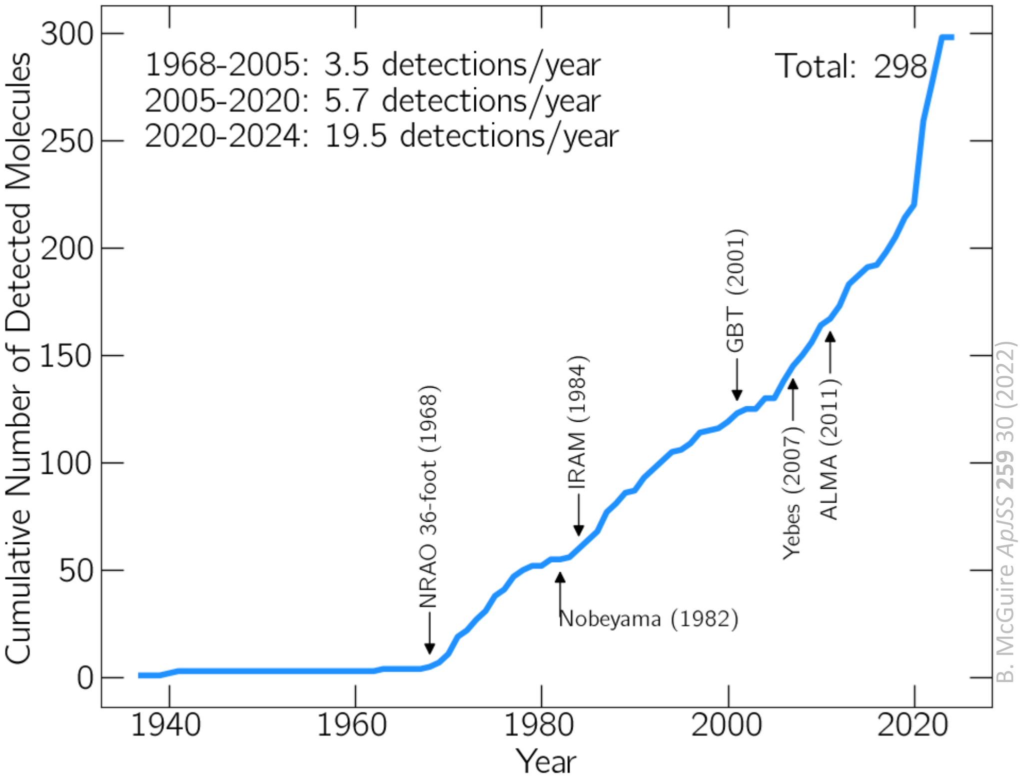
8 Atoms
$HCOOCH_3$, CH_3C_3N, C_7H, CH_3COOH, H_2C_6, CH_2OHCHO, HC_6H, CH_2CHCHO, CH_2CCHCN, NH_2CH_2CN, CH_3CHNH, CH_3SiH_3, NH_2CONH_2, $HCCCH_2CN$, CH_2CHCCH, MgC_6H, $C_2H_3NH_2$, HOCHCHOH, HCCCHCCC, C_7N^-, CH_3CHCO, MgC_6H^+

9 Atoms
CH_3OCH_3, CH_3CH_2OH, CH_3CH_2CN, HC_7N, CH_3C_4H, C_8H, CH_3CONH_2, C_8H^-, CH_2CHCH_3, CH_3CH_2SH, HC_7O, CH_3NHCHO, $H_2CCCHCCH$, HCCCHCHCN, H_2CCHC_3N

10 Atoms
CH_3COCH_3, $HOCH_2CH_2OH$, CH_3CH_2CHO, CH_3C_5N, CH_3CHCH_2O, CH_3OCH_2OH, H_2CCCHC_3N, C_6H_4, C_2H_5NCO, HC_7NH^+, $CH_3CHCHCN$, CH_2CCH_3CN, CH_2CHCH_2CN, NH_2COCH_2OH

11 Atoms
HC_9N, CH_3C_6H, C_2H_5OCHO, CH_3COOCH_3, CH_3COCH_2OH, C_5H_6, $NH_2CH_2CH_2OH$, CH_2CCHC_4H, $C_{10}H^-$, C_4H_5CN

13+ Atoms
C_6H_5CN, $HC_{11}N$, *c*-$C_5H_4CCH_2$, *c*-C_6H_5CCH, 1-$C_{10}H_7CN$, 2-$C_{10}H_7CN$, C_9H_8, 2-C_9H_7CN, C_{60}, C_{60}^+, C_{70}



Unique spectra for each molecule and its isotopologues

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3 Atoms

H_2O, HCO^+, HCN, OCS, HNC, H_2S, N_2H^+, C_2H, SO_2, HCO, HNO, HCS^+, HOC^+, SiC_2, C_2S, C_3, CO_2, CH_2, C_2O, MgNC, NH_2, NaCN, N_2O, MgCN, H_3^+, SiCN, AlNC, SiNC, HCP, CCP, AlOH, H_2O^+, H_2Cl^+, KCN, FeCN, HO_2, TiO_2, CCN, SiCSi, S_2H, HCS, HSC, NCO, CaNC, NCS, MgC_2, HSO

4 Atoms

NH_3, H_2CO, HNCO, H_2CS, C_2H_2, C_3N, HNCS, $HOCO^+$, C_3O, *l*-C_3H, $HCNH^+$, H_3O^+, C_3S, *c*-C_3H, HC_2N, H_2CN, SiC_3, CH_3, C_3N^-, PH_3, HCNO, HOCN, HSCN, HOOH, *l*-C_3H^+, HMgNC, HCCO, CNCN, HONO, MgCCH, HCCS, HNCN, H_2NC, $HCCS^+$, CH_3^+

5 Atoms

HC_3N, HCOOH, CH_2NH, NH_2CN, H_2CCO, C_4H, SiH_4, *c*-C_3H_2, CH_2CN, C_5, SiC_4, H_2CCC, CH_4, HCCNC, HNCCC, H_2COH^+, C_4H^-, CNCHO, HNCNH, CH_3O, NH_3D^+, H_2NCO^+, $NCCNH^+$, CH_3Cl, MgC_3N, HC_3O^+, NH_2OH, HC_3S^+, H_2CCS, C_4S, CHOSH, HCSCN, HC_3O, NaCCCN, MgC_3N^+

6 Atoms

CH_3OH, CH_3CN, NH_2CHO, CH_3SH, C_2H_4, C_5H, CH_3NC, HC_2CHO, H_2C_4, C_5S, HC_3NH^+, C_5N, HC_4H, HC_4N, *c*-H_2C_3O, CH_2CNH, C_5N^-, HNCHCN, SiH_3CN, MgC_4H, CH_3CO^+, H_2CCCS, CH_2CCH, HCSCCH, C_5O, $HCCNCH^+$, C_5H^+, *c*-C_5H, HC_4S, HMgCCCN, MgC_4H^+, $H_2C_3H^+$, HOCOOH, H_2C_3N

307 Molecules

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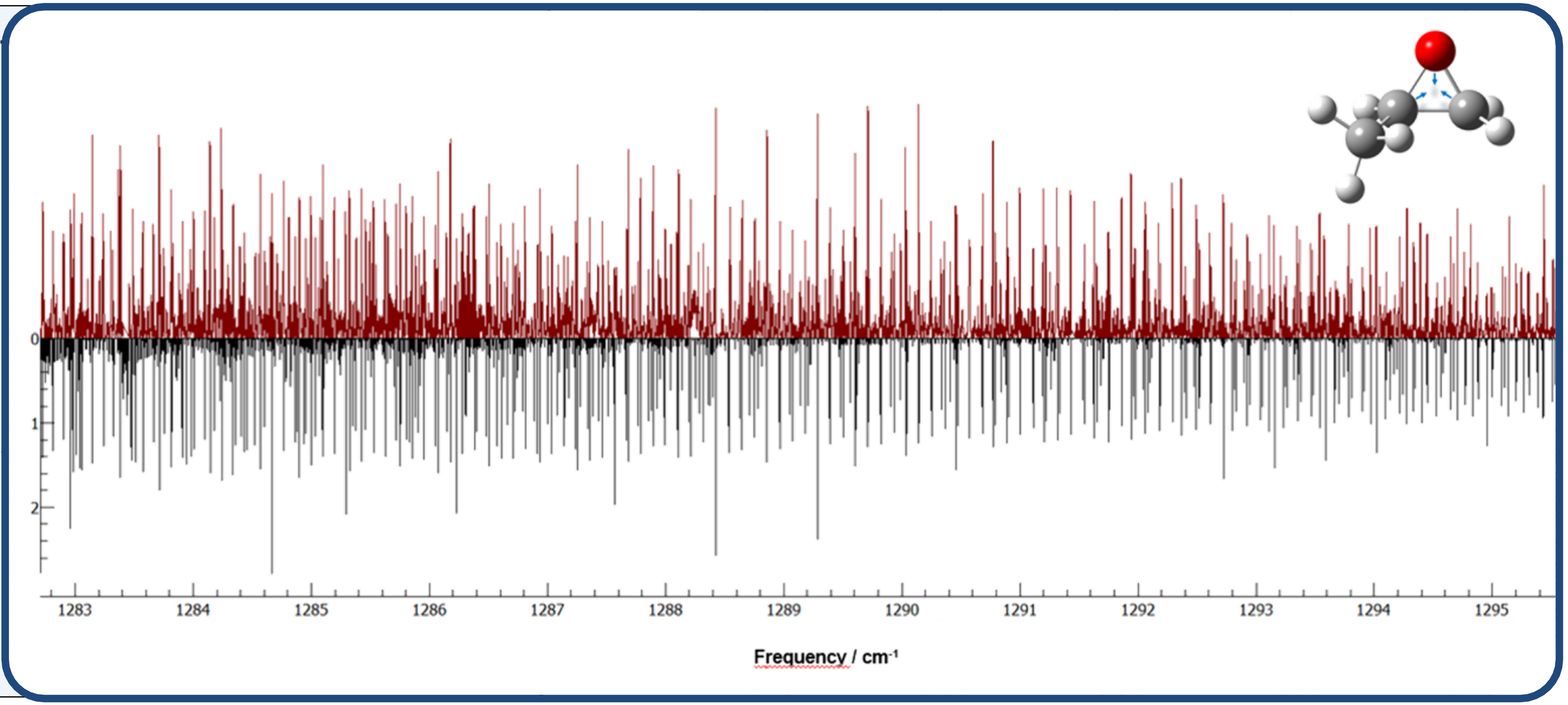
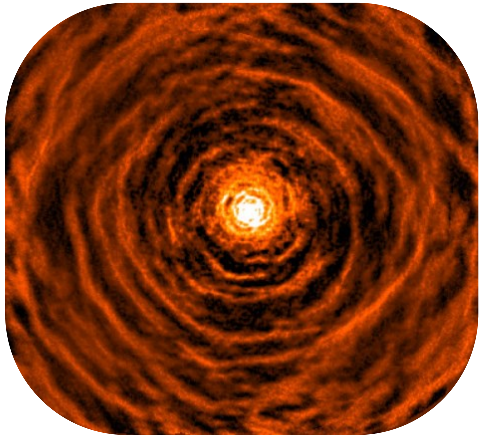


Year

Unique spectra for each molecule and its isotopologues

Stellar environments: Astrochemistry

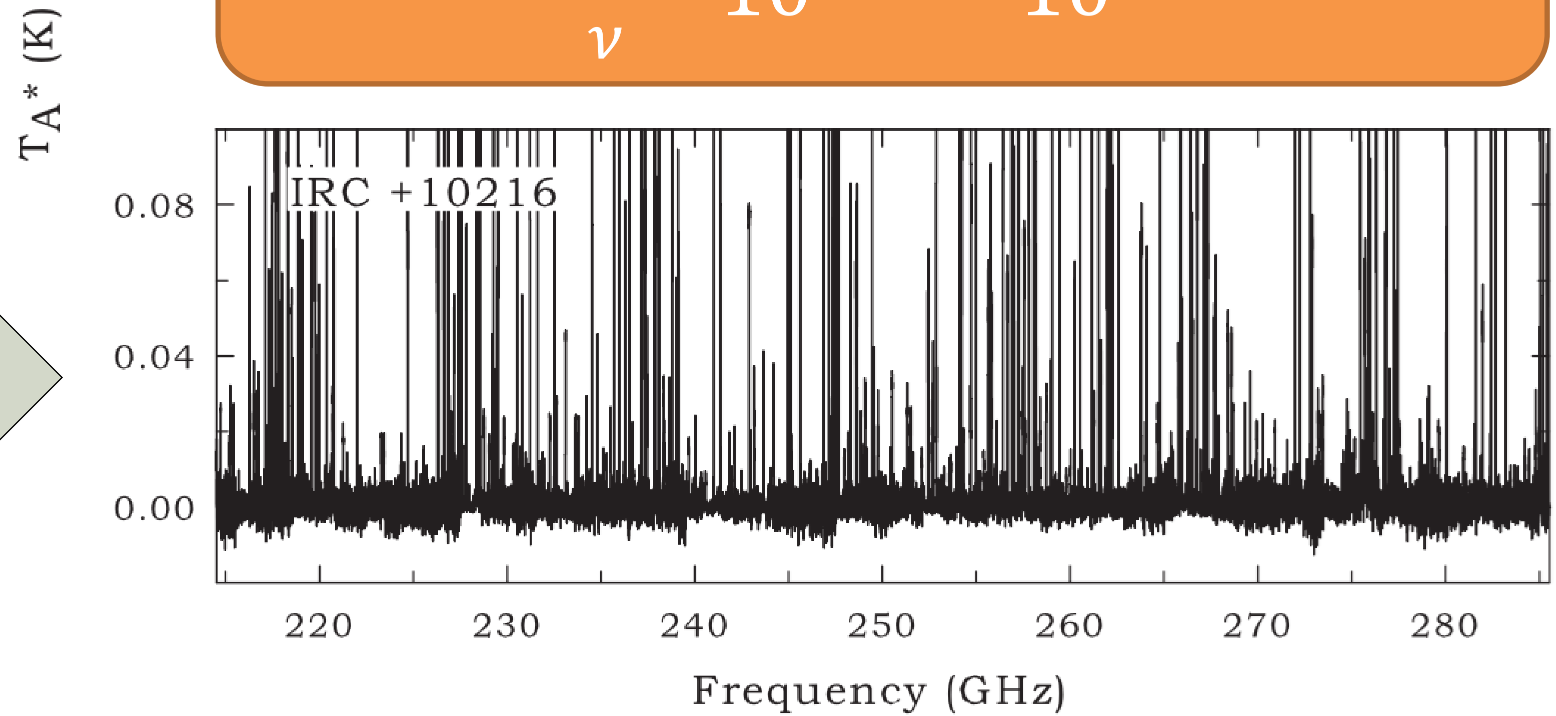
Guélin *et al* A&A 610, A4 (2018)



C/O >1

Precision demand:

$$\frac{\Delta\nu}{\nu} \sim 10^{-7} \dots 10^{-9}$$

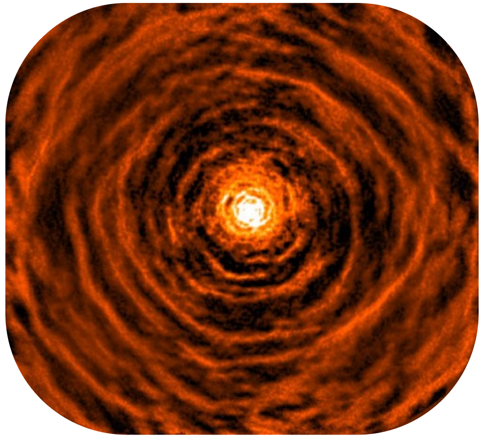


E. D. Tenenbaum *et al* ApJL **720** L102 (2010)

Stellar environments: Astrochemistry

Credit: NASA/ESA/R. Humphreys

C/O <1



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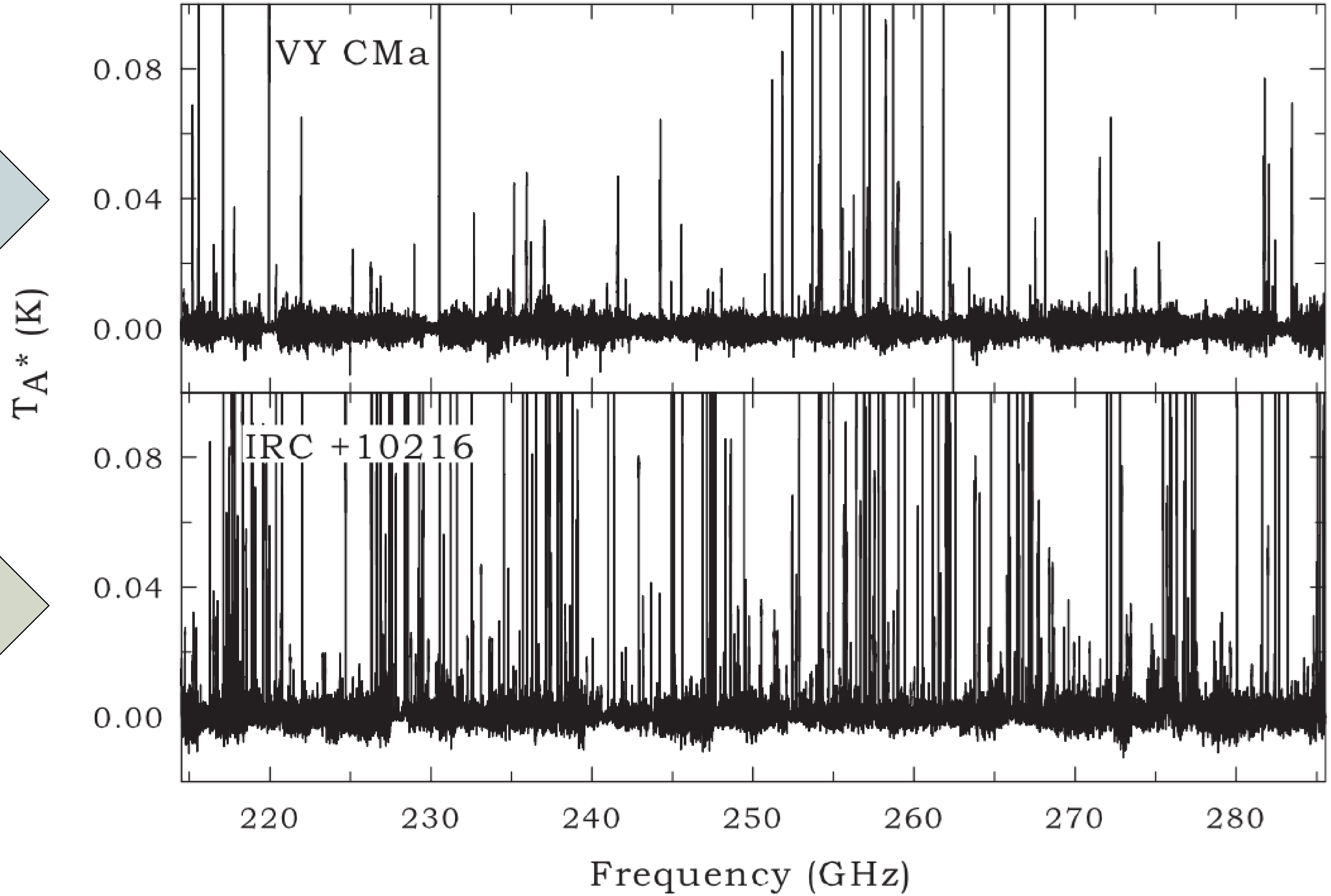

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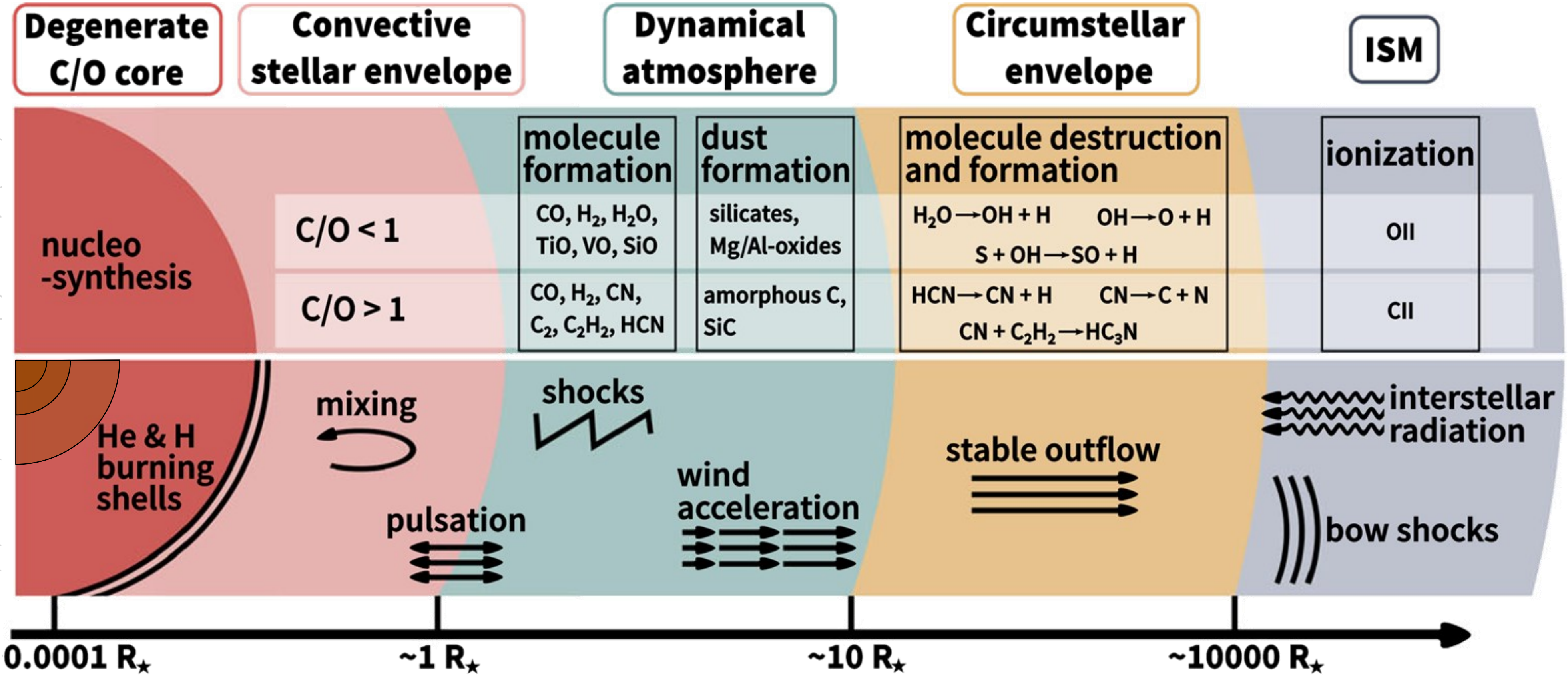
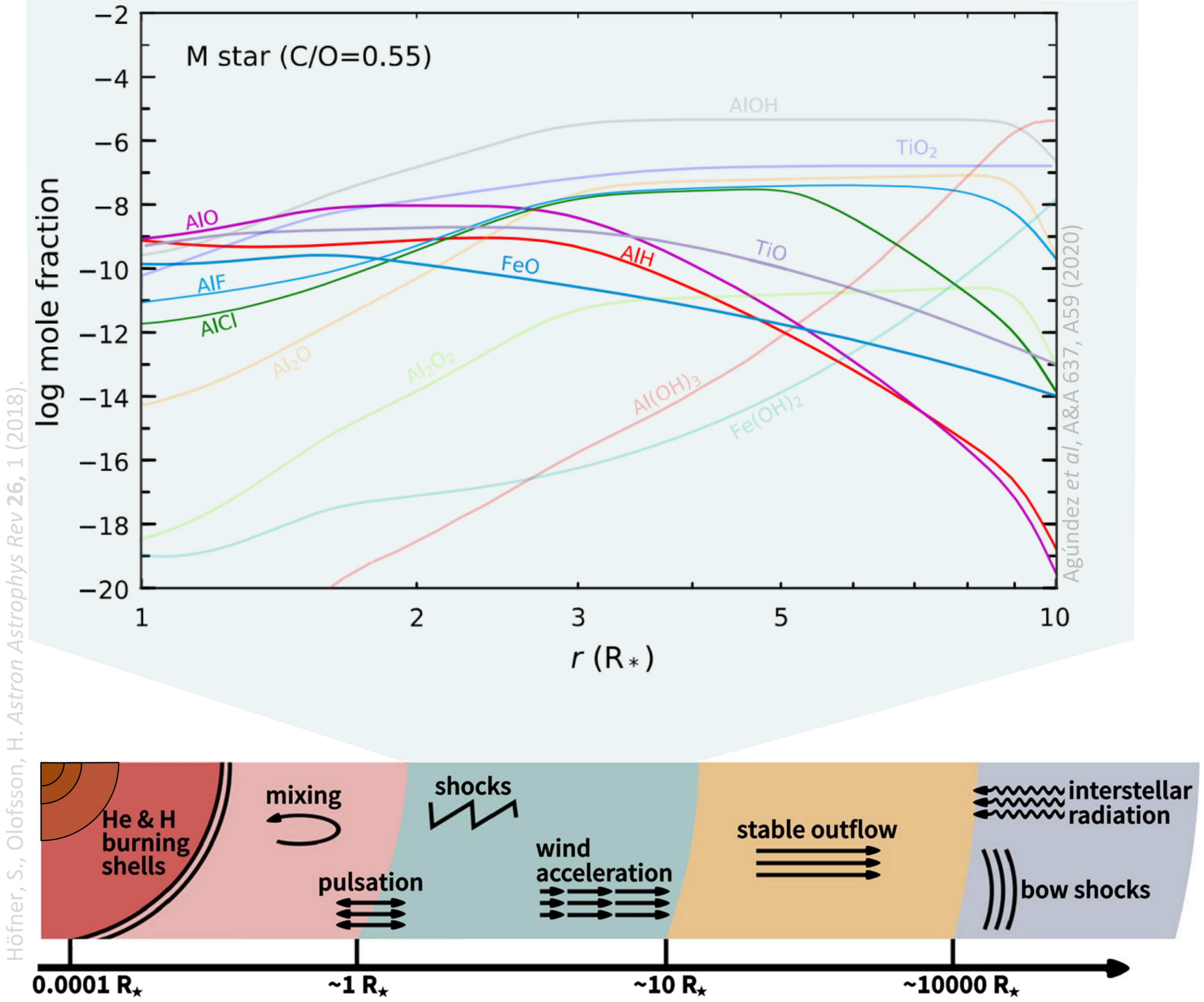
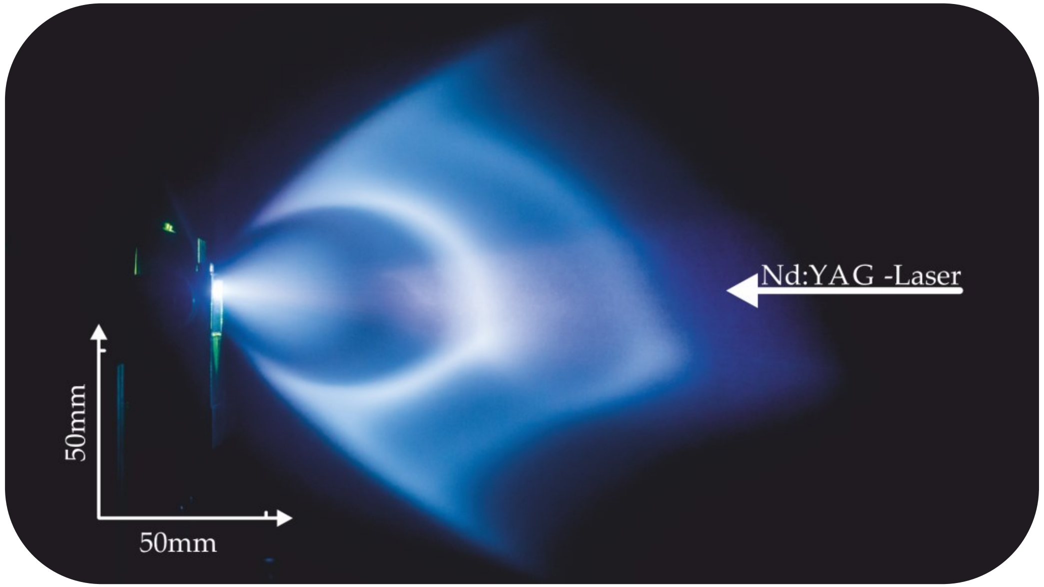
Molecular Species near Stellar Objects



Höfner, S., Olofsson, H. *Astron Astrophys Rev* **26**, 1 (2018).

Molecular Species near Stellar Objects





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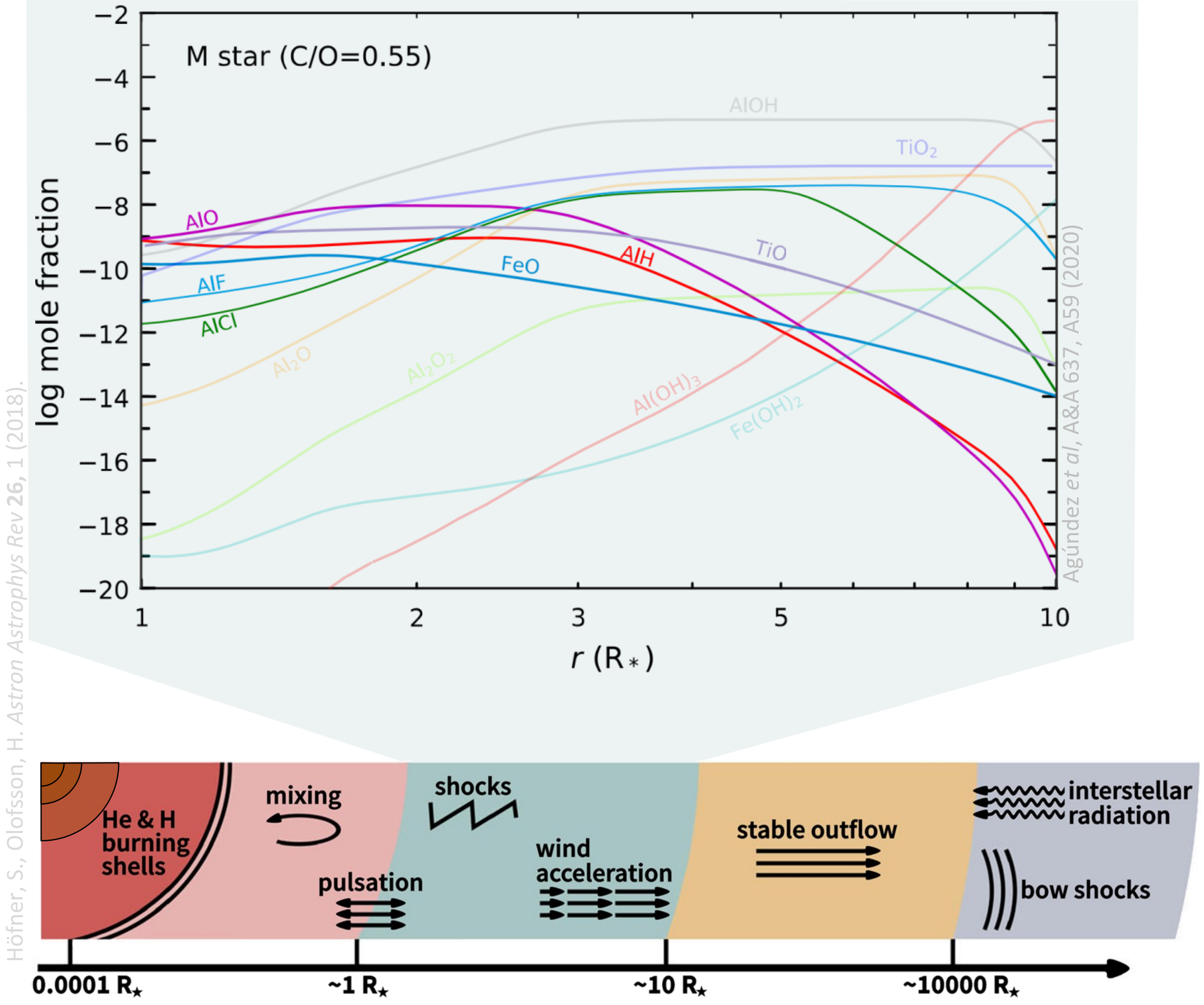


Radioactive diatomic molecules

Breier *et al.*, JMS **350**, 43 (2018)

^{26}AlO

^{26}AlF

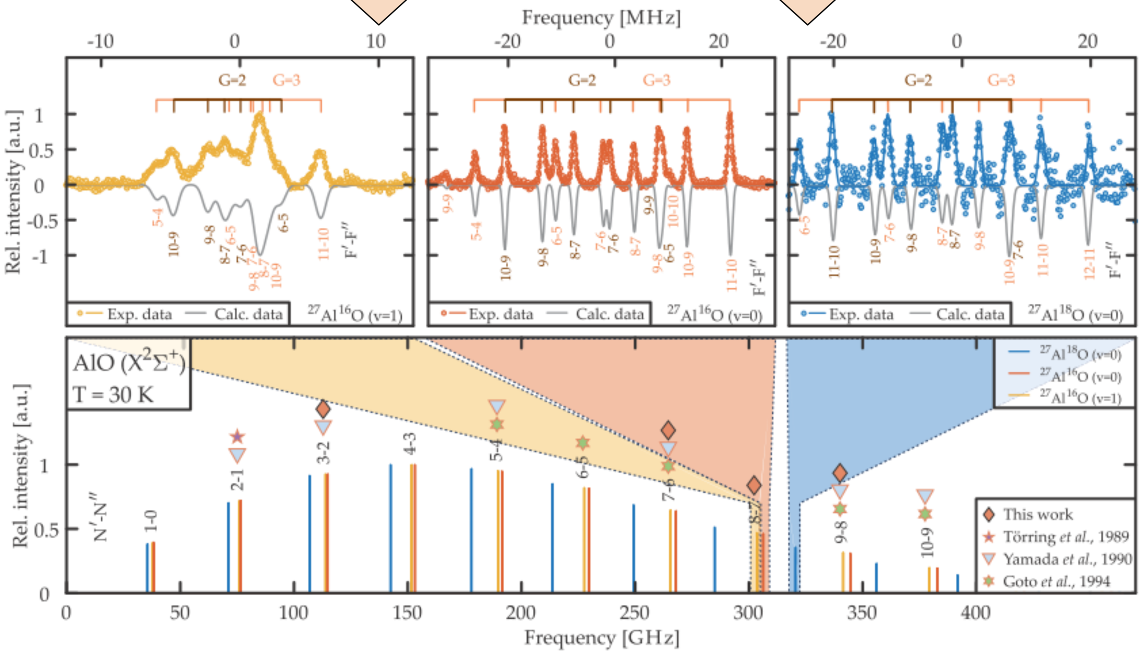
Breier *et al.*, JMS **355**, 46 (2019)

^{44}TiO

^{60}FeO

Waßmuth, Breier *et al.*, *MolPhys 1774087* (2020)

scalable



Molecular structure is a spectroscopic puzzle

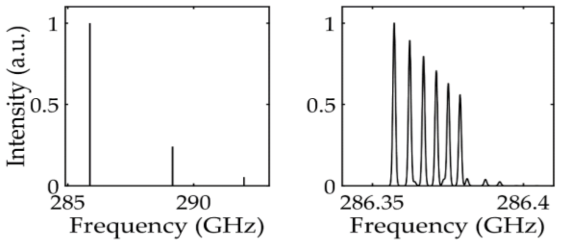
Mass-independent description

$$B_v = \sum_k \mu^{-(k/2+1)} \left(1 + \sum_{i=A,B} \frac{m_e}{M_i}\Delta^i_{kl}\right) U_{kl} \left(v + \frac{1}{2}\right)^k$$

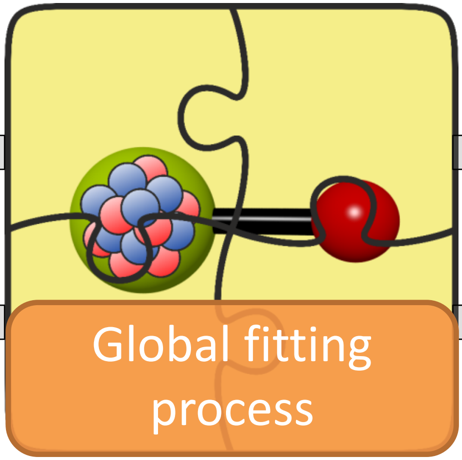
$B_v \rightarrow r_v$

- Ro-vibrational coupling → r_e
- Ro-‘e⁻-motion‘ coupling → r_e^{BO}

(Hyper-)Fine-structure



$$X_{v,\alpha} = \sum_k \eta \cdot \mu_\alpha^{-\frac{2l+k}{2}} \cdot \left(1 + \sum_{i=A,B} \frac{m_e}{M^i_\alpha}\Delta^i_{\hat{O}_{k,l}}\right)_{BO} \cdot \hat{O}_{k,l} \cdot \left(v + \frac{1}{2}\right)^k$$



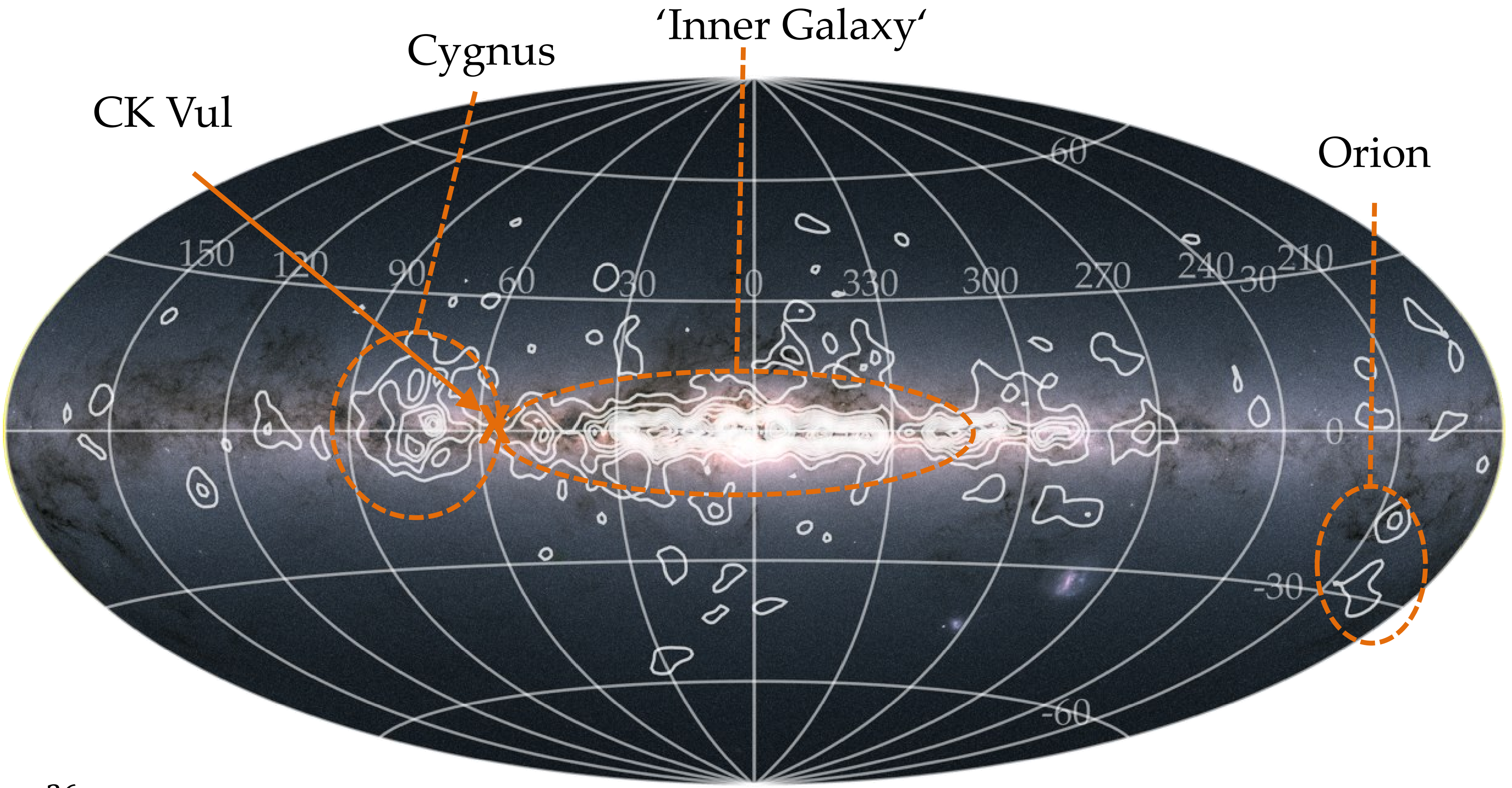
Already observed

- Optical/IR/MW transitions

Lab observation

- Rotational transitions
- Vibrational transitions
- Optical transitions

Galactic ^{26}Al distribution



Credit: ESA/Gaia/DPAC & Plüschke (2001)

$$m_{total}^{^{26}Al} = 2.8(8) \times M_{\odot}$$

Diehl *et al.,* Nature **439**, 45 (2006)

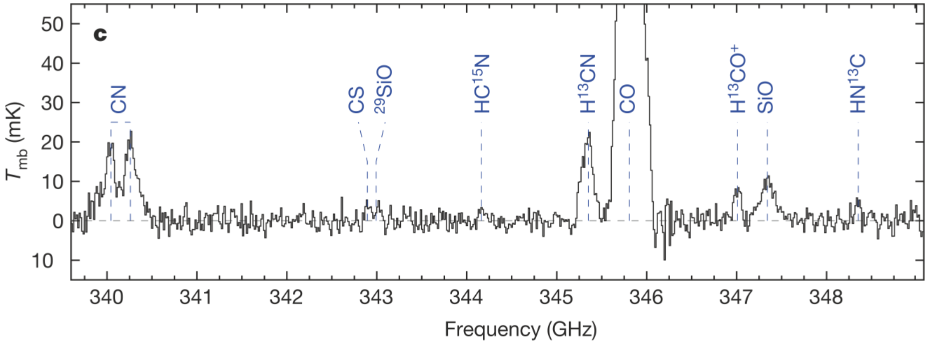
Global structures as big as 100pc

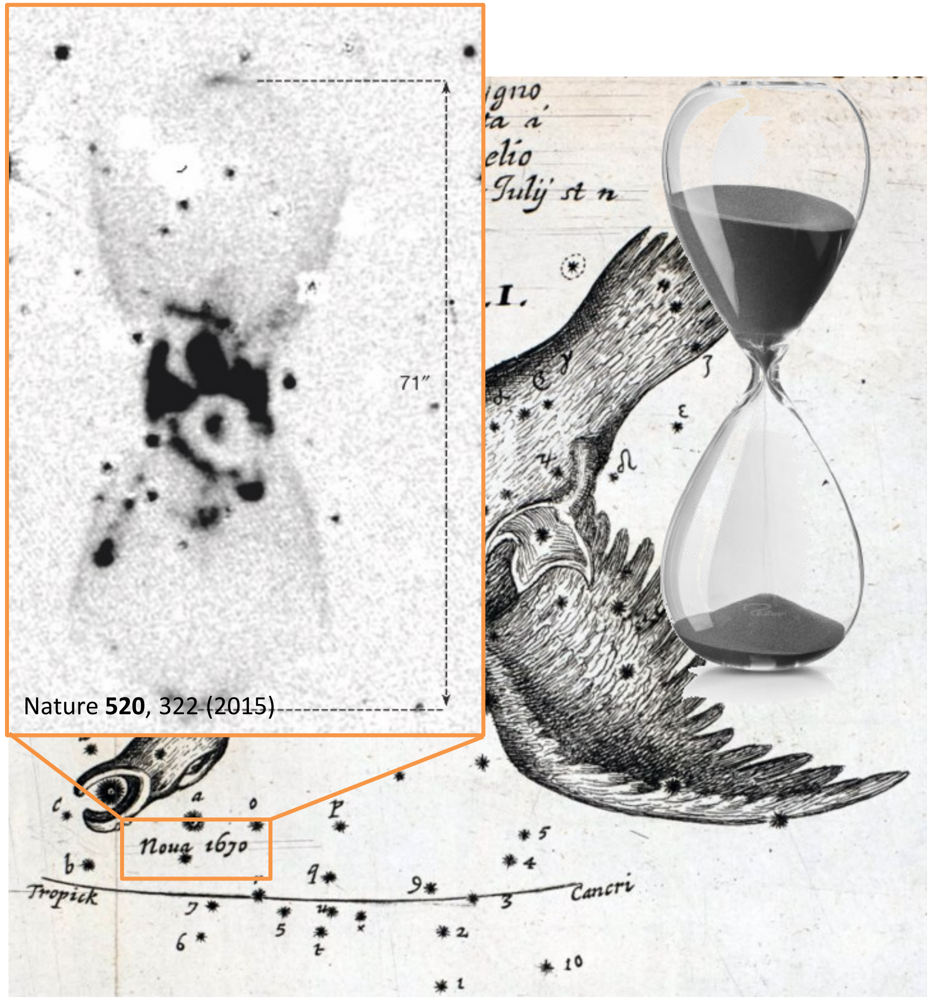
Pinpoint source: CK Vulpeculae (CK Vul)

Key facts

- 1670(1) CK Vul outburst observed
- 1982 Bipolar nebula was found
- ‘Red’ nova object
- 27 molecules detected

  containing H, C, N, O, F, Al, Si, P, S





Nuclear ashes and outflow in the eruptive star Nova Vul 1670

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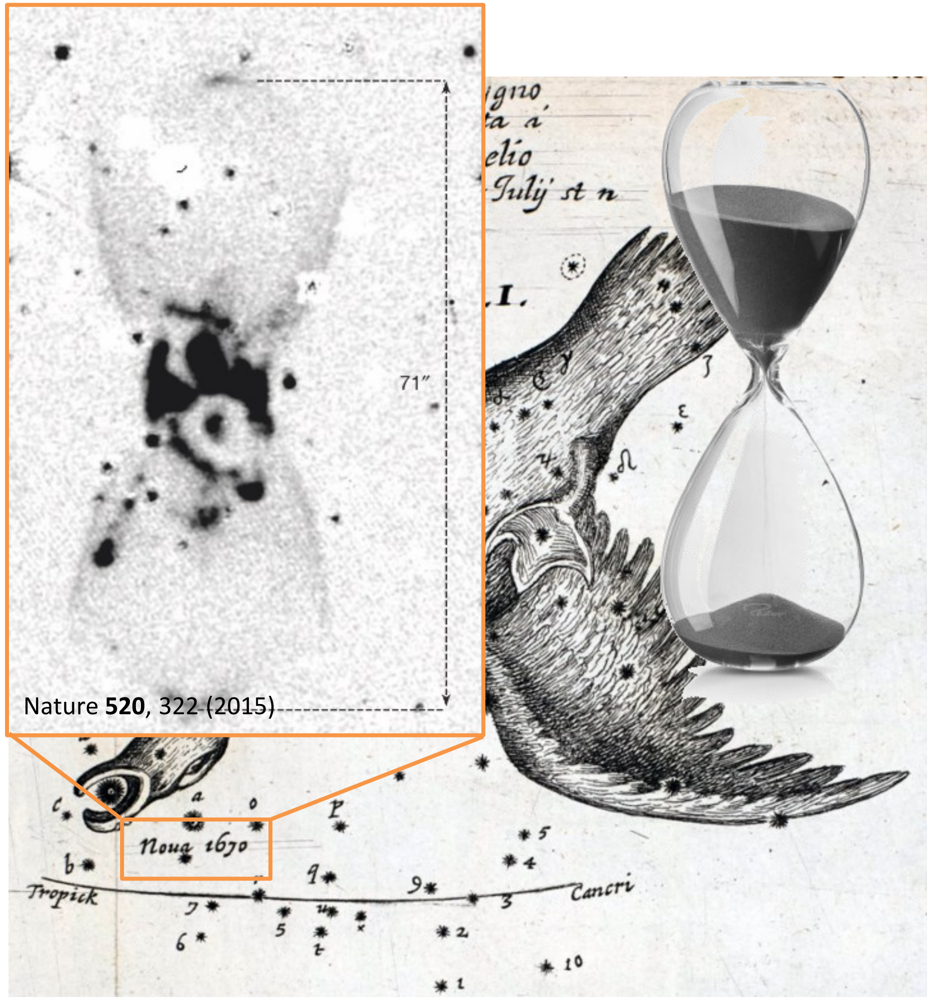
Isotopic ratios

	CK Vul	Sun
$^{12}C/^{13}C$	3.8(10)	90
$^{14}N/^{15}N$	20(10)	440
$^{16}O/^{18}O$	36(14)	500
$^{16}O/^{17}O$	>180	2600
$^{28}Si/^{29}Si$	6.7(4)	20



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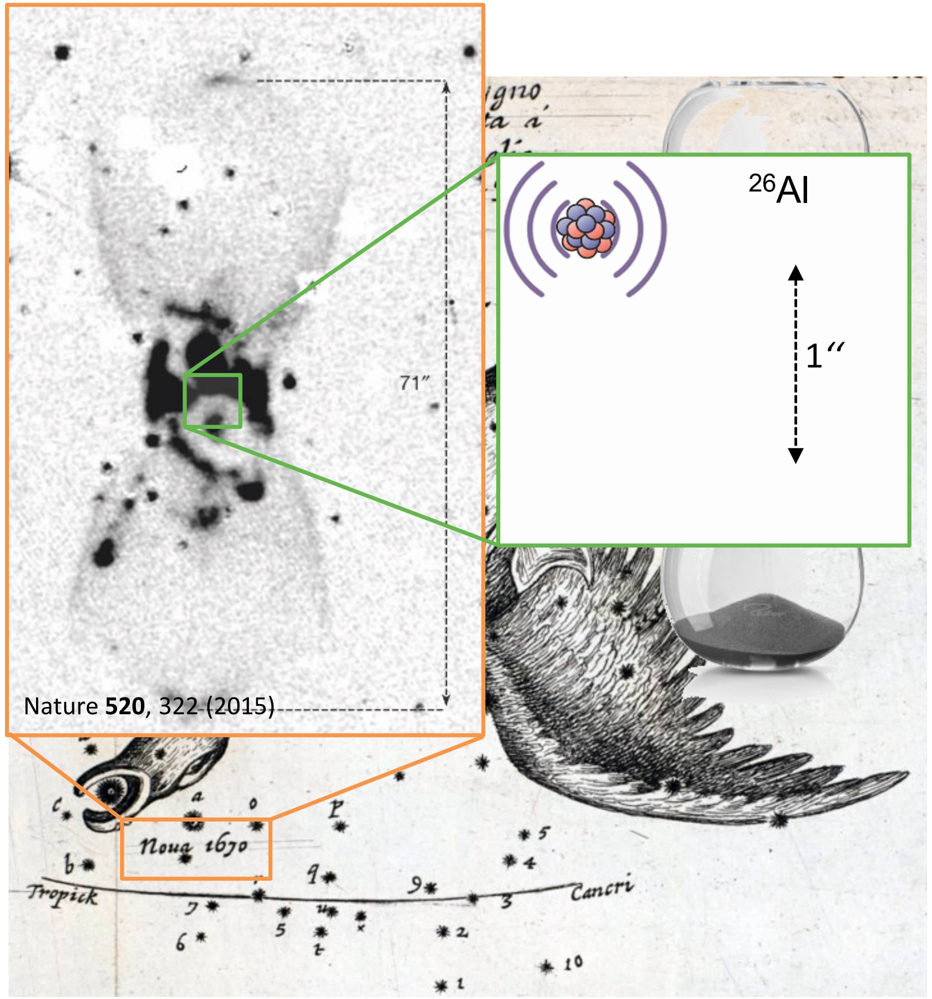
	CK Vul	Sun
$^{12}C/^{13}C$	3.8(10)	90
$^{14}N/^{15}N$	20(10)	440
$^{16}O/^{18}O$	36(14)	500
$^{16}O/^{17}O$	>180	2600
$^{28}Si/^{29}Si$	6.7(4)	20



Nuclear ashes and outflow in the eruptive star Nova Vul 1670

Pinpoint source: CK Vulpeculae (CK Vul)

Key facts

- 1670(1) CK Vul outburst observed
- 1982 Bipolar nebula was found
- ‘Red’ nova object
- 27 molecules detected

  containing H, C, N, O, F, Al, Si, P, S

Isotopic ratios

	CK Vul	Sun
$^{12}C/^{13}C$	3.8(10)	90
$^{14}N/^{15}N$	20(10)	440
$^{16}O/^{18}O$	36(14)	500
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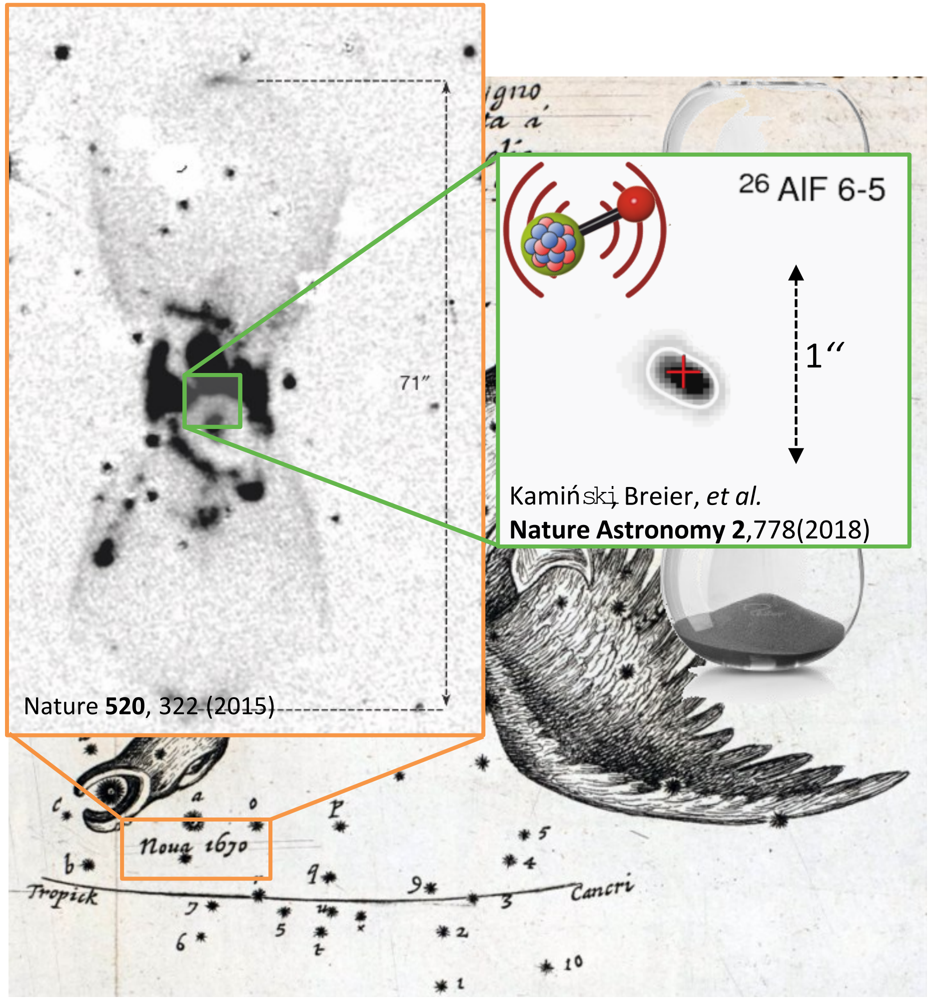


Nuclear ashes and outflow in the eruptive star Nova Vul 1670

Mass-independent description of AlF

AlF

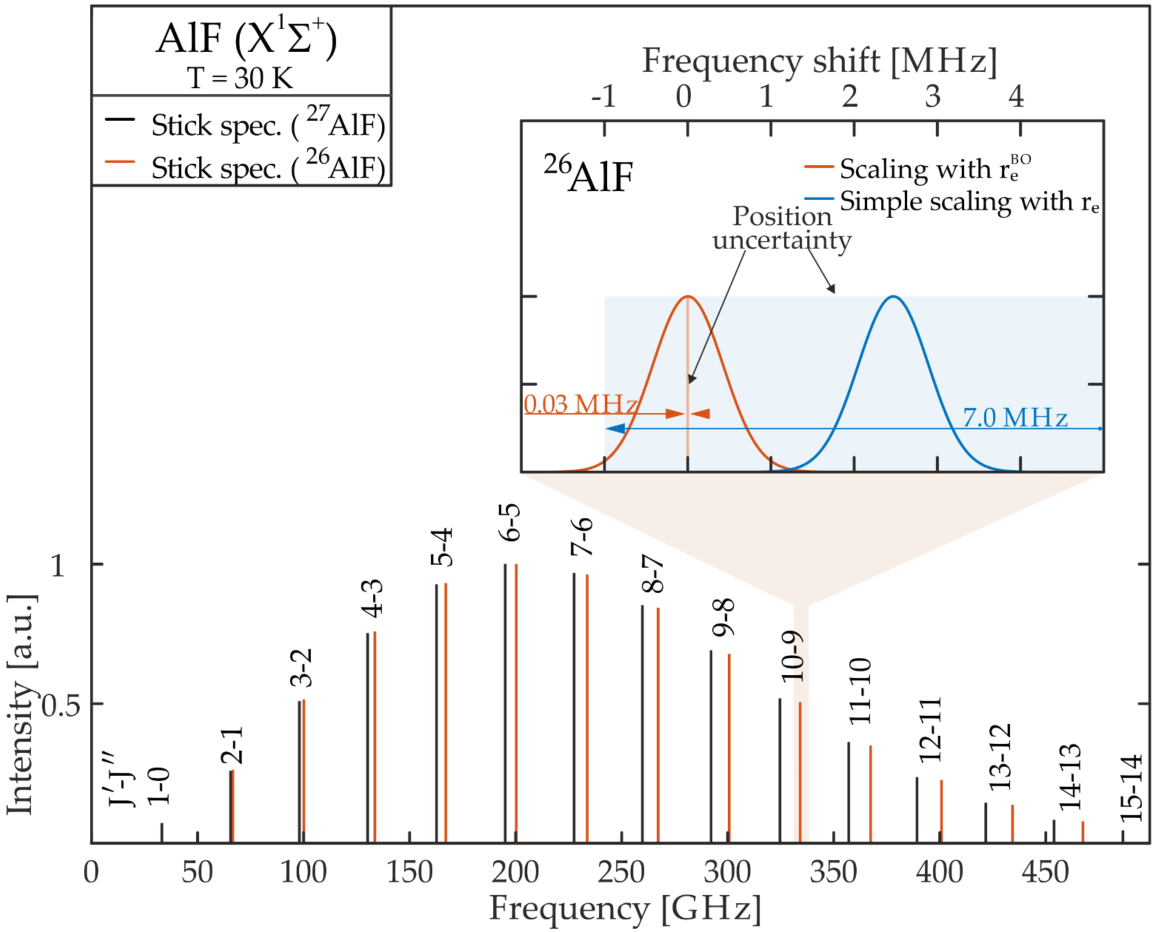
$$B_v = \sum_k \mu^{-(k/2+1)} \left(1 + \sum_{i=A,B} \frac{m_e}{M_i} \Delta^i_{k1}\right) U_{k1} \left(v + \frac{1}{2}\right)^k$$

$$U_{01} = 184655.12(23)\ \mathrm{MHz} \cdot \mathrm{u}$$
$$r_e^{BO} = 1.65435196(103)\ \text{Å}$$

AB	Δ^A_{U01}	Δ^B_{U01}
BF	-1.84(6)	-1.4*
AlF [theo]	[-0.96]	[-1.45]
GaF	-0.66(20)	-1.5*

*Using wobble-stretch theory

I (^{26}Al/^{19}F)	5/0.5
Q(^{26}Al) [mb]	265(32)



→Reducing uncertainty from 10^{-5} to 10^{-7}

Mass-independent description of AlF

AlF

$$B_\nu = \sum_k \mu^{-(k/2+1)} \left(1 + \sum_{i=A,B} \frac{m_e}{M_i} \Delta^i_{k1}\right) U_{k1} \left(\nu + \frac{1}{2}\right)^k$$

$$U_{01} = 184655.12(23)\ \mathrm{MHz \cdot u}$$

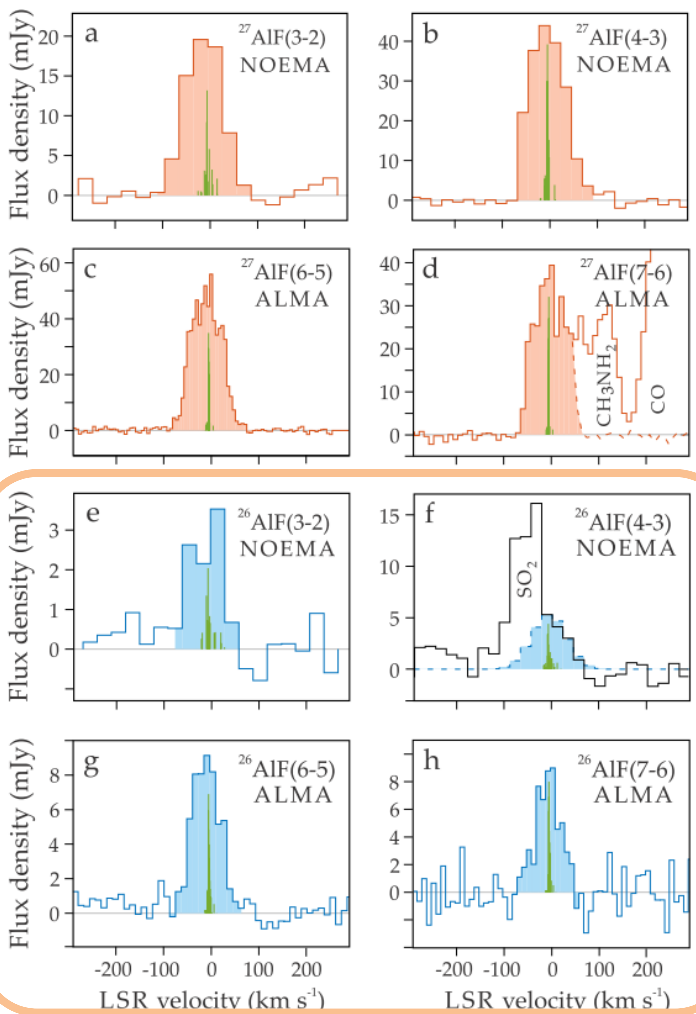
$$r_e^{BO} = 1.65435196(103)\ \text{Å}$$

AB	Δ^A_{U01}	Δ^B_{U01}
BF	-1.84(6)	-1.4*
AlF	-0.97(6)	-1.2*
[theo]	[-0.96]	[-1.45]
GaF	-0.66(20)	-1.5*

*Using wobble-stretch theory

I (^{26}Al/^{19}F)	5/0.5
Q(^{26}Al) [mb]	265(32)

Astronomical observation



Kamiński ...,Breier,..., Nature Astronomy 2 778 (2018)

Why so much ^{26}AlF in CK Vul ?

The origin of ^{26}Al

CK Vul

$$N_{27} = 3.0^{+0.5}_{-0.6} \times 10^{15}\ \mathrm{cm}^{-2}$$

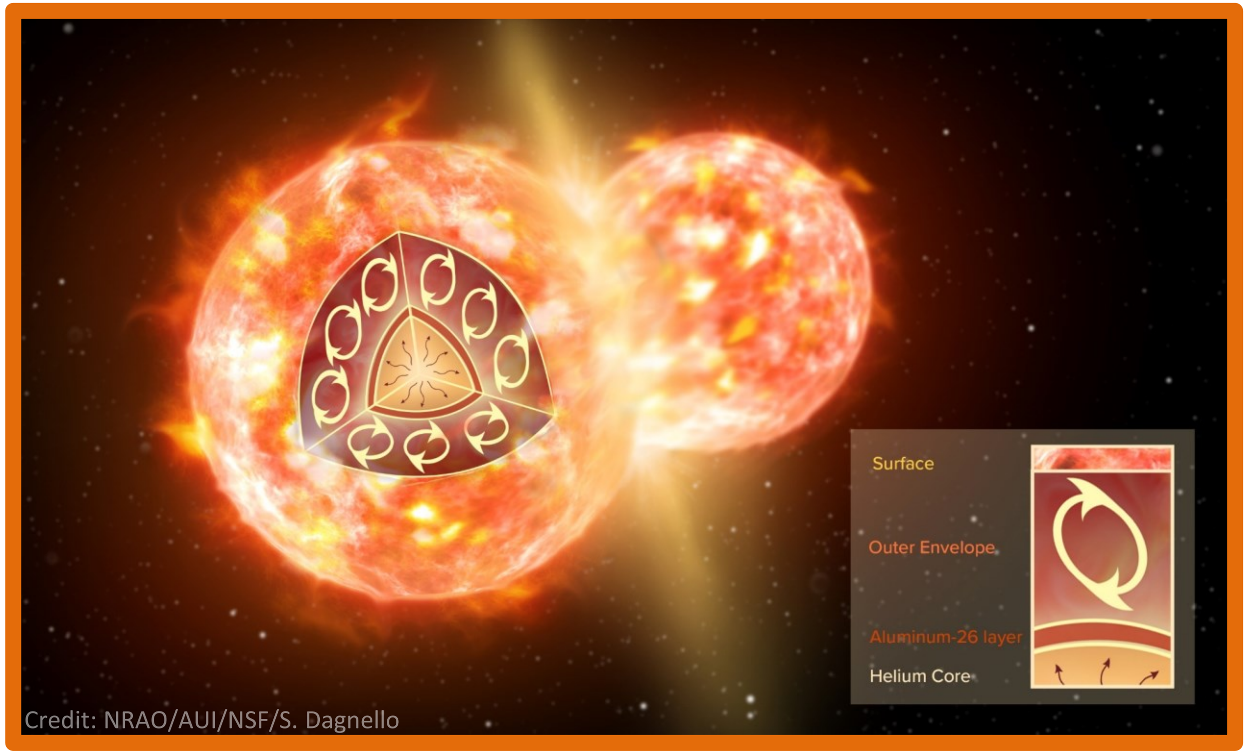
$$N_{27}/N_{26} = 7.1^{+3.2}_{-2.2}$$

AGB

$$\bar{N}_{27}/\bar{N}_{26} \approx 120000$$

Diehl *et al.*, Nature **439**, 45 (2006)

Why so much ^{26}AlF in CK Vul ?



Merging scenario

- Stellar Merger: two low mass star being one in the RGB phase

Kamiński *et al.*, Nature Astronomy **2**, 778 (2018)

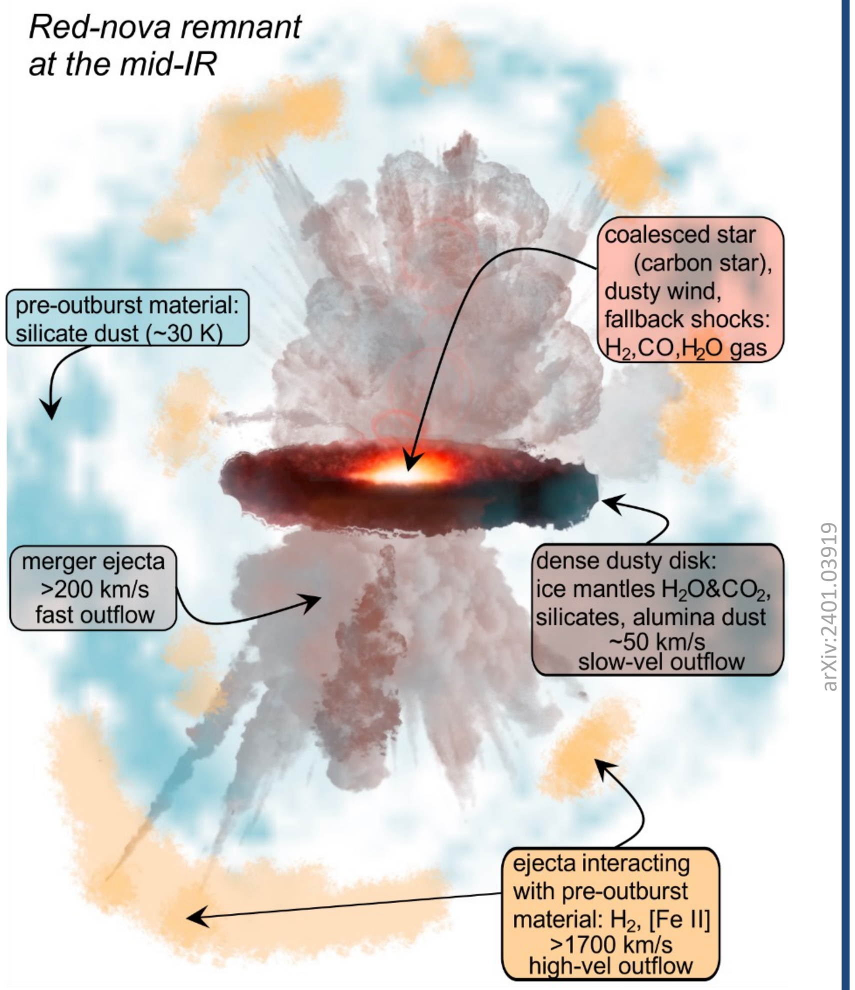
Or

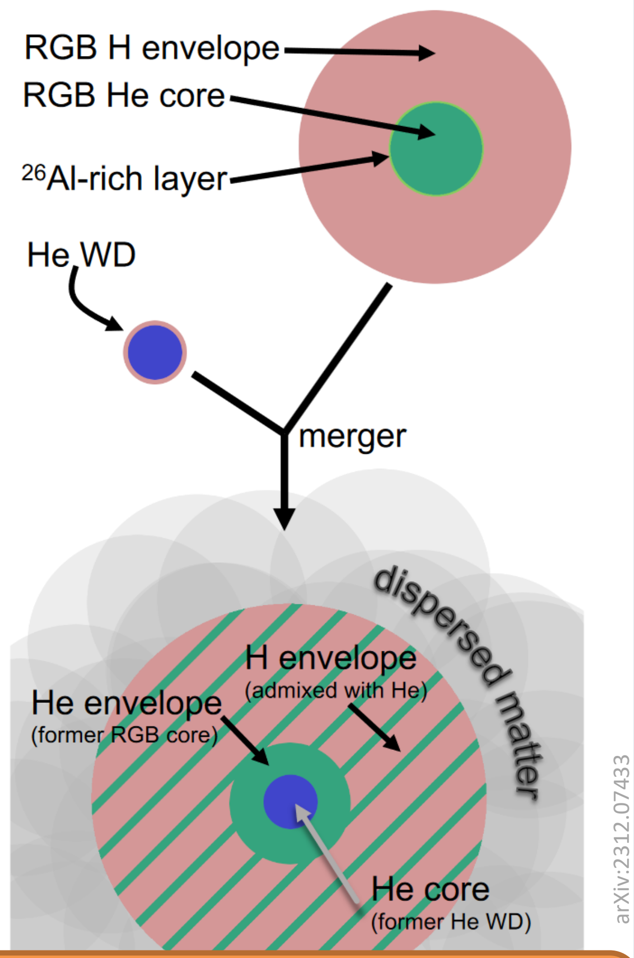
- Merger event between a white and brown dwarf

Eyres *et al.*, MNRAS **481**, 4931 (2018)

Reconstruction of merger event

Relative abundances by number			
	CK Vul	Error	Sun
He/H	0.260	±21%	0.085
N/H	1.69E–4	±29%	6.76E–5
O/H	1.22E–4	±34%	4.90E–4
Ne/H	7.45E–5	±29%	8.50E–5
S/H	5.70E–6	±9%	1.32E–5
Ar/H	1.35E–6	±15%	2.50E–6
Abundances by mass			
H	0.488	±18%	0.740
He	0.509	±28%	0.252
N	1.15E–3	±35%	7.01E–4
O	9.50E–4	±40%	5.80E–3
Ne	7.27E–4	±35%	1.26E–3
S	8.91E–5	±16%	3.13E–4
Ar	2.64E–5	±21%	7.40E–5





Re-definition of ‚red‘ nova!

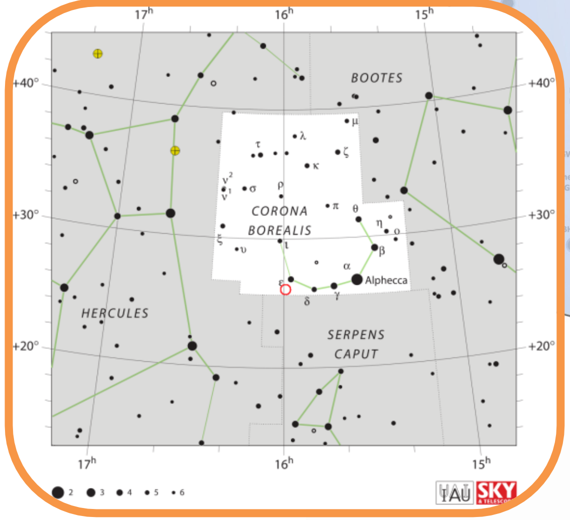
Common envelope events

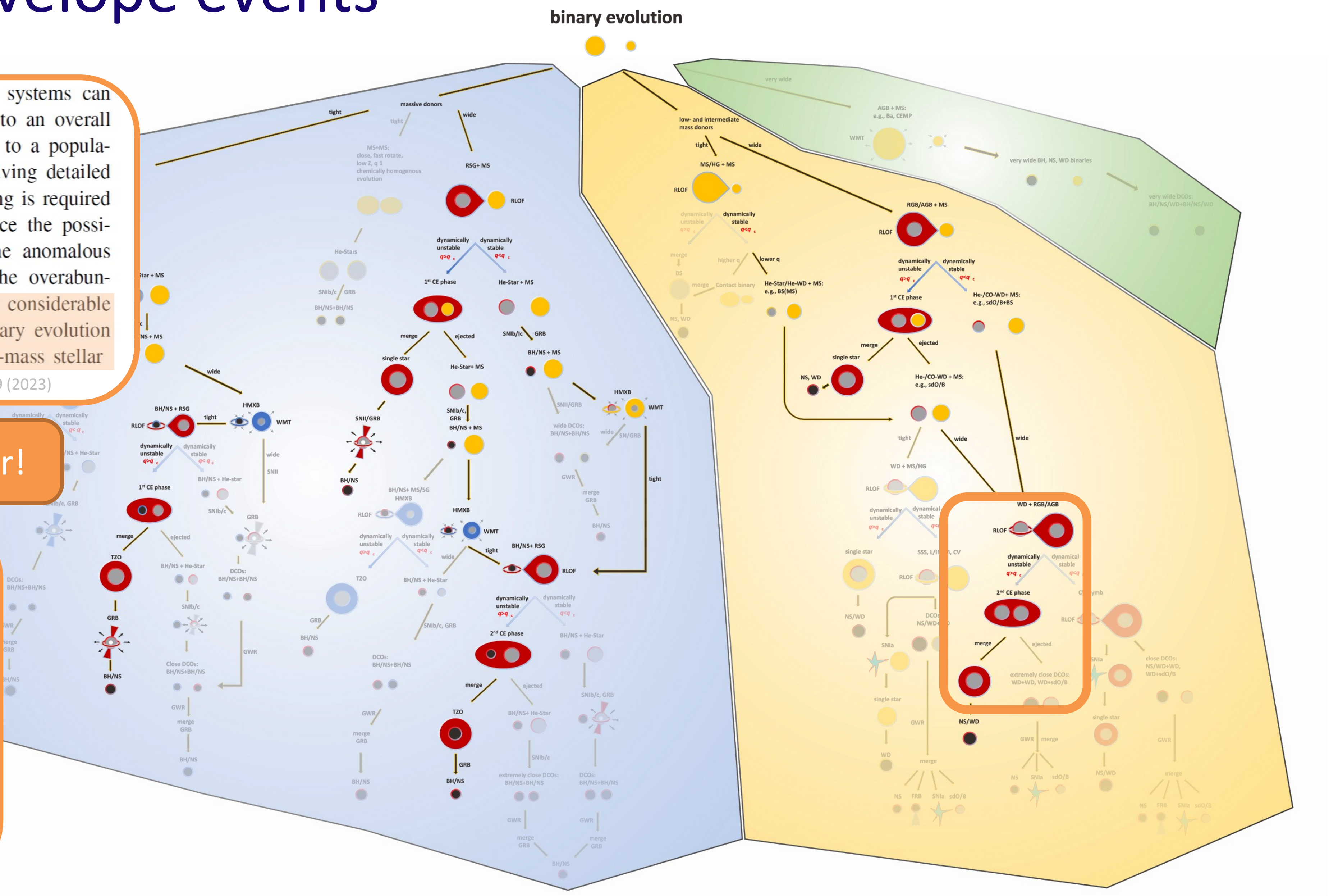
Our results show that ^{26}Al yields of individual systems can be extremely sensitive to binary evolution leading to an overall overproduction in a stellar population as compared to a population of only single-stars. Further investigation involving detailed models including core growth during core He-burning is required to verify our synthetic models. Our results introduce the possibility of binary evolution being responsible for the anomalous abundances observed in globular clusters or for the overabundance of ^{26}Al in our solar system. Our results show considerable promise in understanding the contribution from binary evolution onto the stellar yields from a low- and intermediate-mass stellar population.

Z. Osborn *et al.*, MNRAS **526**.4 6059 (2023)

Many events to discover!

T Coronae Borealis



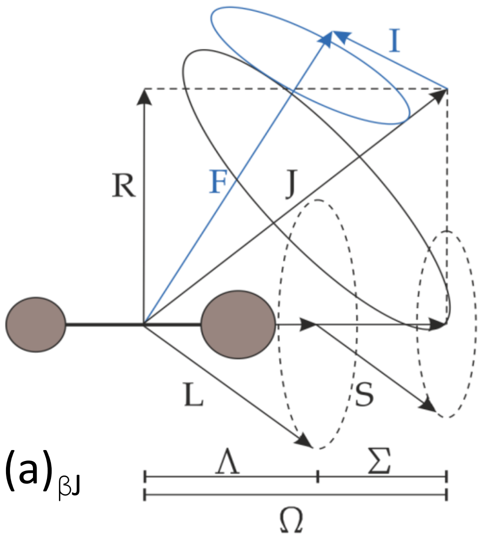


Han *et al.*, Res. Astron. Astrophys **20**.10, 161 (2020)

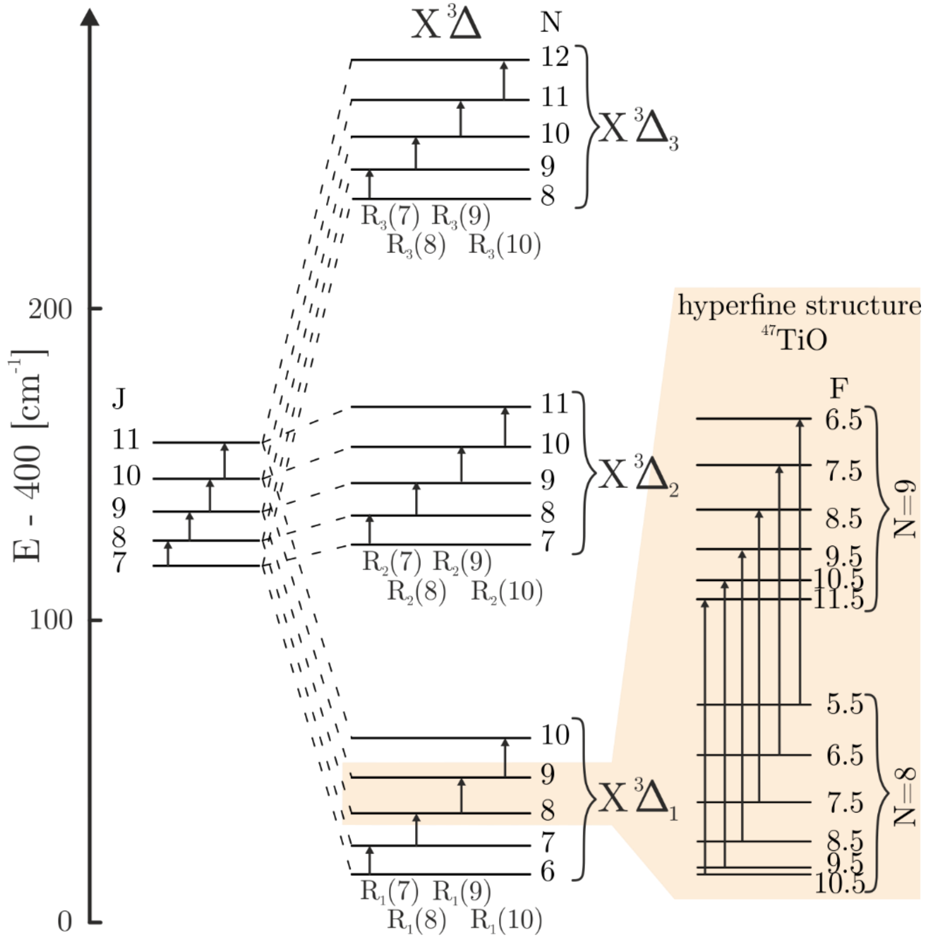
Another Diatomic case: TiO – a more complex one

Spectroscopic facts

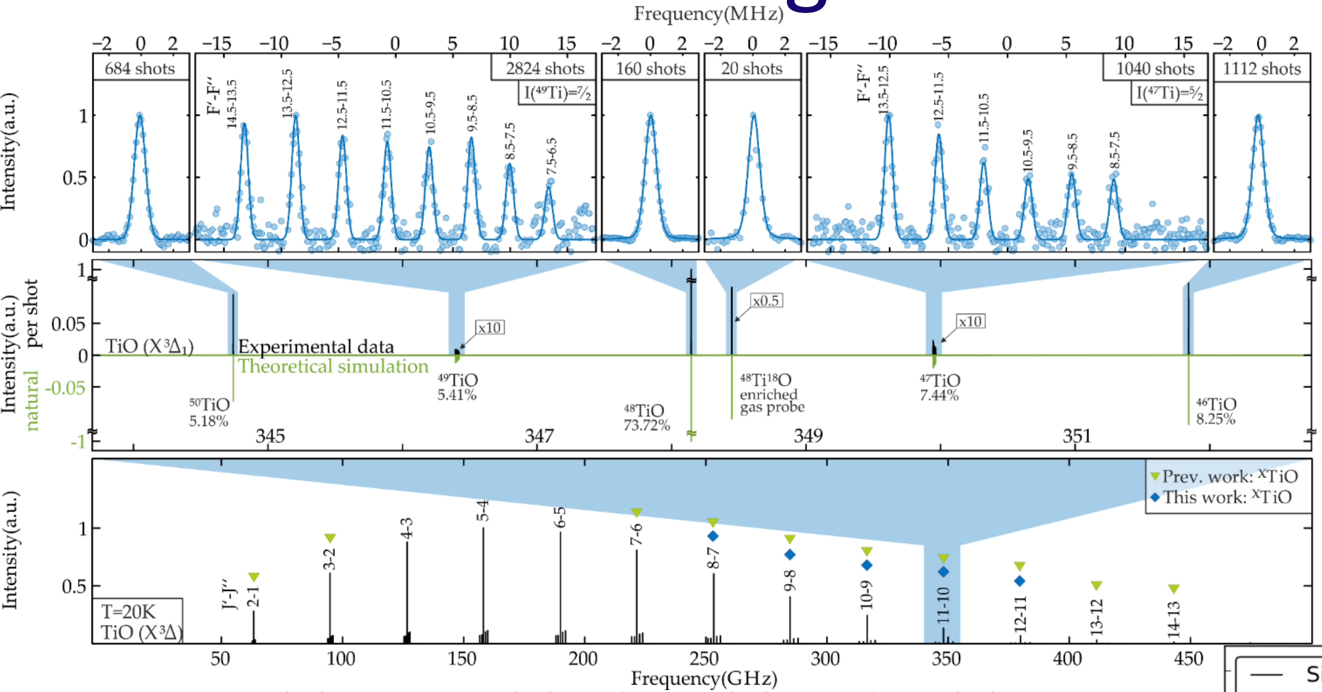
Observed in Lab since	1929
Valence conf.	$9\sigma^1 1\delta^1$
Ground state	$X^3\Delta$
Dipole moment [D]	3.34
Nuclear spin I ($^{47}Ti/^{49}Ti$)	2.5/3.5
Q($^{47}Ti/^{49}Ti$) [mb]	302/247



Hund's case (a)$_{\beta J}$

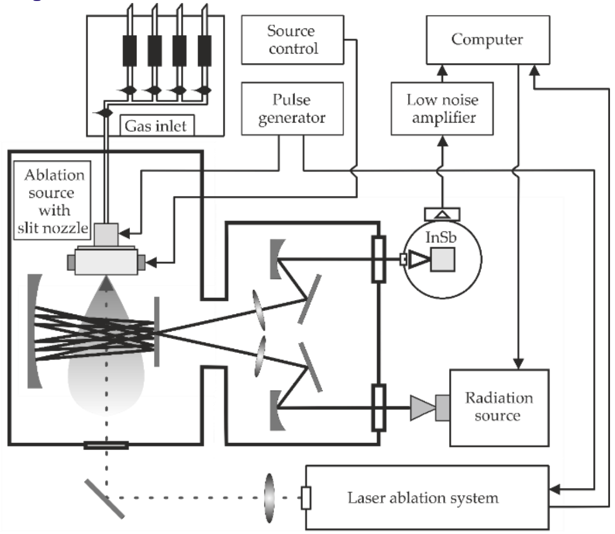


TiO – High-resolution experimental spectra

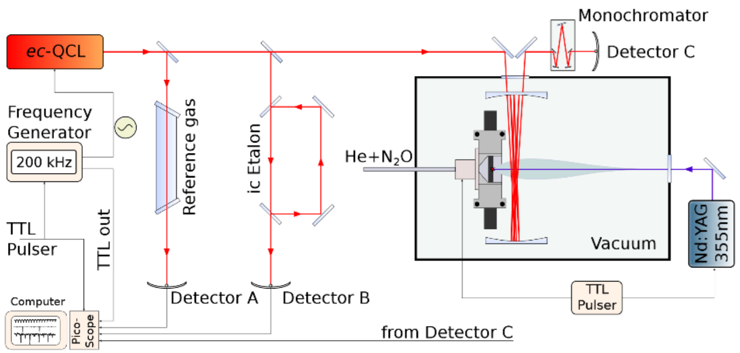


Prev. work: Amiot *et al.*, *JCP* **102**, 4375 (1995); Namiki *et al.*, *JMS* **191**, 176 (1998); Ram *et al.*, *ApJS* **122**, 331 (1999); Lincowski *et al.*, *ApJ* **883**, 9 (2016)

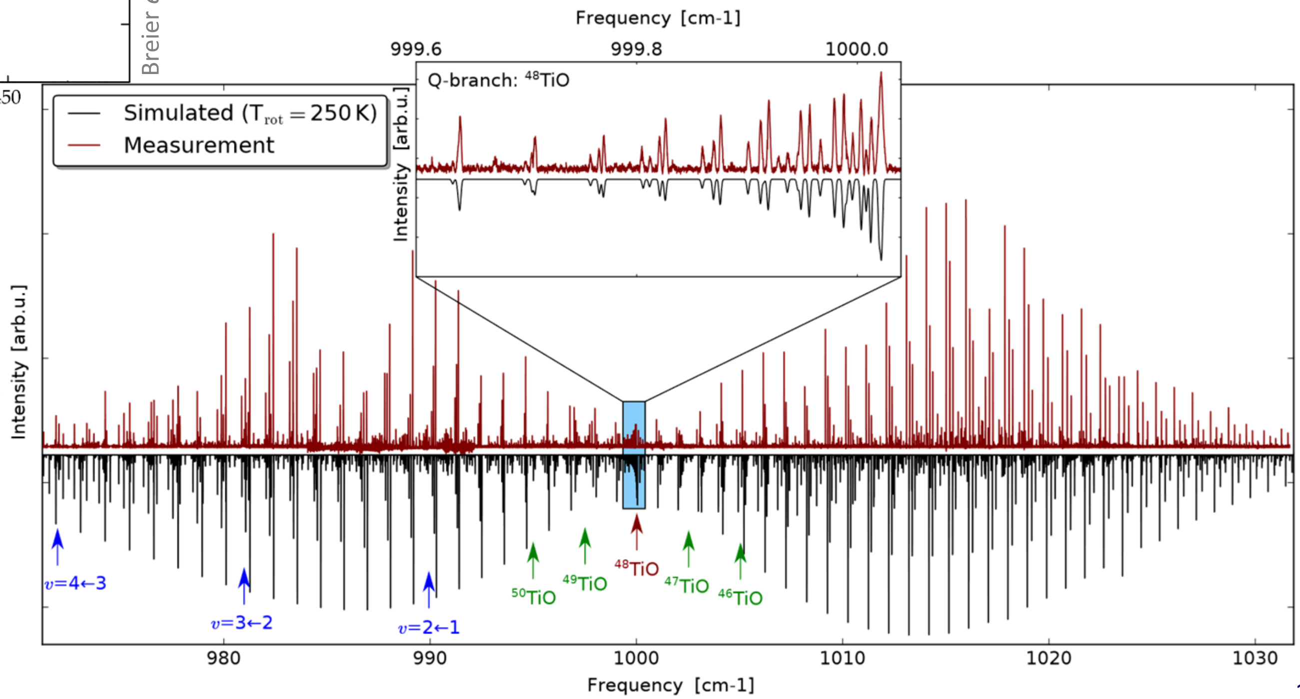
Breier *et al.*, JMS **355**, 46 (2019)



Rotational spectra



IR spectra



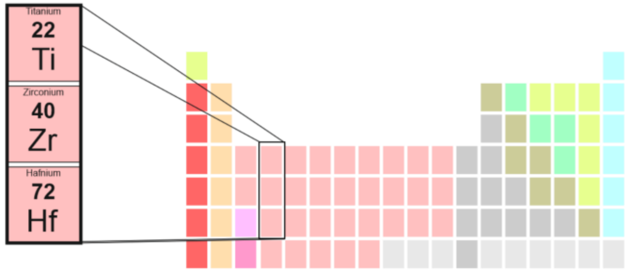
Witsch *et al.*, JMS **377**, 111439 (2021)

Mass-independent description of open-shell system

Born-Oppenheimer breakdown

$$U_{01} = 192547.813(75)\ \mathrm{MHz} \cdot \mathrm{u}$$

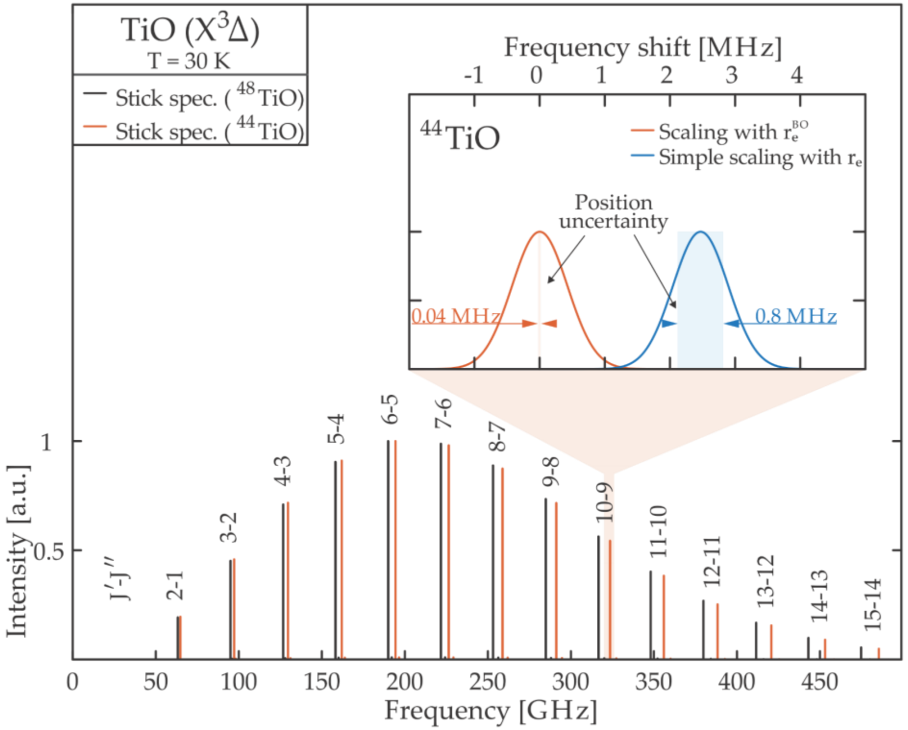
$$r_e^{BO} = 1.62009060(31)\ \text{Å}$$



Molecule(AB)	Δ^A_{U01}	Δ^B_{U01}
$TiO(X^3\Delta)$	-8.17(3)	-6.10(2)
$ZrO(X^1\Sigma^+)$	-4.87(4)	-6.19(1)
$HfO(X^1\Sigma^+)$	-3.4(6)	-5.66(2)

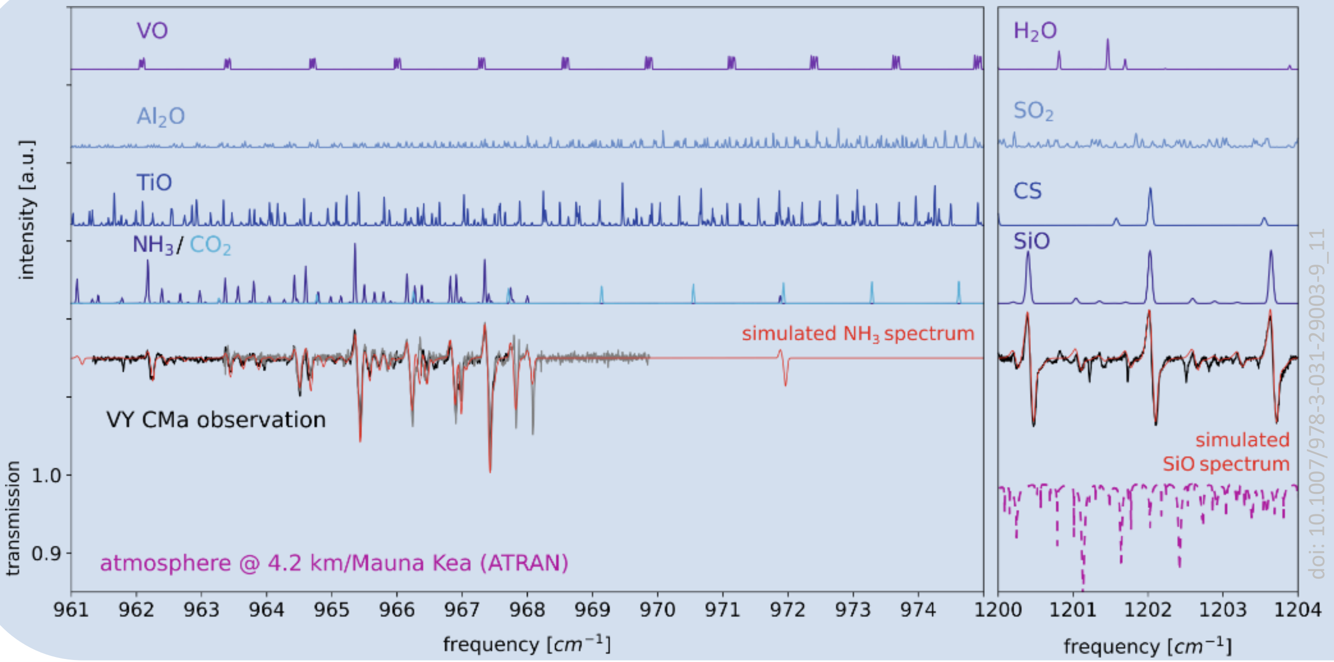
- 34 Dunham parameters (>500 molecular para.)

$$B_v = \sum_k \mu^{-(k/2+1)} \left(1 + \sum_{i=A,B} \frac{m_e}{M_i} \Delta^i_{k1}\right) U_{k1} \left(v + \frac{1}{2}\right)^k$$

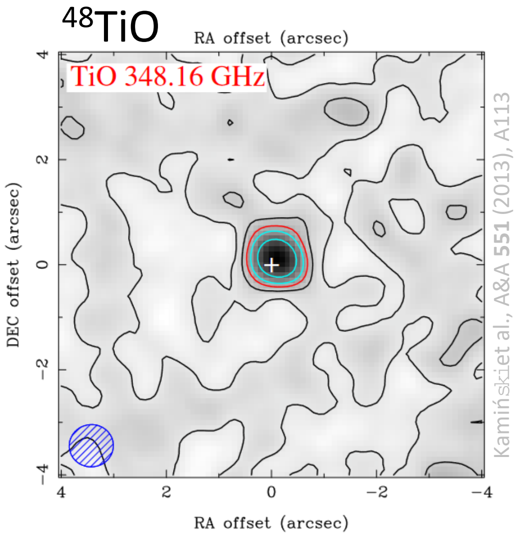


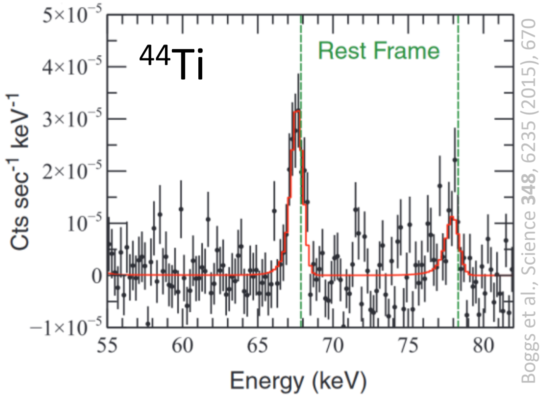
→Accurate transition frequencies

^{44}TiO in stellar objects?

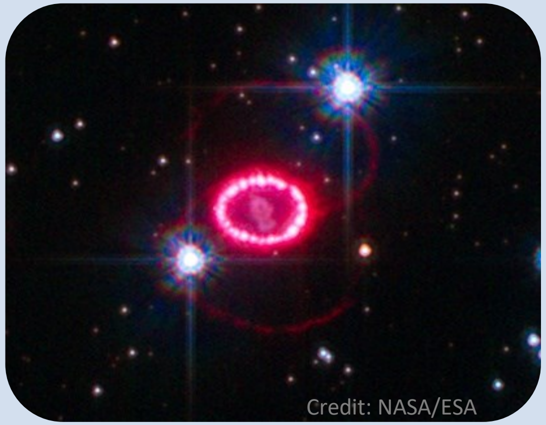


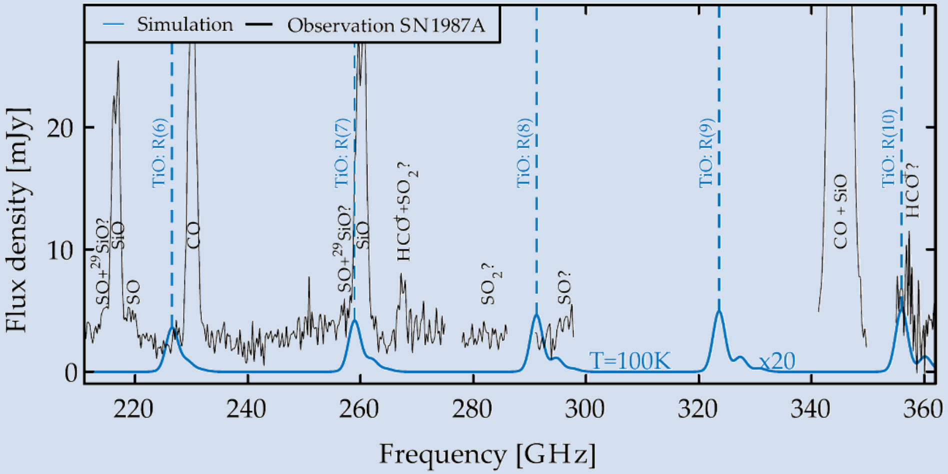
Aging stars



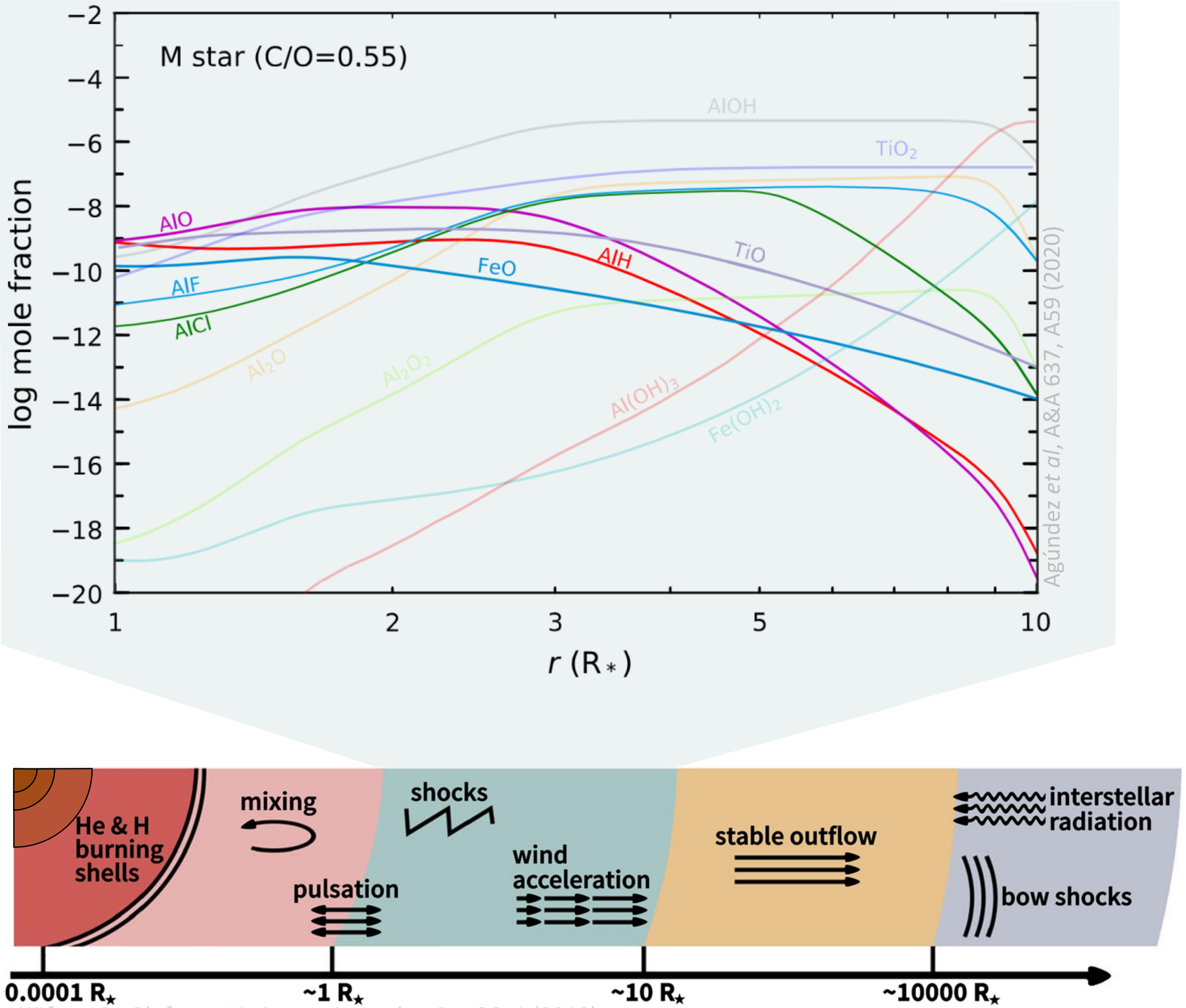


Supernova





Larger Molecular Species



Höfner, S., Olofsson, H. *Astron Astrophys Rev* **26,** 1 (2018).

Radioactive diatomic molecules

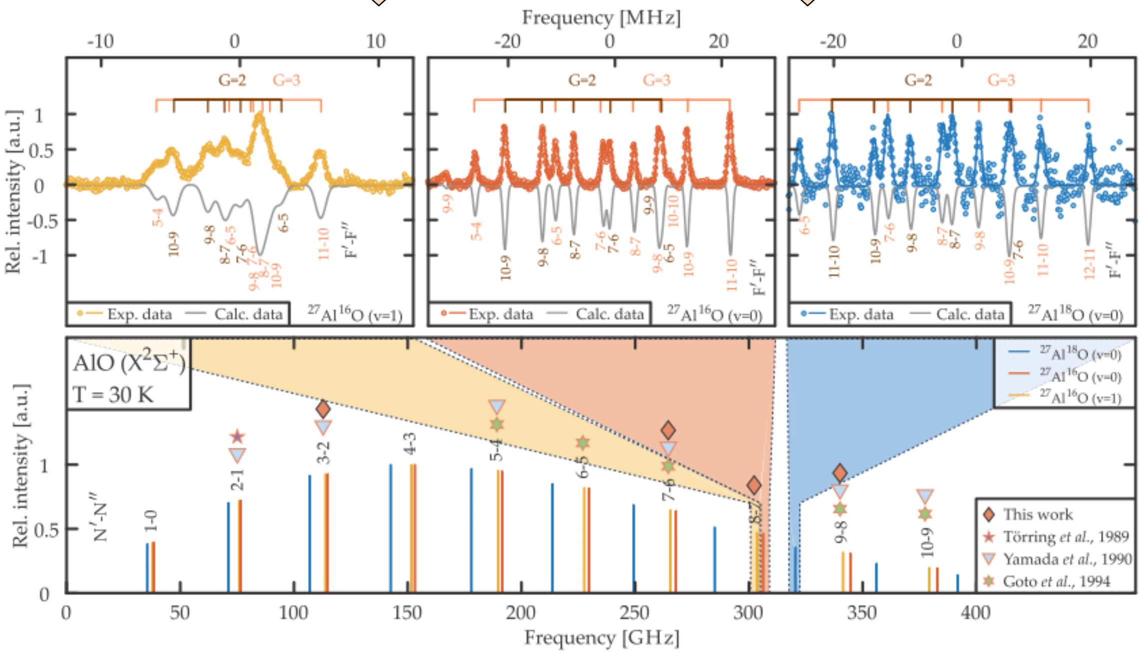
^{26}AlO ?

^{44}TiO

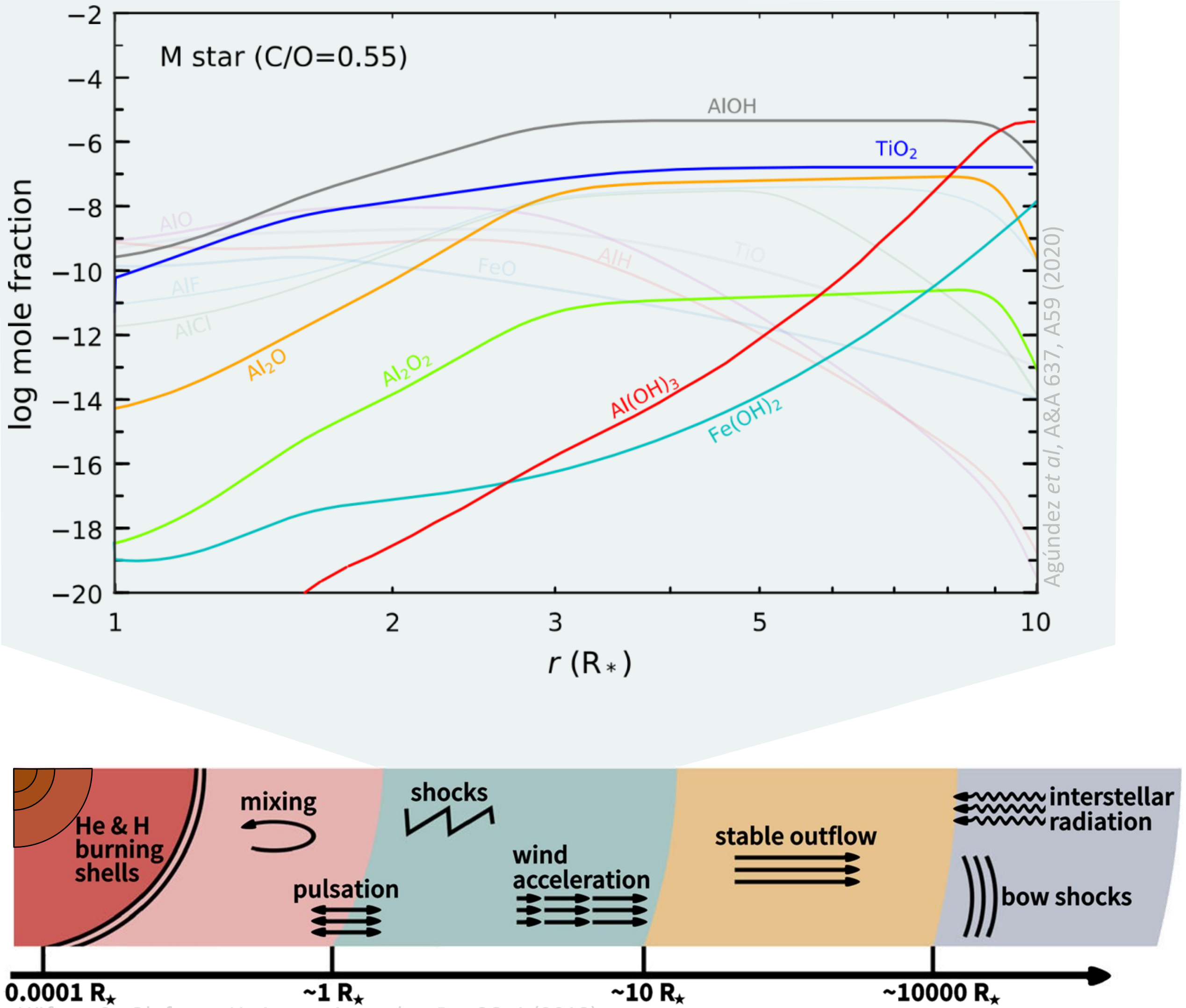
^{26}AlF

^{60}FeO

scalable

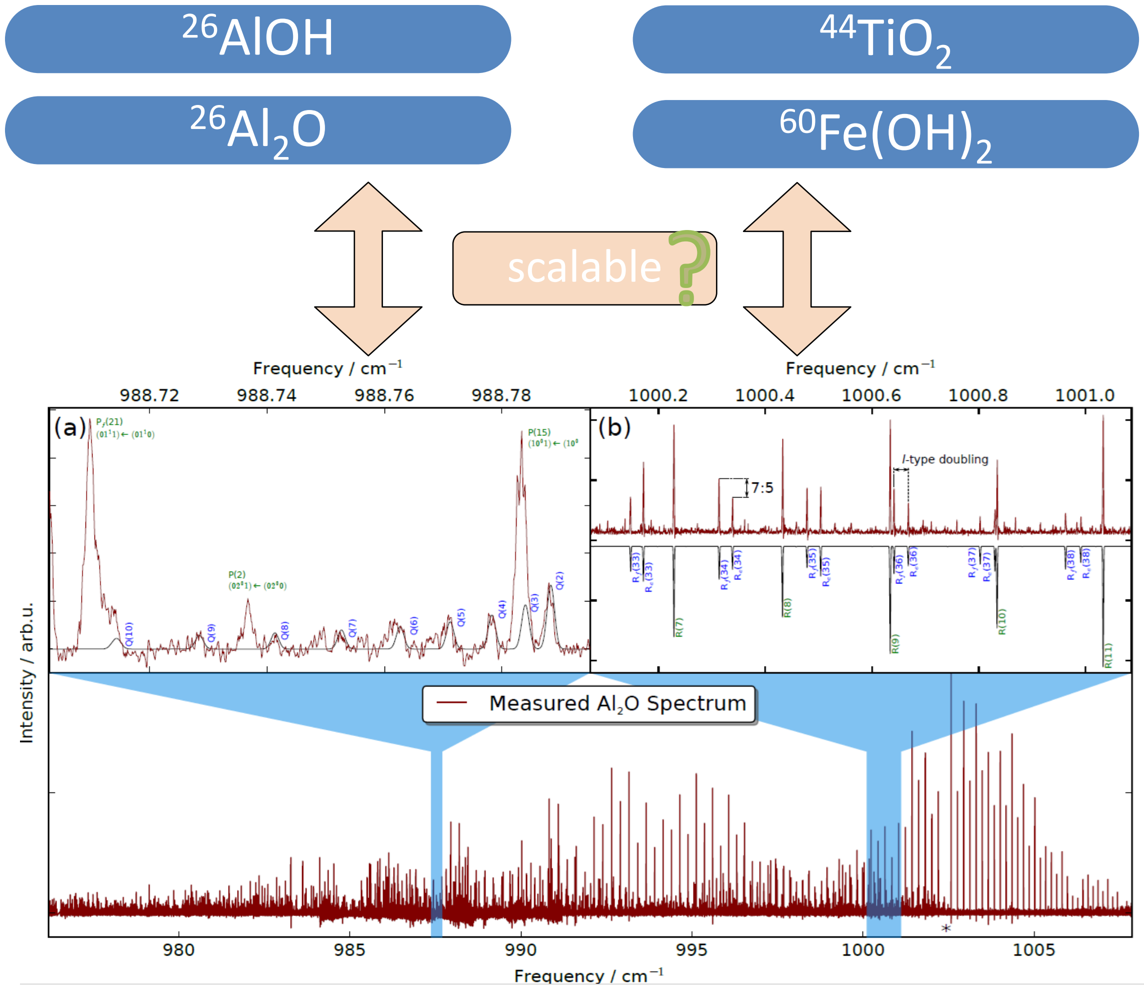


Larger Molecular Species

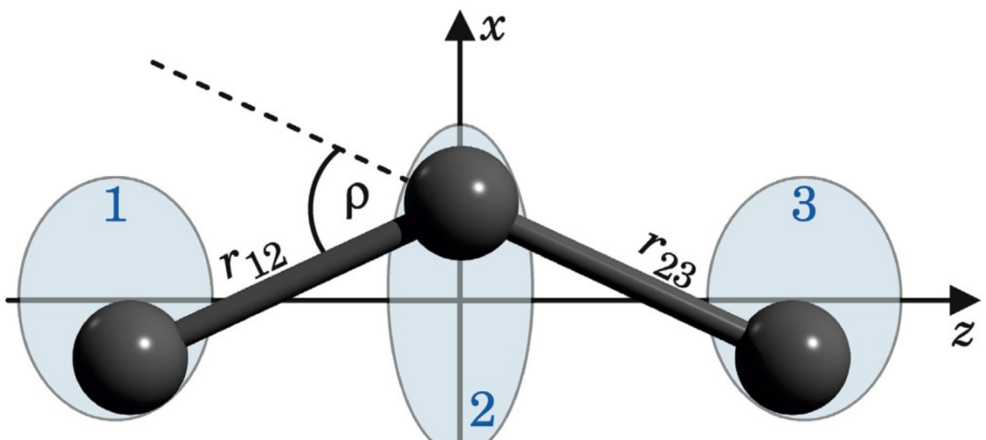


Höfner, S., Olofsson, H. *Astron Astrophys Rev* **26,** 1 (2018).

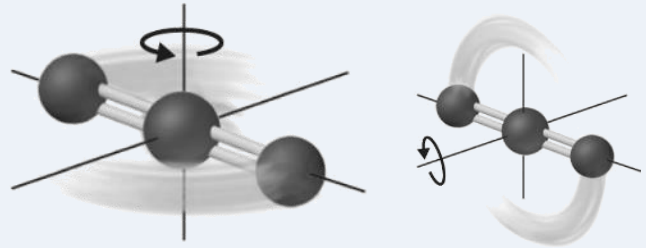
Radioactive polyatomic molecules



Molecular structure of polyatomic species



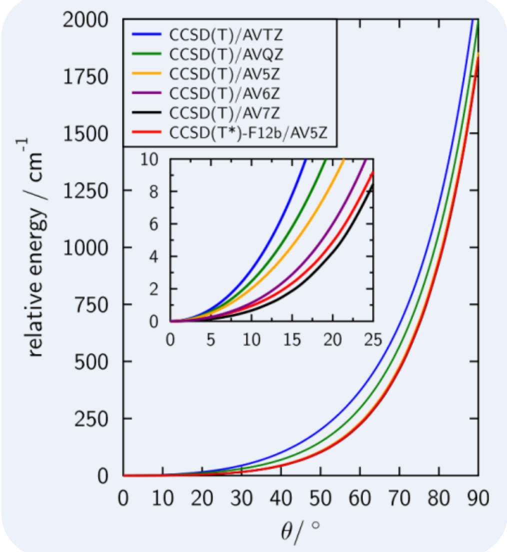
Breier et al., J. Mol. Struc. **1219** (2020) 128329



$$A = A_e - \sum_i \alpha_i^A \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^A \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$
$$B = B_e - \sum_i \alpha_i^B \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^B \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$
$$C = C_e - \sum_i \alpha_i^C \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^C \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$

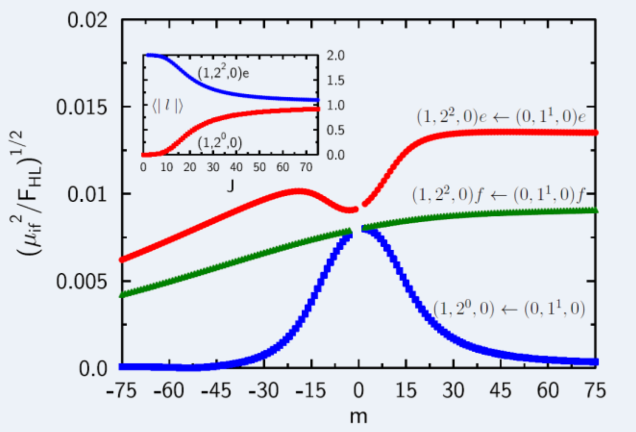
$$\hat{\mathbf{H}}_{\text{rig}} = \left(A - \frac{B+C}{2}\right)\hat{J}_a^2 + \frac{B+C}{2}\hat{\mathbf{J}}^2 + \frac{B-C}{4}\left(\hat{J}_+^2 + \hat{J}_-^2\right)$$

Anharmonic Potential

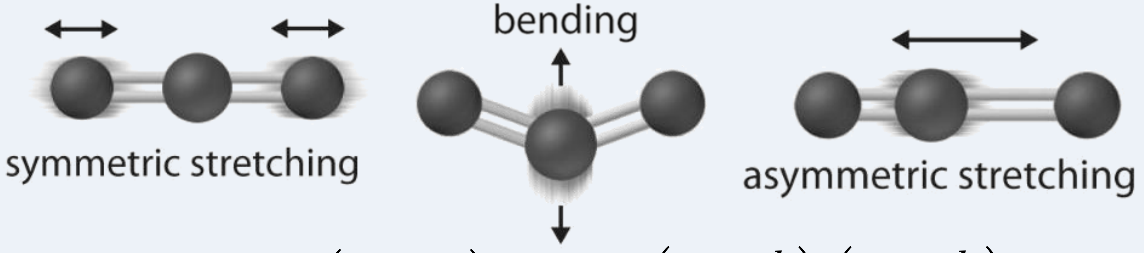


B. Schröder, P. Sebald, J. Chem. Phys. **144**, 044307 (2016)

Pertupations



$$\left\langle v', J, K_a \middle| \hat{\mathbf{H}}^c_{\text{cor}} \middle| v'', J, K_a \pm 1 \right\rangle = \mp \frac{\xi^c_{v',v''}}{2}\sqrt{J(J+1) - K_a(K_a \pm 1)}$$



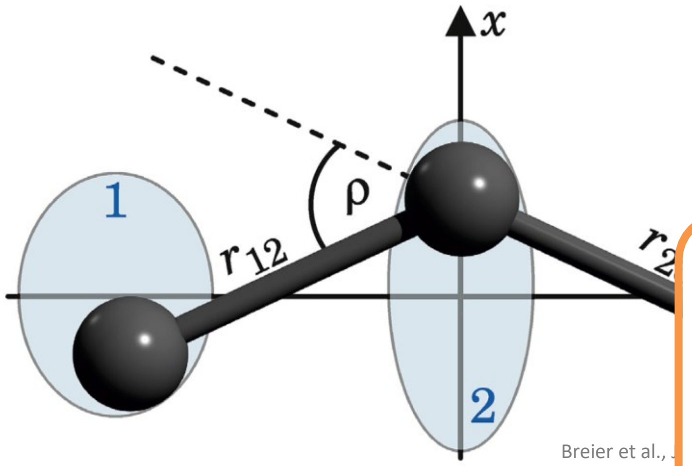
$$E_{\text{vib}}(v_i) = \sum_i \omega_i \left(v_i + \frac{d_i}{2}\right) + \sum_{i \le s} \chi_i \left(v_i + \frac{d_i}{2}\right)\left(v_s + \frac{d_s}{2}\right) + g l^2$$

Structure info

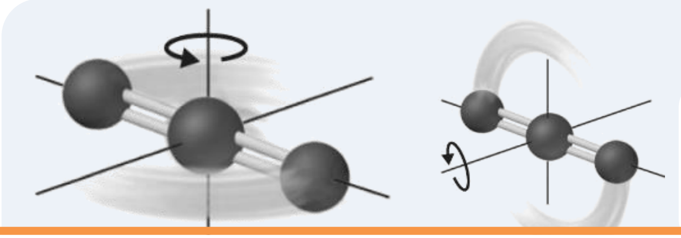
$$\frac{u_{r_{e,\text{poly}}}}{r_{e,\text{poly}}} \ge 10^3 \frac{u_{r_{e,\text{Dia}}}}{r_{e,\text{Dia}}}$$

Scaling error‘s are too big to be useful

Molecular structure of polyatomic species



Breier et al., …

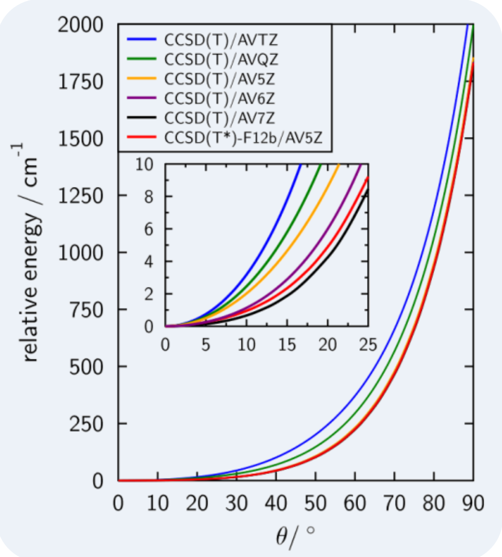


$$A = A_e - \sum_i \alpha_i^A \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^A \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$

$$B = B_e - \sum_i \alpha_i^B \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^B \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$

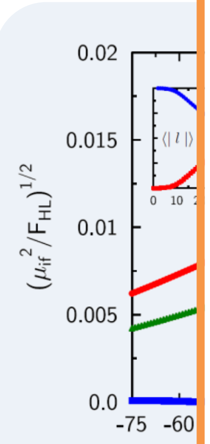
$$C = C_e - \sum_i \alpha_i^C \left(v_i + \tfrac{1}{2}\right) + \sum_{i \le j} \gamma_{ij}^C \left(v_i + \tfrac{1}{2}\right)\left(v_j + \tfrac{1}{2}\right) + \cdots$$

Anharmonic Potential

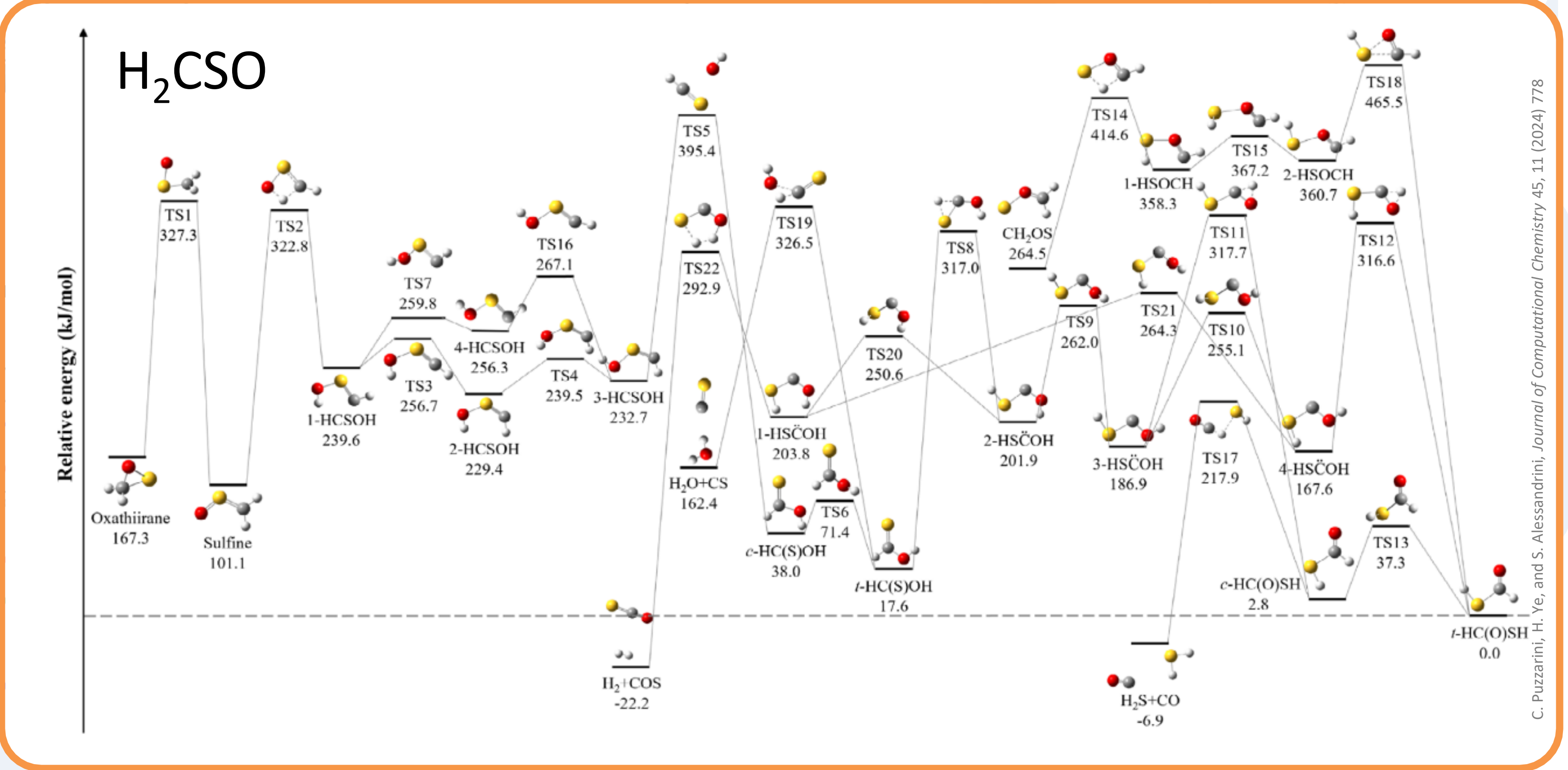


B. Schröder, P. Sebald, J. Chem. Phys. 144, 044307 (2016)

F



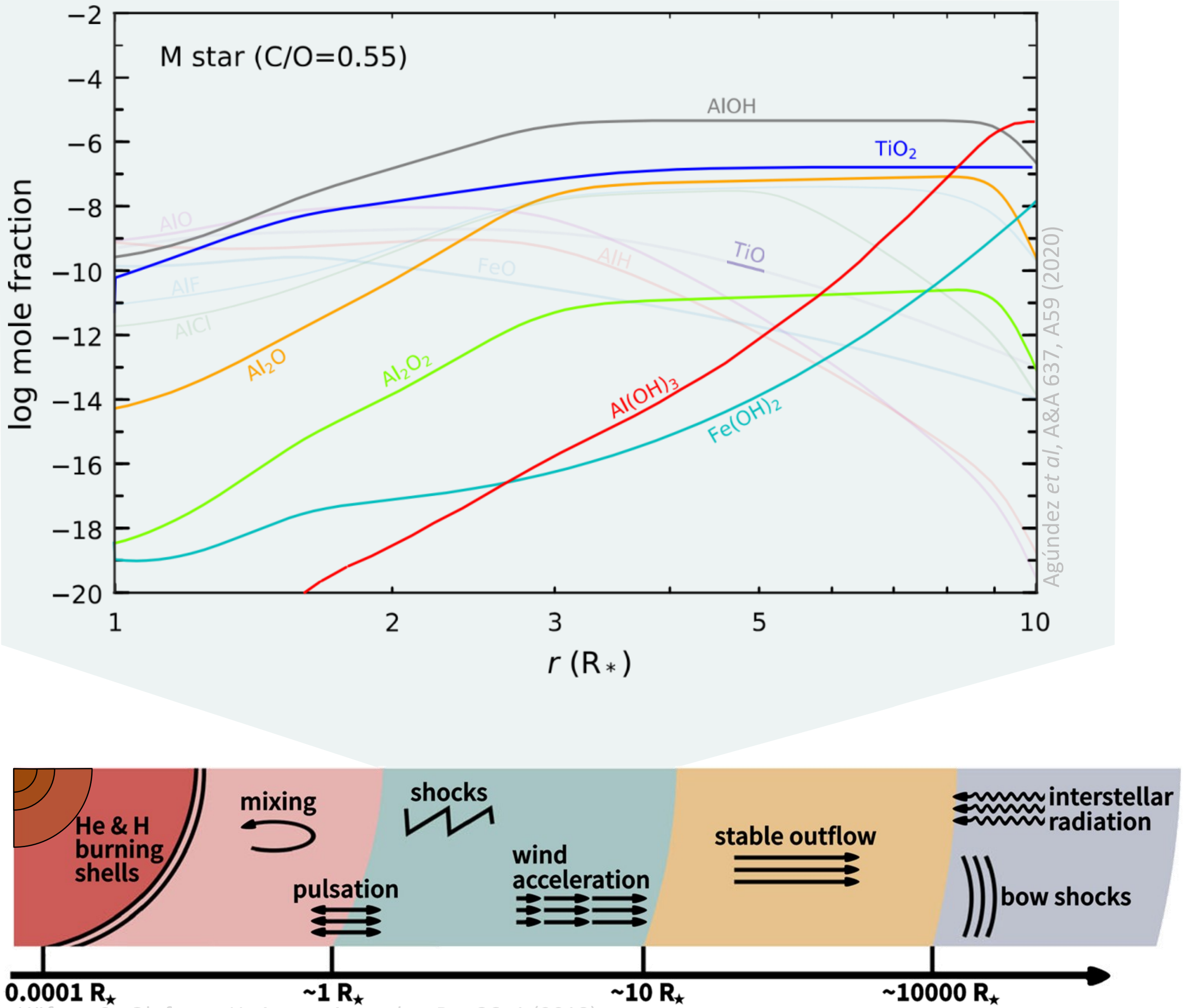
$$\left\langle v', J, K_a \left| \hat{\mathbf{H}}^c_{\mathrm{cor}} \right| v'', J, K_a \pm 1 \right\rangle = \mp \frac{\varsigma_{v',v''}}{2} \sqrt{J(J+1) - K_a(K_a \pm 1)}$$



C. Puzzarini, H. Ye, and S. Alessandrini, Journal of Computational Chemistry 45, 11 (2024) 778

Scaling error‘s are too big to be useful

Larger Molecular Species



Höfner, S., Olofsson, H. *Astron Astrophys Rev* **26,** 1 (2018).

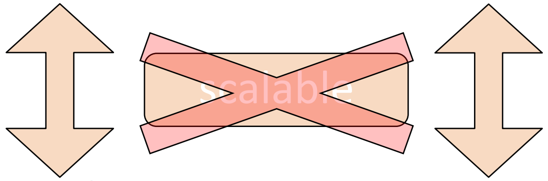
Radioactive polyatomic molecules

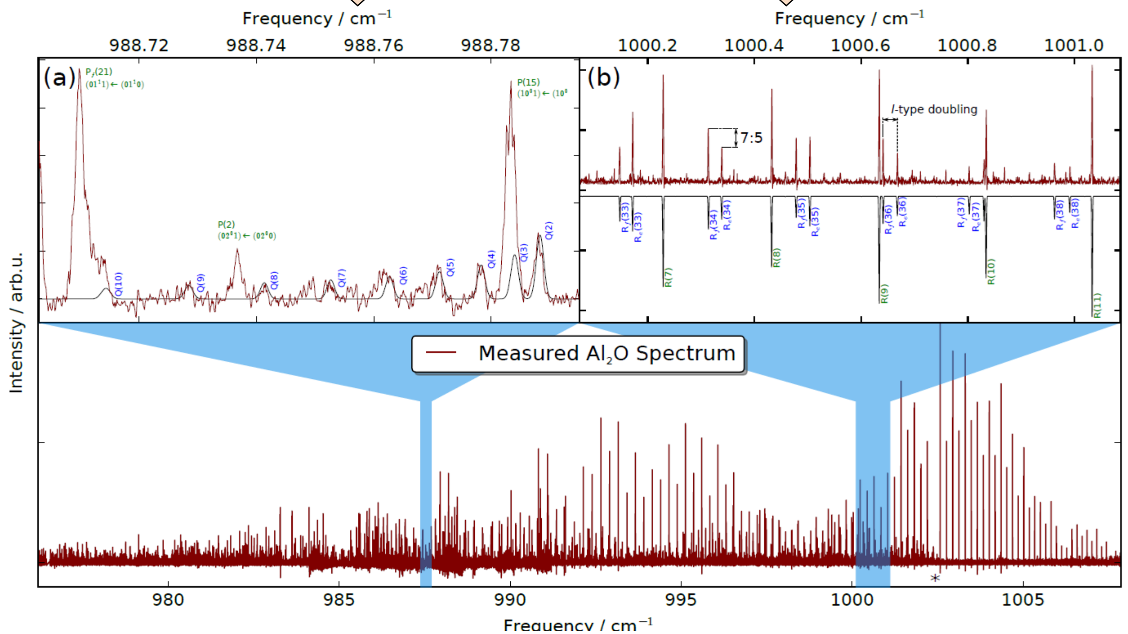
$^{26}AlOH$

$^{44}TiO_2$

$^{26}Al_2O$

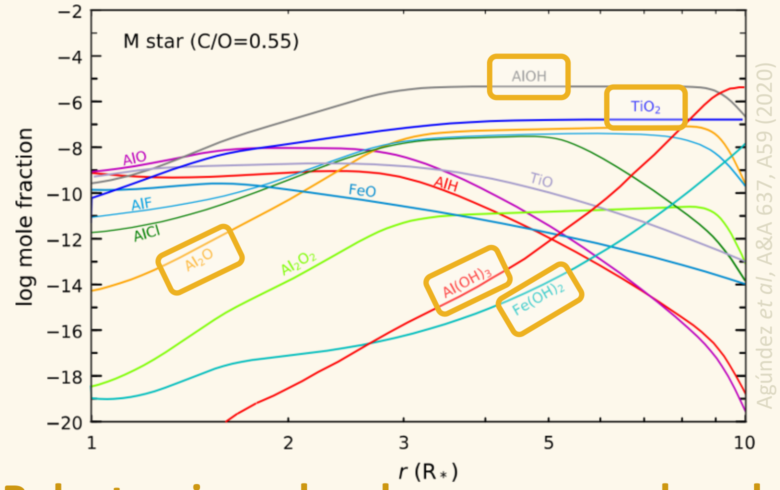
$^{60}Fe(OH)_2$



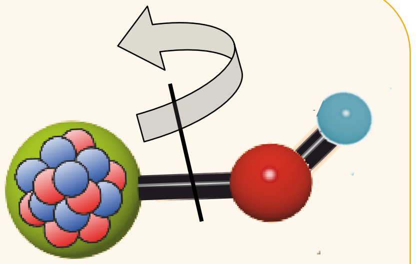


Polyatomic radioactive molecules as tracers

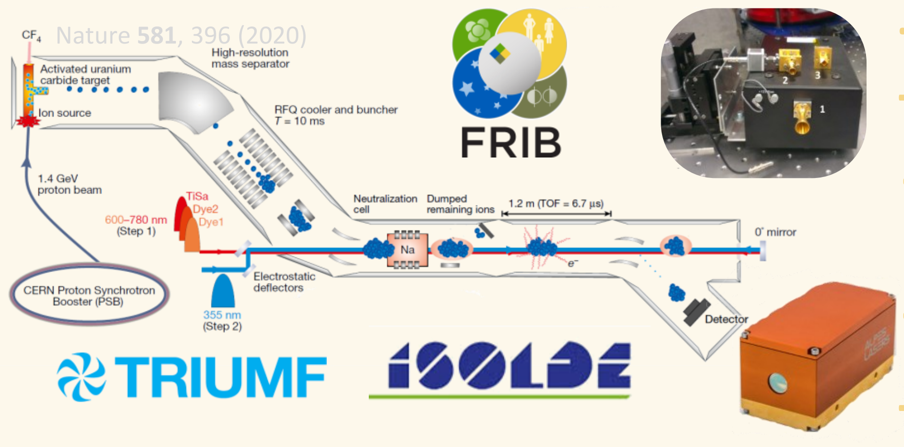
Astrochemistry



Polyatomic molecules are more abundant



3-atomic: i.e. AlOH



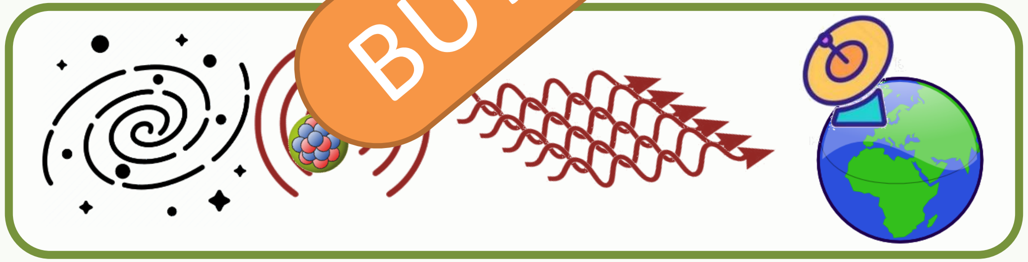
Direct measurements needed

Laboratory astrophysics

Tracer Molecules

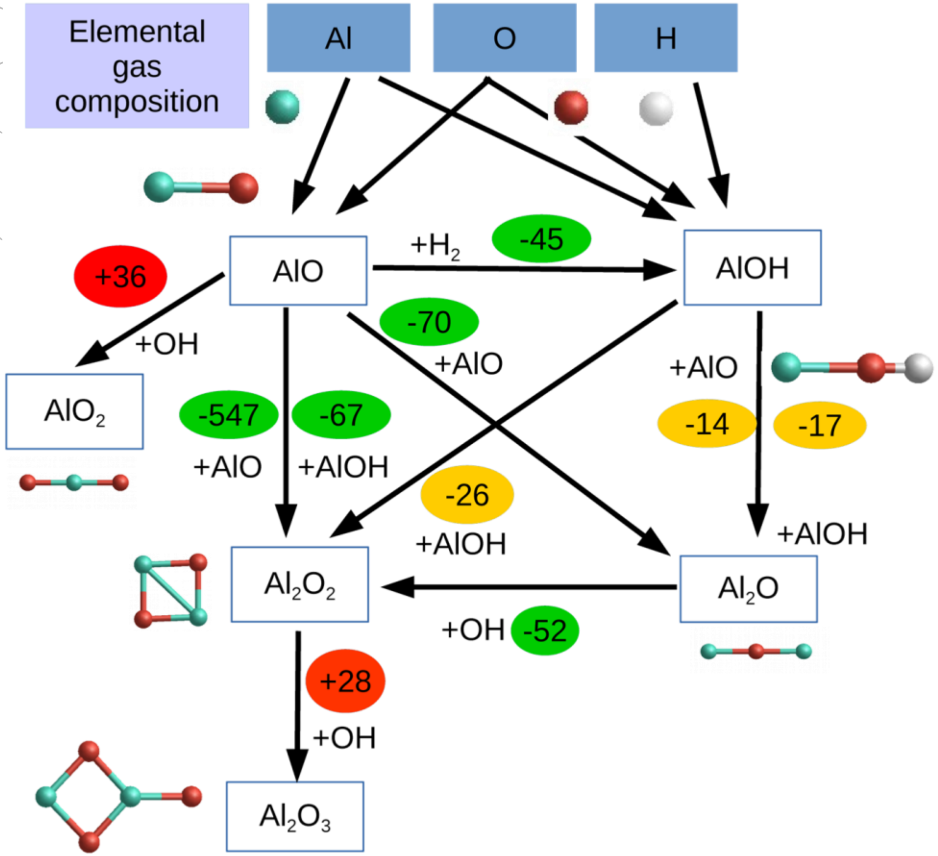
C/O <1 | ^{26}AlOH | $^{44}TiO_2$ | ^{60}Fe | $^{26}Al_2O$ | $^{32}Si_2C$ | $^{32}SiC_2$ | C/O >1

BUT …

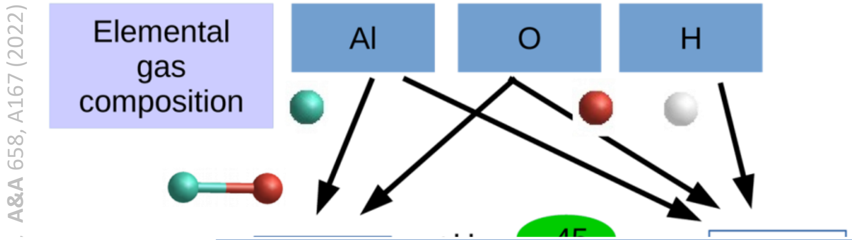


Structure information towards (Ultra)high-resolution spectroscopy

D. Gobrecht *et al.*, **A&A** 658, A167 (2022)



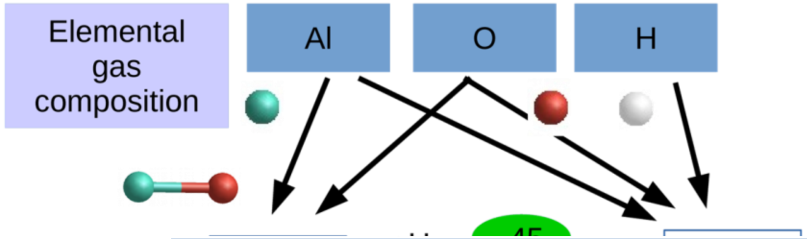
Structure information towards (Ultra)high-resolution spectroscopy



	Spectral information			
Molecule	**Rotation**	**Vibration**	**Excited states**	**ISM observed?**
AlO	✓	(✓)	✓	✓
AlOH	✓	?	?	✓
AlO_2	-	?	?	?
Al_2O	-	✓	?	?
Al_2O_2	-	?	?	?
Al_2O_3	-	?	?	(?)

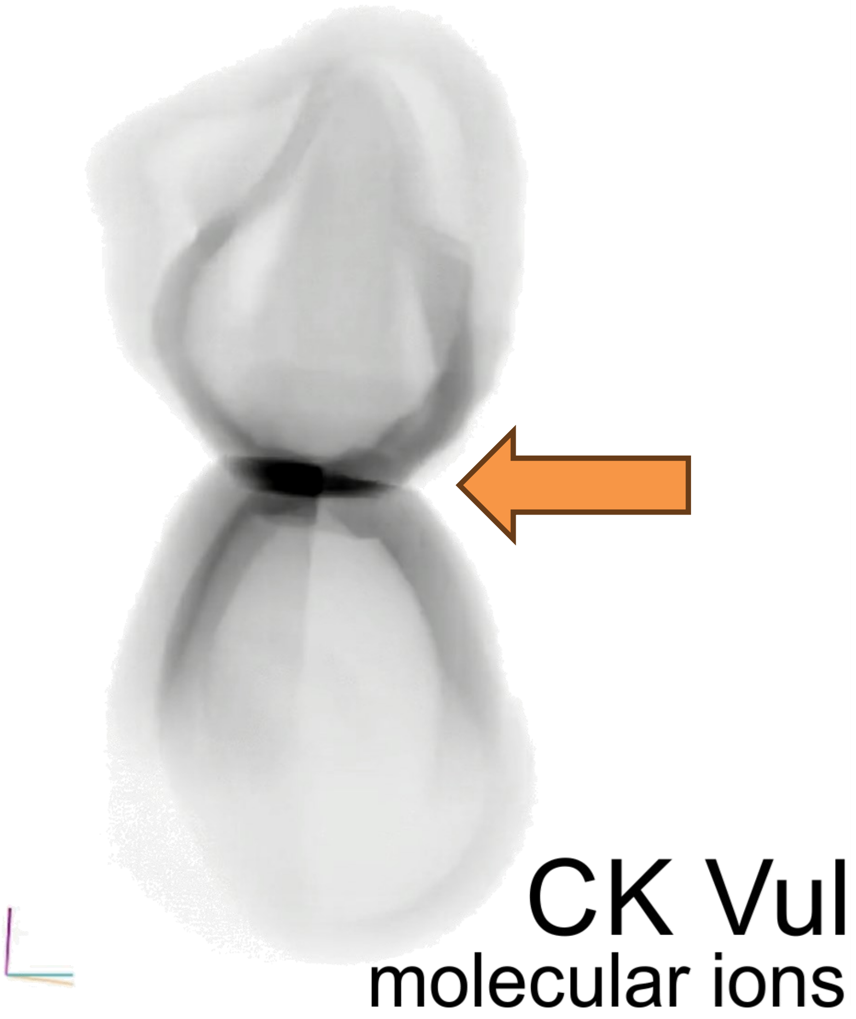
Structure information towards (Ultra)high-resolution spectroscopy

A&A 658, A167 (2022)

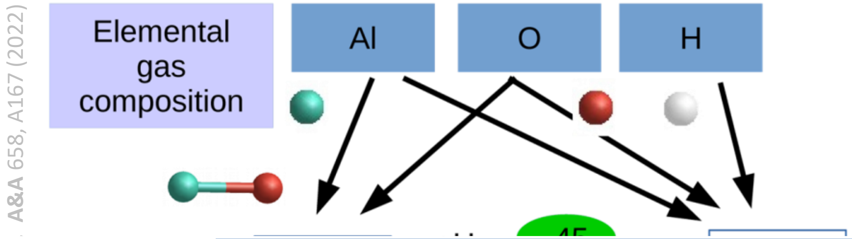


	Spectral information			
Molecule	**Rotation**	**Vibration**	**Excited states**	**ISM observed?**
AlO^+	?	?	?	?
$AlOH^+$	?	?	?	?
AlO_2^+	?	?	?	?
Al_2O^+	?	?	?	?
$Al_2O_2^+$	?	?	?	?
$Al_2O_3^+$	?	?	?	?

Neutral-neutral reactions?! No ions?



Structure information towards (Ultra)high-resolution spectroscopy



	Spectral information			
Molecule	**Rotation**	**Vibration**	**Excited states**	**ISM observed?**
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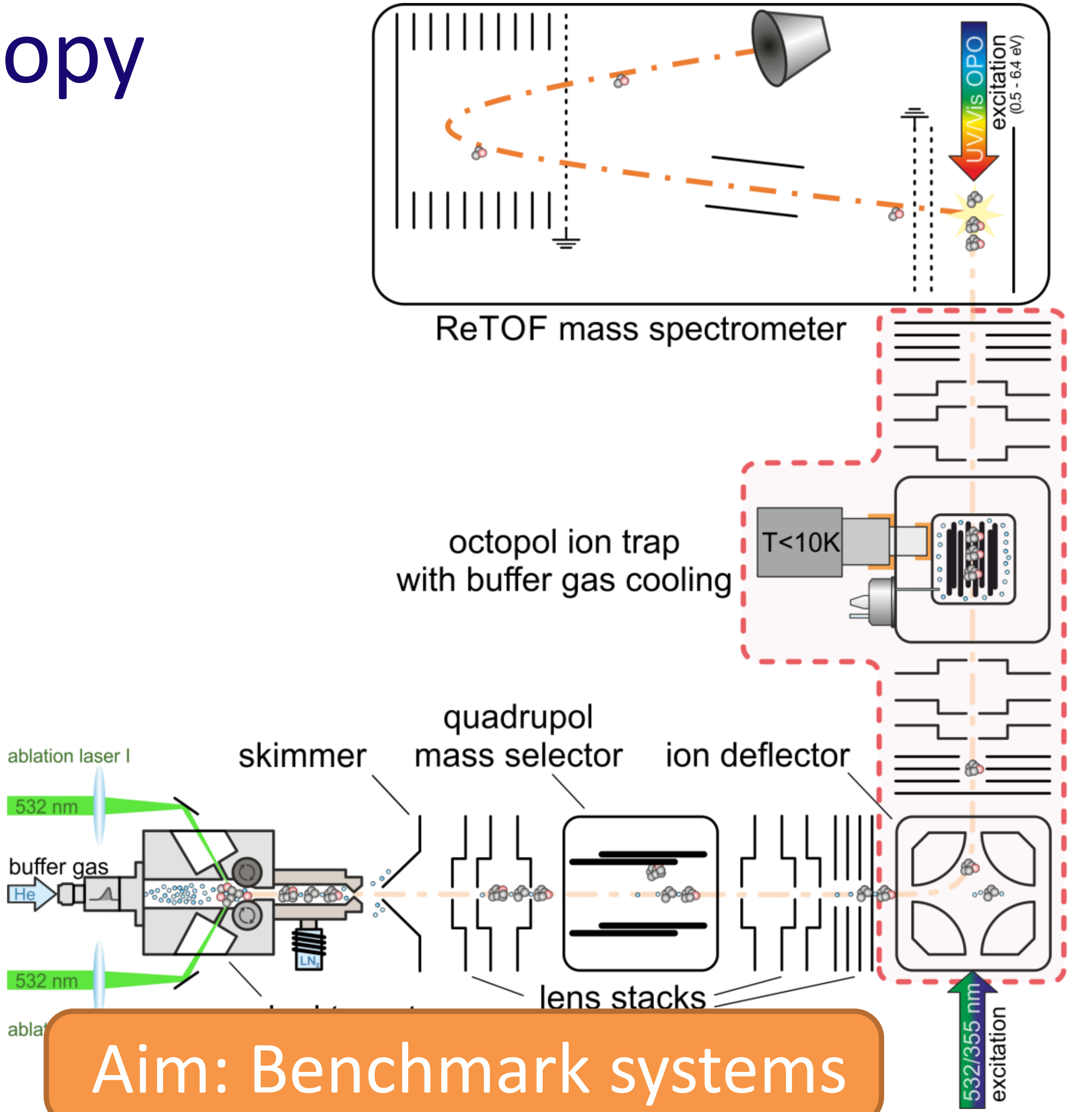
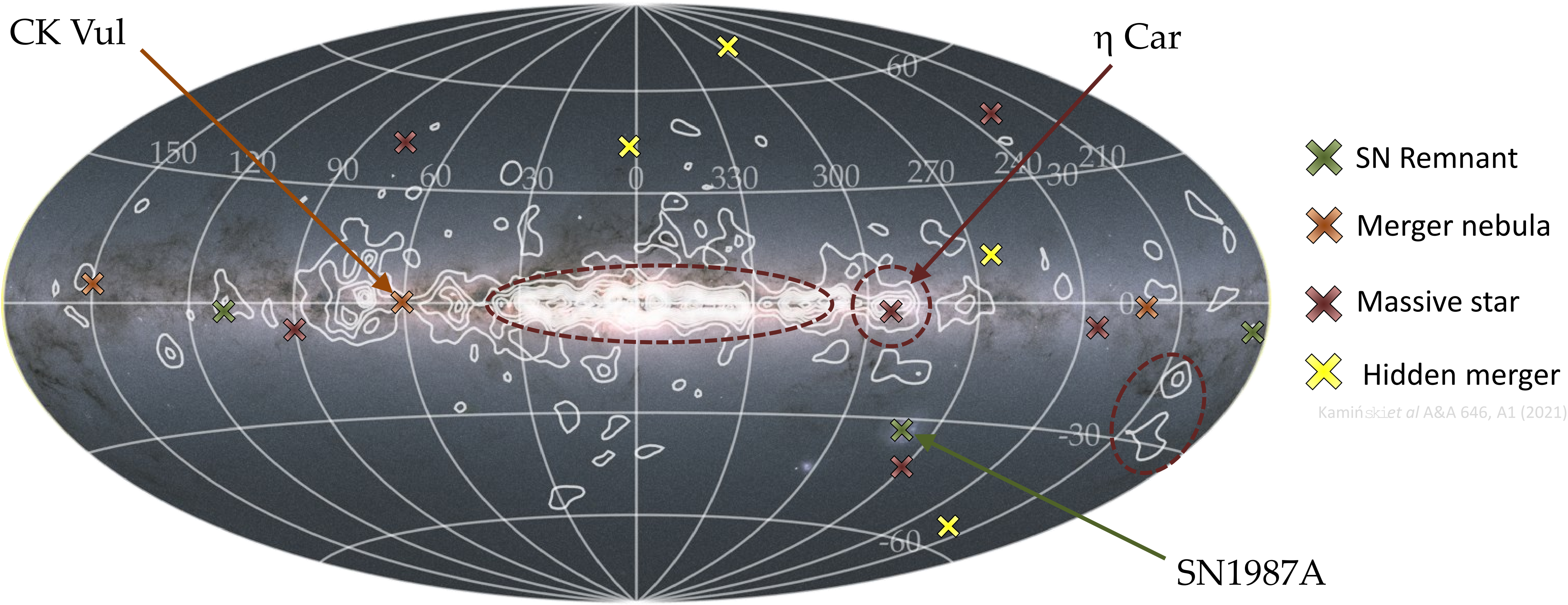
AlO_2^+	?	?	?	?
Al_2O^+	?	?	?	?
$Al_2O_2^+$	?	?	?	?
$Al_2O_3^+$	?	?	?	?

Neutral-neutral reactions?! No ions?



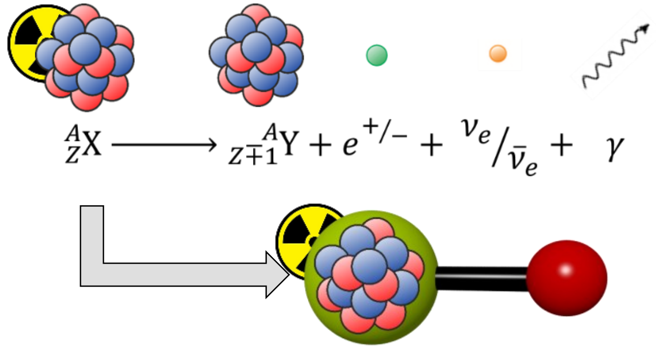
Aim: Benchmark systems

Pinpoint more sources? Yes!

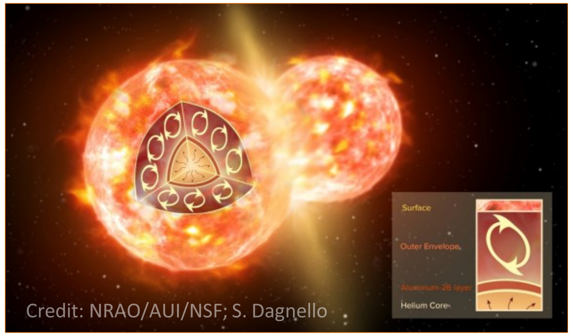


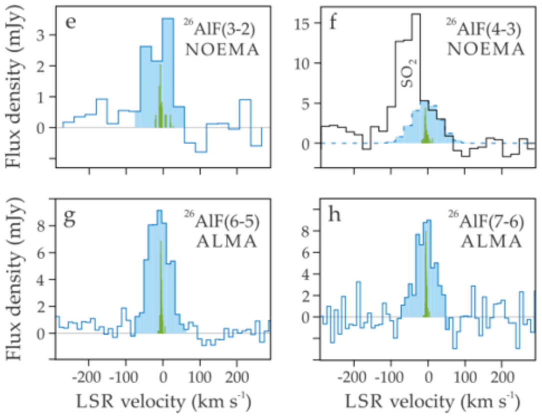
Credit: ESA/Gaia/DPAC & Plüschke (2001)

Conclusion

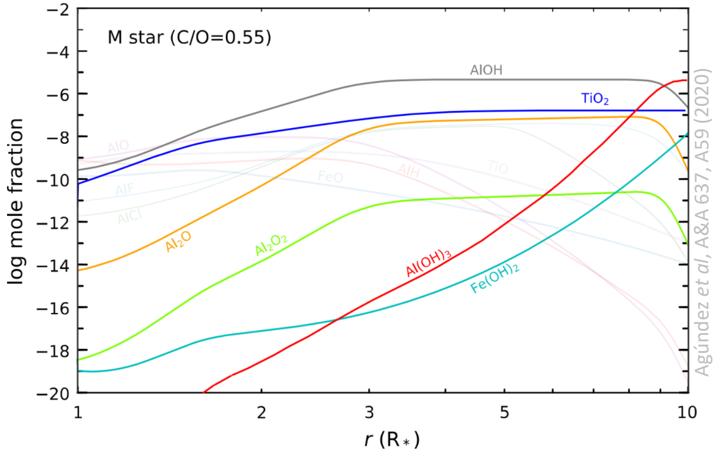


- Radioactive molecule:
  as additional tracers for stellar dynamics





- Mass-independent description on diatomic molecules,…



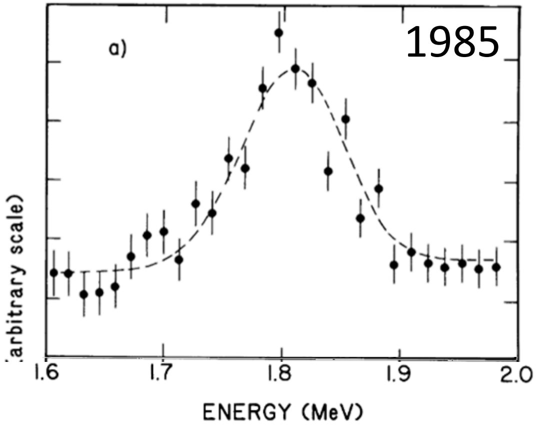
- …but radioactive polyatomic molecules need direct measurements

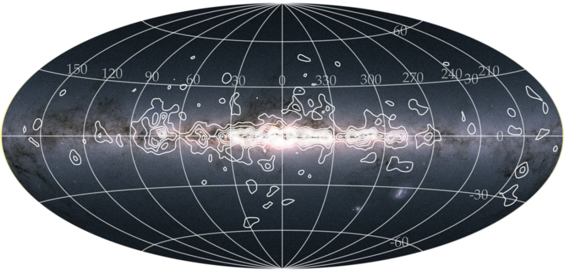
C/O <1 | $^{26}AlOH$ | $^{44}TiO_2$ | $^{60}Fe(OH)_2$ | $^{26}Al_2O$ | $^{32}Si_2C$ | $^{32}SiC_2$ | C/O >1

Multimessenger approach

^{26}Al

Share *et al.*, ApJ **292**, *1985, L61*





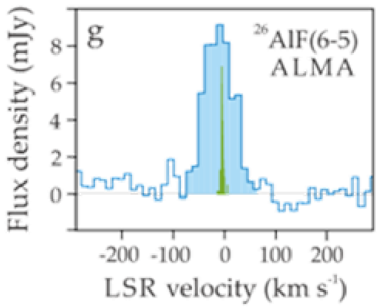
Until now

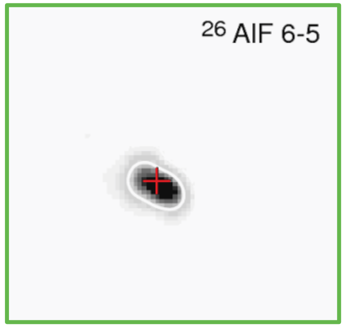
Advances in sub-mm spectroscopy with the ALMA observatory and corresponding advances in laboratory studies have led to prospects to identify lines for molecules that include a radioactive isotope. In a first such success, rotational lines of ^{26}AlF could be measured from a point nova-like source called CK Vul [147]; spatial resolution in sub-mm astronomy allowed to pinpoint the source directly. We caution, however, that molecule production such as in this case will only occur under very special conditions. Therefore, it is difficult to merge such unique molecule-biased observational results with general conclusions on ^{26}Al sources and on compositional evolution of galactic gas in general.

R. Diehl, N. Prantzos, Handbook of Nuclear Physics, 2023,3261

^{26}AlF

2018





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Thank you for your attention!

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