The history and evolution of the UMIST Database for Astrochemistry

OR

How to construct and maintain a database: the gas-phase example I

T. J. Millar
Catherine Walsh
Andrew Markwick
Daniel McElroy
Martin Cordiner
Ken Smith
Outline

❖ Historical origins, motivation, and philosophy
❖ Evolution of the database
  - RATE91
  - RATE95
  - RATE99: first online only version
  - RATE06: second online version
  - RATE12: current version (http://www.udfa.net/)
❖ The future of the UMIST Database for Astrochemistry
❖ What Tom would have done differently
❖ Closing remarks
History

- Motivated by detection of complex molecules in dark clouds, TMC1 and L134N, in early 1980s
  - Cyanopolyynes: HCₙN (n = 3, 5, 7, 9)
  - Hydrocarbons: C₄H, CH₃CCH, CH₃C₄H

- Early versions - personal compilation from the literature (C, N, O)
  - Prasad & Huntress 1980
  - Freeman, A. 1982, PhD thesis, UMIST
  - Freeman & Millar 1983: cyanopolyynes in TMC-1
  - Millar & Freeman 1984: TMC-1 and L134N
  - Millar & Nejad 1985: laboratory data and time dependence
History

Most reaction rate coefficients in this scheme were measured in the laboratory (Bohme et al. 1982, Herbst et al. 1983)

*Figure 1. Entering the hydrocarbon chemistry.*

From Millar & Freeman, 1984
History


❖ Subsequent versions
  - Millar, Bennett, & Herbst, 1987: phosphorus chemistry added
  - Millar et al. 1988: dissociative recombination
  - Herbst et al. 1989: silicon chemistry added
  - Millar & Herbst 1990: sulphur chemistry added

❖ Personal compilation of multiple reaction files: dark clouds, hot cores, circumstellar envelopes - merged into one database
Philosophy

❖ Adopt an ‘optimistic’ approach for molecular synthesis

❖ Adopt laboratory-measured and calculated rate coefficients where available: critical analysis reaction-by-reaction by a dedicated team

❖ Bench-marking with previous versions and alternative networks

❖ Inclusion of reactions also important at high temperatures (> 10 K)

❖ Updated versions of the network anticipated accompanied by a paper describing the each updated version of the database
First public release of the UMIST database

Gas phase reactions and rate coefficients for use in Astrochemistry. The UMIST ratefile

T.J. Millar¹, J.M.C. Rawlings¹,², A. Bennett¹, P.D. Brown¹,³ and S.B. Charnley¹,⁴

¹ Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD, U.K.
² Institut für extraterrestrische Physik, Max-Planck-Institut für Physik und Astrophysik, D-8046 Garching bei München, F.R.G.
³ Canadian Institute of Theoretical Astrophysics, McLennan Physical Laboratory, 60 St. George Street, Toronto M5S 1A1, Canada
⁴ Department of Physics, Rensselaer Polytechnic Institute, Troy, NY 12180-3590, U.S.A.

Some discussion on release of database: decision made it was best for the community
RATE91

- 313 atomic and molecular species
- 12 elements: H, He, C, N, O, Na, Mg, Si, P, S, Cl, and Fe
- 2880 reactions
  - neutral-neutral reactions (338)
  - ion-neutral reactions (2397; Smith & Adams - SIFT)
  - cosmic-ray ionisations (11)
  - photoreactions (134; van Dishoeck 1987, 1988)
- Additional data and tools
  - formulae for calculating rate coefficients
  - dipole moments for neutral molecules
  - dark cloud model results
  - code available on request to generate ODEs
Rate91

- Format of the database
  - tabulated in the paper and available electronically on request

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<th>Index</th>
<th>Reactants</th>
<th>Products</th>
<th>α</th>
<th>β</th>
<th>γ</th>
<th>Note</th>
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</tbody>
</table>

Flags:
- measured (1)
- reaction type (2)
- importance (1)
- accuracy (1)
- reference (4)

Parametrisation of the rate coefficient:

\[ k = \alpha \frac{(T/300)^\beta}{\exp(-\gamma/T)} \text{cm}^3\text{s}^{-1}, \text{for two body reactions,} \]

\[ k = \alpha s^{-1}, \text{for cosmic-ray ionisations, and} \]

\[ k = \alpha \exp(-\gamma A_v) s^{-1}, \text{for photoreactions.} \]
**RATE95**

- Second public release of the UMIST database
  - First instance of name, “UDfA”, and release, “RATEXX”

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**Astronomy & Astrophysics**

**Supplement Series**

_Astron. Astrophys. Suppl. Ser. 121, 139-185 (1997)_

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**The UMIST database for astrochemistry 1995***

T.J. Millar, P.R.A. Farquhar and K. Willacy

Department of Physics, UMIST, P.O. Box 88, Manchester, M60 1QD, UK

Received February 12; accepted May 14, 1996

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- 395 (313) species
- 3864 (2880) reactions

XX = year up to which database is complete (i.e., not year of publication)
RATE95

- Updates to the chemistry (examples)
  - Chemistry for newly detected species (e.g., CCO)
  - Neutral-neutral chemistry cross-referenced with NIST database
  - Negative ion reactions
  - Isomer-specific chemistry (e.g., \( l \)-C3H2 and \( c \)-C3H2)
  - Updated photoreactions (Roberge 1991)
  - Cosmic-ray-induced photodissociation (Gredel et al. 1988, 1987)

- Additional data and tools
  - Heats of formation of each species

- Format as for RATE91; however, all data also available for download
RATE99

- Third public release of the UMIST database

The UMIST database for astrochemistry 1999*

Y.H. Le Teuff, T.J. Millar, and A.J. Markwick

Department of Physics, UMIST, PO Box 88, Manchester M60 1QD, UK

- 396 (395) species
- 4113 (3864) reactions
Rate99

- Updates to chemistry
  - Reactions applicable to environments beyond cold ISM
  - Three-body reactions
  - Collisional dissociation

- Additional data and tools
  - Photoreaction cross sections (radiation fields other than ISM)
  - Deuterium chemistry

- Format of rate file updated to ensure all reactions
  - are flagged as ‘measured’, ‘calculated’, ‘literature’, or ‘estimated’
  - have temperatures ranges
  - have estimated uncertainties (‘A’ to ‘E’ from < 25% to highly uncertain)
Rate99

❖ First version available online in electronic form only
  - http://www.rate99.co.uk (no longer live)
❖ Java applet developed to allow searches for reactions based on:
  - species or element
  - validity at a particular temperature
  - source
❖ Available data per reaction:
  - formula for calculating rate coefficient
  - temperature range over which rate coefficient is valid
  - full reference information
  - plot showing rate coefficient as a function of temperature (or visual extinction or dust albedo)
Forth public release of the UMIST database

The UMIST database for astrochemistry 2006

J. Woodall¹, M. Agúndez², A. J. Markwick-Kemper¹,³, and T. J. Millar¹,⁴

¹ Jodrell Bank Centre for Astrophysics, School of Physics and Astronomy, University of Manchester, Sackville Street Building, Manchester M60 1QD, UK
e-mail: Tom.Millar@qub.ac.uk
² Departamento de Astrofísica Molecular e Infrarroja, Instituto de Estructura de la Materia, CSIC, Serrano 121 28006 Madrid, Spain
³ Department of Astronomy, University of Virginia, PO Box 3818, Charlottesville, VA 22903, USA
⁴ Astrophysics Research Centre, School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, UK

- 420 (396) species
- 4573 (4113) reactions

Naming convention retained despite:
(i) UMIST subsumed by the University of Manchester
(ii) T. J. Millar now at Queen’s University Belfast
**RATE06**

- Critical reassessment of all reaction rate coefficients in database

- Updates to chemistry (examples)
  - Fluorine chemistry (detection of HF and CF⁺)
  - Ion-neutral chemistry cross-referenced with Anicich database (2004) and new low-temperature data (Smith et al. 2004)
  - Neutral-neutral chemistry cross-referenced with IUPAC atmospheric chemistry database and NIST
  - Dissociative recombination rates and products updated (wealth of data from storage ring experiments in Stockholm)

- Additional data and tools
  - Dipole-enhanced version of network
RATE06 compared with RATE99

- Just over 1/3 of reaction rates are measured
- Increase in number of measured reaction rate coefficients
- Increase in accuracy of rate coefficients
RATE06

- Second version available online in electronic form only
  - http://www.udfa.net (no longer live)
- Full current rate file available for download
- Search available by species and reaction
  - All legacy data listed (from RATE95 onwards)
  - Full reference
  - Accuracy
RATE12

- Fifth (and current) public release of the UMIST database

**The UMIST database for astrochemistry 2012**

D. McElroy¹, C. Walsh¹, A. J. Markwick², M. A. Cordiner³,⁴, K. Smith¹, and T. J. Millar¹

¹ Astrophysics Research Centre, School of Mathematics and Physics, Queen’s University Belfast, Belfast BT7 1NN, UK
e-mail: dmcelroy@qub.ac.uk
² Jodrell Bank Centre for Astrophysics, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK
³ Astrochemistry Laboratory and the Goddard Center for Astrobiology, Mailstop 691, NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20770, USA
⁴ Institute for Astrophysics and Computational Sciences, The Catholic University of America, Washington, DC 20064, USA

- 467 (420) species
- 6173 (4573) reactions
RATE12

- A further critical reassessment of all reaction rate coefficients

- Updates to chemistry (examples)
  - Anion chemistry ($C_n^-$, $C_nH^-$, $C_nN^-$ following detection)
  - Dissociative recombination (CRYRING data)
  - Low-temperature neutral-neutral reactions (CRESU data)
  - Photoreaction rates (van Dishoeck)
  - HNCO isomers (following detection, Quan et al. 2010)
  - Refit of temperature behaviour of problematic reaction rates (Rollig 2011)

- Integration with VAMDC (Virtual Atomic and Molecular Data Centre)
RATE12

- New website
  - Search by species: reactions sorted by formation/destruction
  - Full legacy reaction data available (from RATE95 onwards)
  - All reaction data have a DOI and/or reference
  - Time-dependent abundances of each species for “standard” dark cloud model

- Additional material
  - Deuterium chemistry: exchange reactions
  - Deuterium chemistry: state (ortho and para) specific reaction rates
  - Binding (desorption) energies
  - Three-body reactions
RATE12

- Coming soon
  - Data evaluation sheets for all reactions
  - Codes to model molecular clouds and circumstellar envelopes
  - Tutorials for running models
  - Output of “standard” dark cloud model for benchmarking

http://www.udfa.net
The future of UDfA

- Implementation in VAMDC (http://www.vamdc.eu/)

- Current lack of funding: Tom is currently sole database administrator (with web support from Andrew Markwick in Manchester)

- Link chemical codes with radiative codes

- Age of high impact, high citation science: general lack of funding for fundamental research

- Strengthen link between database and original references (databases have high citation rates, original references very few)
What would Tom have done differently?

❖ Maintained deuterium chemistry database (was ‘lost’ between RATE99 and RATE12 databases)

❖ Greater control over the web version of the database: reflective of distance between Manchester and Belfast (QUB)

❖ Early universe chemistry

❖ Links to other astrochemistry-related databases on the website

❖ Accuracy of “accuracy” labels - important for sensitivity analyses
Closing thoughts

❖ Database name, logo, and host

❖ Data legacy
  - Regularly updated “live” version
  - Regular releases with accompanying publication
  - Benchmarking with some “standard” model

❖ Database maintenance and collation
  - Conducted by a dedicated team (e.g., UDfA)
  - Reliant also on the community (e.g., KIDA)
  - Evaluation of data in event of multiple datasets (what to trust)
  - Preparation of data sheets with recommended rates/data

❖ Provision of tools/models

❖ Citation of original work via citation of the database - essential!