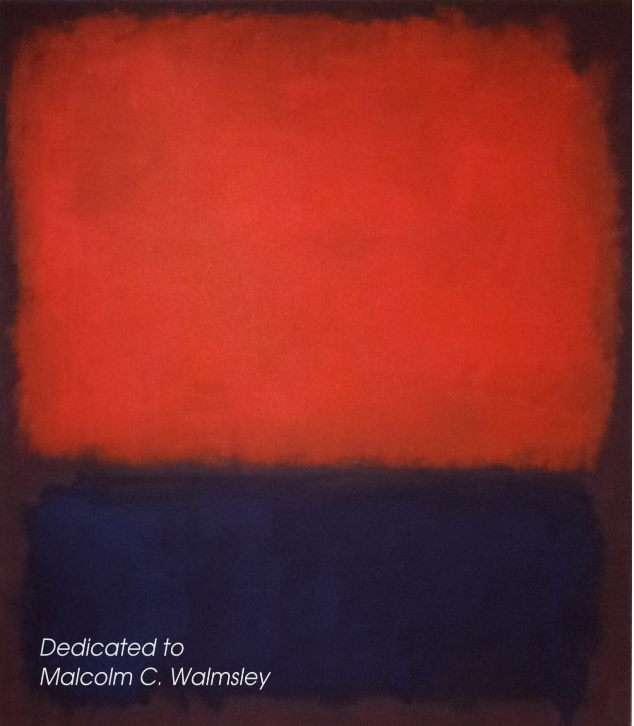

Steady-state nuclear-spin chemistry in dark clouds

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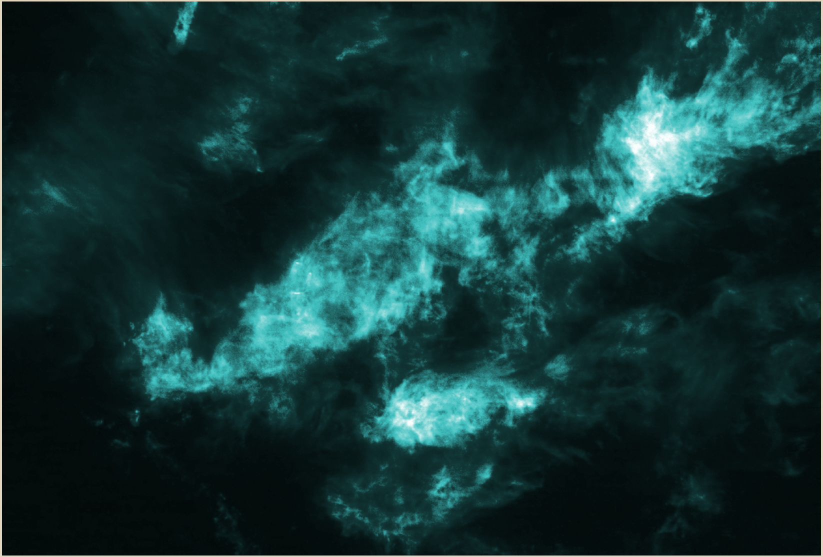
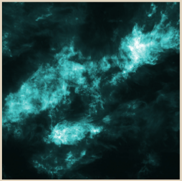
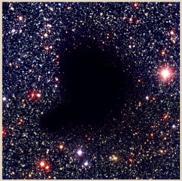
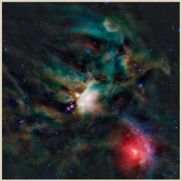
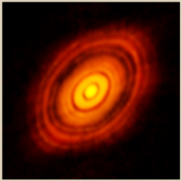
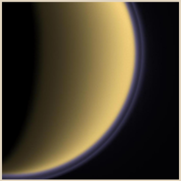


Starless cores: a pivotal state

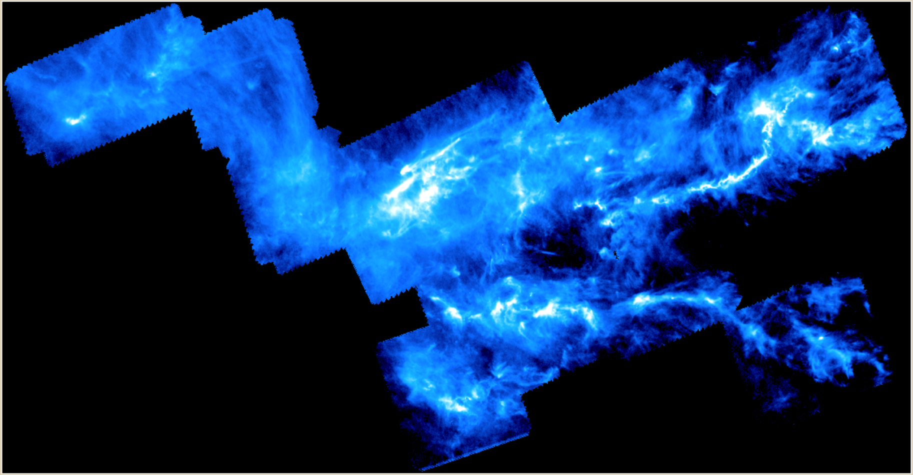
From clouds to cores to planetary systems

Clouds | Cores | Protostars | Disks | Planets

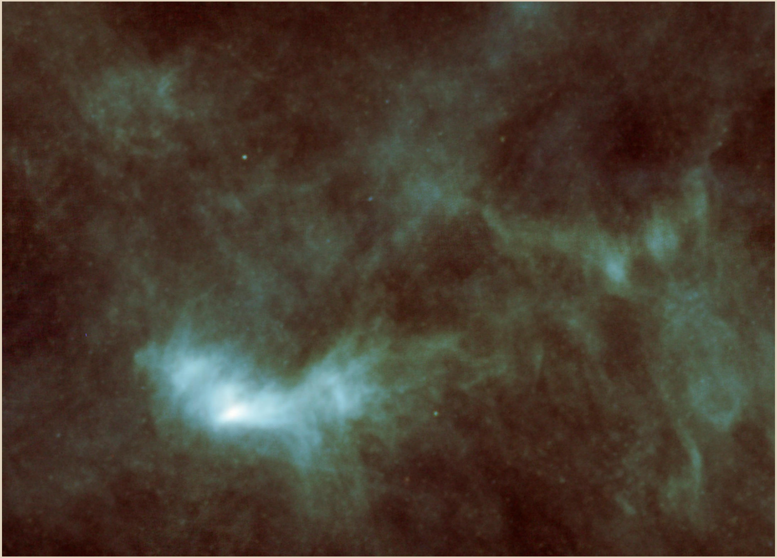






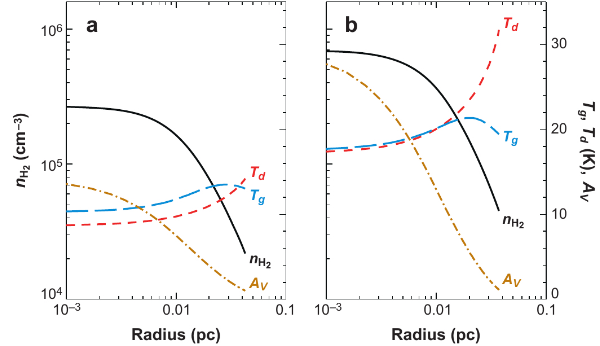
- Physics of star and planet formation
- Chemical conditions in starless cores ?
- Timescales of star formation ?

Starless cores within molecular clouds



Starless cores: L1544

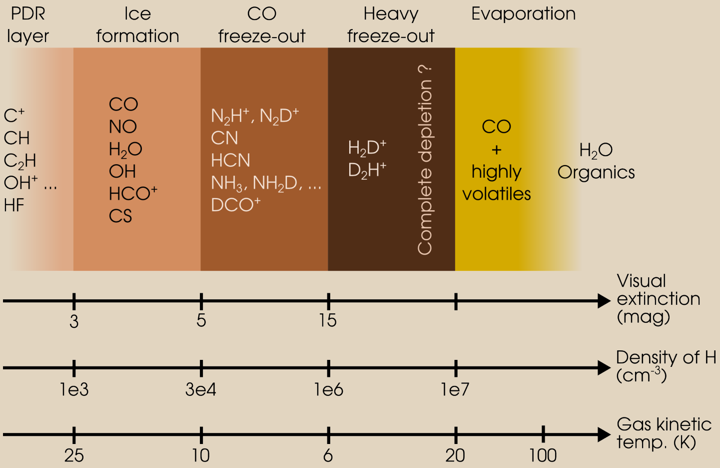




Galli, Walmsley, Gonçalves, A&A 2002

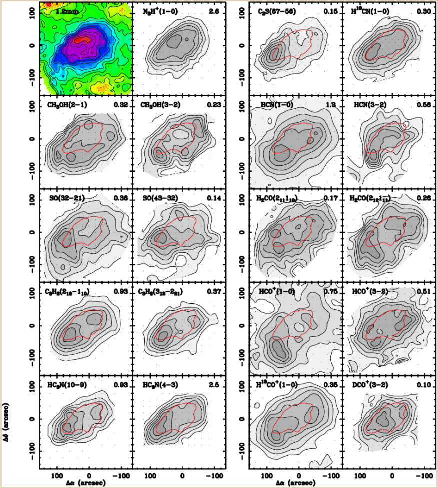
- cold (10 K), dense ($n_{\rm H} > 10^4\,{\rm cm}^{-3}$)
- dark: $A_{\rm V} > 10$ mag (CR + UV from secondary photons)

Starless cores: chemical factories



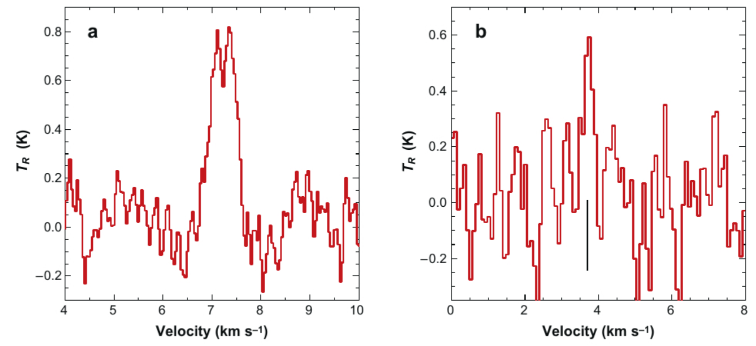
adapted from Bergin & Tafalla 2007

Molecular depletion



Tafalla et al. (2006)

- Depletion affects most species
- Nitrogen bearing species (CN, NH_3, N_2H^+) less affected Hily-Blant et al. (2008)
- Complete depletion ? Walmsley et al. (2004)
- Lightest species remain in the gas phase: H_3^+ and D-isotopologues



o-H_2D^+ at 372.4 GHz (Caselli et al. 2008), p-D_2H^+ at 692 GHz (Vastel et al. 2004)

- Observations: usually one symmetry only: e.g. o-H_2D^+, p-D_2H^+, NH_3
- OPRs required to derive total column density

Why OPRs are important ?

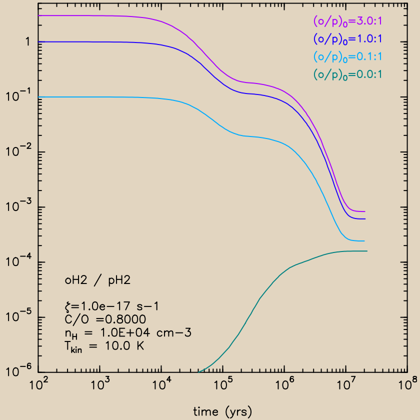
- Derive total column densities
- Disentangle between formation pathways (Faure et al. 2013)
- Gas-phase vs surface chemistry
- Derive physical conditions and impact on thermodynamics

Can OPRs be used as astrochemical clocks ?

- Updated network for the complete depletion scenario
- Time-dependent chemical calculations
- New network and preliminary results

- Deuteration: $H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 + \Delta E$
- internal energy of o-H_2 promotes endoergic reactive collisions, mitigating deuterium fractionation
- Metals and electrons also decrease deuteration (destroy H_2D^+)
- Milestones: Dalgarno et al. (1973); Pagani et al. (1992); Gerlich et al. (2002); Walmsley et al. (2004)
- OPR of H_2 regulates deuteration, and OPR depends on timescale for NSC
- Idea: measure the deuteration to constrain the OPR of H_2
- Brünken et al. (2014): ortho and para H_2D^+ towards IRAS16293-2422; dense core chemical age ~ 1 Myr (Sipillä's talk)
- Timescale for OPRs to reach steady-state: ~ 1 Myr (Flower et al. 2006; Kong et al. 2015; Furuya et al. 2015)

Timescale to reach steady-state

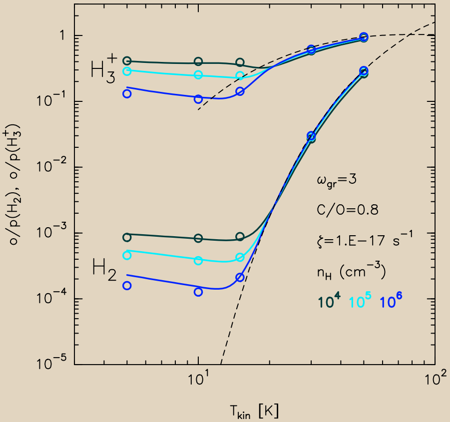


Initial conditions are lost after $\sim$ few 10^6 yr

The OPR of H_2 in dense gas phase

- Competition between: formation on grain surfaces, spin conversion in the gas phase
- $H_2 + XH^+ \rightleftharpoons H_2 + XH^+$
- $H_3^+ + e^- \rightleftharpoons H_3^+ + e^-$,
- $H_3^+ + X \rightleftharpoons H_2 + XH^+$
- Conversion in the gas phase: Hugo et al. (2009), state-to-state rates for $H_3^+ + H_2$ reactions

Thermalized OPR of H_2: T_{crit}

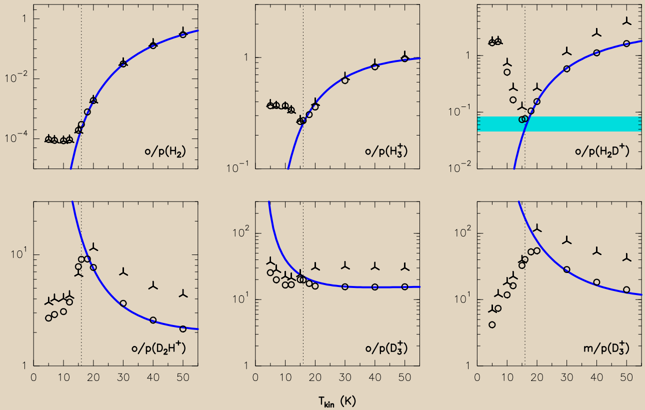


- Competition between formation on grains and gas-phase conversion
- formation of o-H_2 from grains $\sim$ from p-H_2
- Thermalized ratios above $T_{crit} \approx 17$ K (Le Bourlot 1991; Flower et al. 2006)

New reaction rates

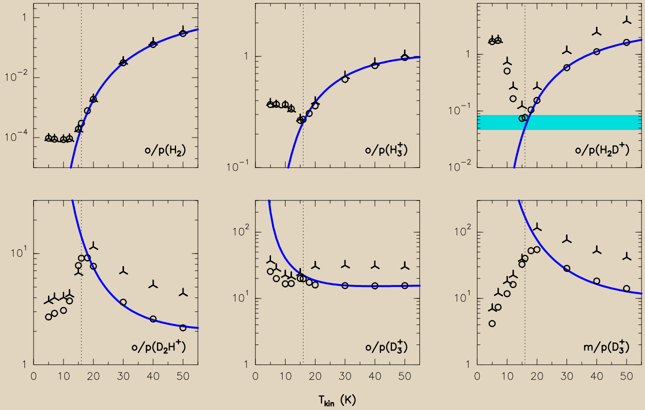
- Published rates: ground-state to species
- New rates *species-to-species*: averaging over Boltzman distribution of reactant populations

Species A	Species B			Number of reactions
H_3^+	HD	H_2	D_2	41
H_2D^+	HD	H_2	D_2	61
D_2H^+	HD	H_2	D_2	68
D_3^+	HD	H_2	D_2	67



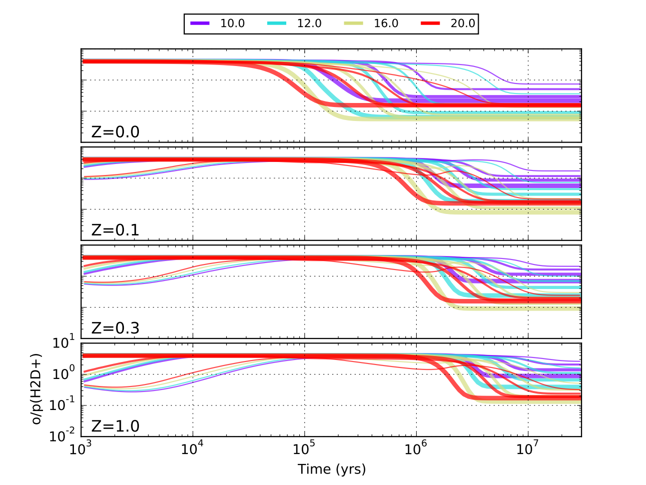
- All OPRs thermalize above $T_{\rm crit}$: leading role of $\rm H_2$
- Discrepancy with previous rates larger for heavier species
- Reality: between the two extremes (ground-state and Boltzmann)

Thermalized OPRs



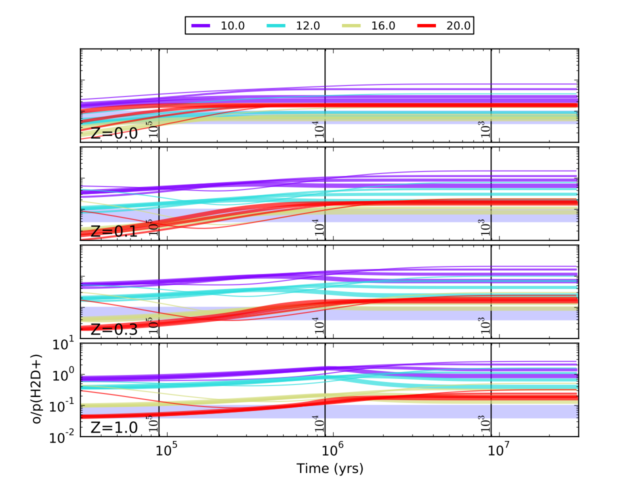
- Observed OPR of H_2D^+: 0.07±0.02, 13–16 K, $t > 5(5)$ yr (Brünken et al. 2014)
- Fully compatible with steady-state predictions

Steady-state OPRs in cores



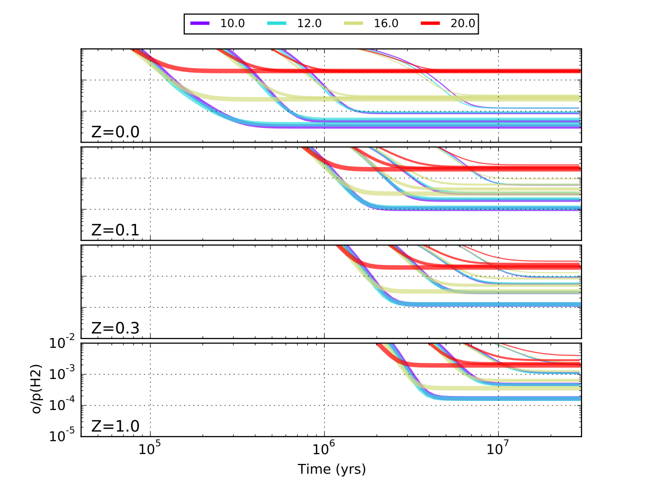
- Depletion factor: $Z \times f$; density; initial conditions: atomic H
- Observations: strong depletion, $T = 12 - 16$ K, high densities

Steady-state OPRs in cores



- Initial conditions: p-H_2
- No constraint from OPR(H_2D^+)

Steady-state OPRs in cores



- Timescales shorten with n_{H}
- Steady-state OPR decreases with Z

- observed OPR of H_2D^+: reflects the age of H_2 since its (last ?) formation
- Minimum age of the embedding molecular cloud
- Bad news: does not tell the age of the core
- Good news: Results do not depend on the (unknown) initial conditions

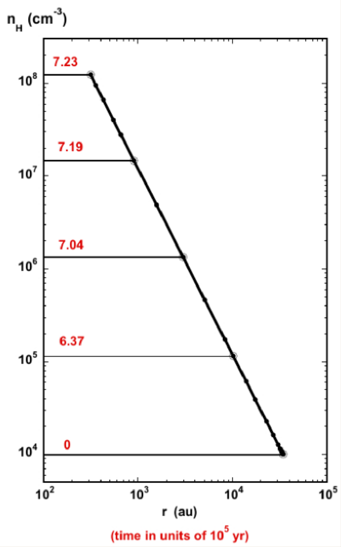
The GRENOBLE network

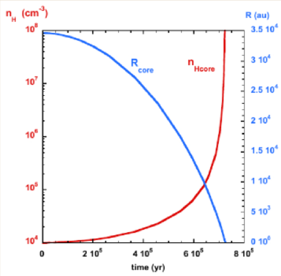
- New network: hydrides of C, N, O, S; Deuterated N-hydrides
- Condensed network: 150 species, 1100 reactions
- Separated network: 205 species, 2900 reactions
- Separation program (`spinstate.f90`): automatic for exothermic; manual for thermoneutral and other specific reactions (e.g. $H_3^+ + e^-$)

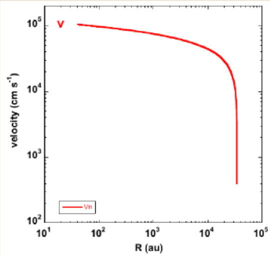
The GRENOBLE model

- Chemical network (gas-phase, ads./des., surface chemistry)
- Self-consistently with Larson-Penston collapsing 1D, isothermal, core (plateau $+ \rho \propto r^{-2}$ envelope)
- 1D-Radiative transfer
- Ray-tracing

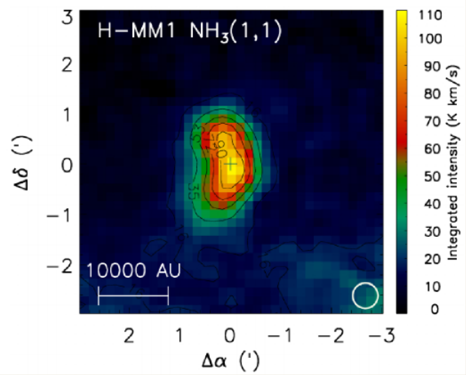
Preliminary results

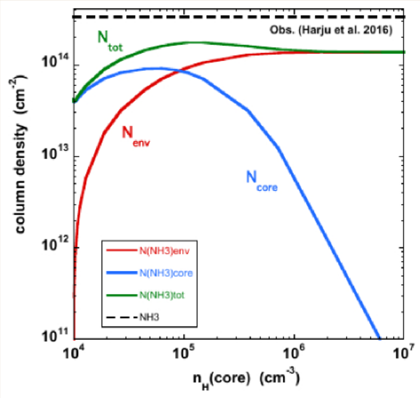




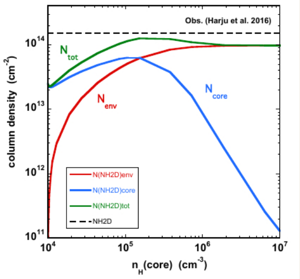


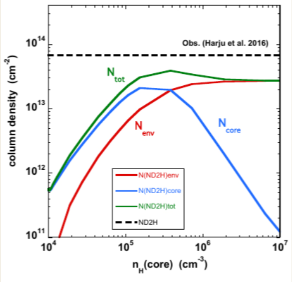
Preliminary results: ammonia

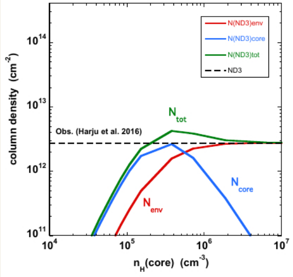




Preliminary results: ammonia







Conclusions

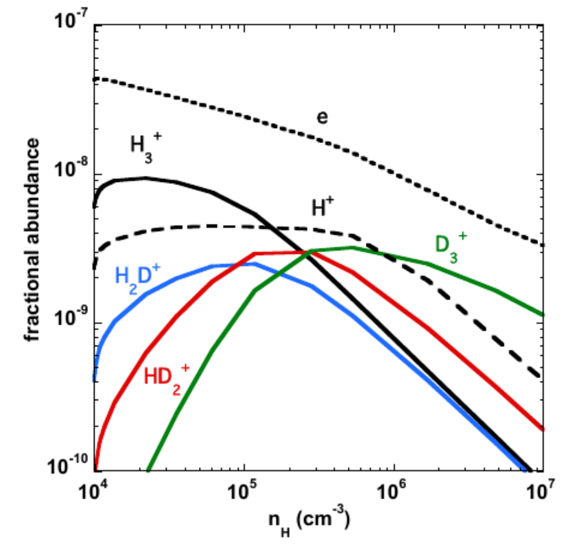
- OPRs of $\mathrm{H_2}$ and H_3^+ are in steady-state
- OPRs: measure the age of $\mathrm{H_2}$

Perspectives

- Are all OPRs in steady-state ?
- Modelling:
- Self-consistent OPRs of C, N, O, and, S hydrides
- The D/H and OPR of water prior to protostar and disk formation
- Tracers of the OPR of $\mathrm{H_2}$
- state-to-state chemistry
- Observations: ALMA


Physical Properties of
Star
Forming Regions
Malcolm Walmsley
Arcetri Observatoy

Preliminary results



References I

Brünken, S., Sipilä, O., Chambers, E. T., et al. 2014, Nature, 516, 219

Caselli, P., Vastel, C., Ceccarelli, C., et al. 2008, A&A, 492, 703

Dalgarno, A., Black, J. H., & Weisheit, J. C. 1973, Astrop. Lett., 14, 77

Faure, A., Hily-Blant, P., Le Gal, R., Rist, C., & Pineau des Forêts, G. 2013, ApJL, 770, L2

Flower, D. R., Pineau des Forêts, G., & Walmsley, C. M. 2006, A&A, 449, 621

Furuya, K., Aikawa, Y., Hincelin, U., et al. 2015, A&A, 584, A124

Gerlich, D., Herbst, E., & Roueff, E. 2002, Planetary and Space Science, 50, 1275

Hily-Blant, P., Walmsley, M., Pineau des Forêts, G., & Flower, D. 2008, A&A, 480, L5

Hugo, E., Asvany, O., & Schlemmer, S. 2009, JCP, 130, 164302

Kong, S., Caselli, P., Tan, J. C., Wakelam, V., & Sipilä, O. 2015, ApJ, 804, 98

Le Bourlot, J. 1991, A&A, 242, 235

Pagani, L., Salez, M., & Wannier, P. G. 1992, A&A, 258, 479

Tafalla, M., Santiago-García, J., Myers, P. C., et al. 2006, A&A, 455, 577

Vastel, C., Phillips, T. G., & Yoshida, H. 2004, ApJL, 606, L127

Walmsley, C. M., Flower, D. R., & Pineau des Forêts, G. 2004, A&A, 418, 1035