A DATABASE OF MOLECULAR LINE DATA FOR ROTATIONAL TRANSITIONS FROM SELECTED SPECIES OF ASTROPHYSICAL INTEREST

Fredrik L. Schöier¹, Floris F. S. van der Tak², Ewine F. van Dishoeck¹, and John H. Black³

¹Leiden Observatory, P.O. Box 9513, 2300 RA Leiden, The Netherlands
²Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany
³Onsala Space Observatory, SE-439 92 Onsala, Sweden

Abstract

Molecular line data for the rotational transitions of a number of astrophysically interesting species have been collected and are made publically available through the www. These data, including energy levels, statistical weights, Einstein A-coefficients and collisional rate coefficients, are essential input for non-LTE molecular radiative transfer programs. A computer program for performing statistical equilibrium calculations is made publically available for use as well. This database should form an important tool in analyzing observations from current and future infrared and (sub)millimetre telescopes.

Key words: Molecular data – Radiative transfer

1. Introduction

A wide variety of molecules has been detected in space to date, ranging from simple molecules like CO to more complex organic molecules including ethers and alcohols. Observations of molecular emission at millimetre and infrared wavelengths, supplemented by careful and detailed modelling, are powerful tools to investigate the physical and chemical conditions of astrophysical objects (e.g., Black 2000). For some objects, lines with a large range of critical densities and excitation temperatures are needed, since the densities can range from \( \sim 10^2 \) – \( 10^9 \) cm\(^{-3}\) and the temperatures from \( \sim 10 \) – 1000 K in the interstellar and circumstellar environments probed by current and future instrumentation.

To extract astrophysical parameters, the excitation and radiative transfer of the lines needs to be calculated. A number of radiative transfer codes have been developed for the interpretation of molecular line emission [see van Zadelhoff et al. (2002) for a review]. The radiative transfer analysis requires molecular data in the form of energy levels, statistical weights and transition frequencies as well as the spontaneous emission probabilities and collisional rate coefficients.

2. Molecular line data

Literature data on the rotational transitions of 23 different molecules are summarized and extrapolation of collisional rate coefficients to higher energy levels and temperatures are made. The data are made available for the community through the www. Many of the data files presented here were adopted by Schöier et al. (2002) to model the circumstellar environment of the protostar IRAS 16293–2422.

2.1. Energy levels and radiative rates

The energy levels and Einstein A-coefficients are obtained from the JPL\(^2\) and CDMS\(^3\) catalogues. In some cases, better or more recent laboratory data have been used instead. Generally, only the ground vibrational state is retained, although in a few cases, e.g. CO and HCN, vibrationally excited levels are included. More study of collisional rate coefficients for vibrational transitions is urgently needed, as there are certainly cases where vibrationally excited molecules are important. Examples include HC\(_3\)N (Wyrowski et al. 1999) and torsionally excited CH\(_3\)OH. In the future, data files including excited vibrational states will be added for more molecules.

Hyperfine splitting can be of importance in line transfer and introduce non-local effects for lines overlapping in frequency (e.g., Lindqvist et al. 2000). However, often the splitting between individual hyperfine components is small compared to the line-broadening, so that it can safely be neglected and treated as a single level for the purpose of excitation analysis. We present data files for some of the relevant molecules, such as HCN and CN, both with and without hyperfine splitting.

\(^1\) http://www.strw.leidenuniv.nl/~moldata
\(^2\) http://spec.jpl.nasa.gov
\(^3\) http://www.cdms.de
2.2. Collisional rate coefficients

The adopted collisional rate coefficients usually pose the largest source of uncertainty of the molecular data input to the radiative transfer analysis. Detailed summaries of the theoretical methods and the uncertainties involved in determining collisional rate coefficients are given by Green (1975) and Flower (1990).

Published collisional rate coefficients cover only a limited range of temperatures and energy levels, and extrapolations are often necessary (see Fig. 1) introducing additional uncertainties. Data files containing the originally calculated set of rates as well as files where an extrapolation has been carried out are available for all molecular species.

In Fig. 2 the predicted line intensities for the 15 lowest rotational transitions of CO of an isothermal homogeneous sphere are shown using different sets of collisional rates. Deviations up to ~ 50% are found for the higher transitions which are sub-thermally excited. The lower transitions are close to LTE and less sensitive to the adopted set of collisional rate coefficients.

3. Radiative transfer

A radiative transfer code, RADEX,

4 http://www.strw.leidenuniv.nl/~moldata/radex.html

is made available for public use as part of the data base. RADEX is a one-dimensional radiative transfer code aimed at solving the statistical equilibrium equations using the escape probability formulation. The code makes no assumption for the geometry or large scale velocity fields and its basic assumption is that of an isothermal and homogeneous medium. RADEX provides a useful tool in rapidly analysing a large set of observational data providing constraints on physical conditions, such as density and kinetic temperature. RADEX provides an alternative to the widely used rotation temperature diagram method (e.g., Blake et al. 1987; Goldsmith & Langer 1999) which relies upon the availability of many transitions of optically thin emission lines and is useful only in roughly constraining the excitation temperature in addition to the column density.

Benchmarking of the RADEX code is presented in Fig. 3 where various expressions for the escape probability...
Figure 3. Comparison of the predicted line strengths for the 10 lowest rotational transitions of CO in a homogeneous isothermal sphere, with $n_{H_2} = 10^5$ cm$^{-3}$ and $T_{\text{kin}} = 50$ K, using different methods. Upper panel – The total optical depth through the sphere at line centre $\tau$ and excitation temperature $T_{\text{ex}}$ as a function of the upper rotational level $J$ involved in the transition. Middle panel – The radiation temperature $T_R$ obtained for each transition using RADEX with different prescriptions of the escape probability, $\beta$, and compared with the result from the Monte-Carlo code (MCC) of Schöier (2000). Also shown are the results for optically thin emission in LTE. Lower panel – $T_R$ obtained from RADEX compared with the results from MCC, $\delta T_R = T_R^{\text{MCC}} - T_R$.

Acknowledgements
FLS and EFvd are grateful to the Leids Kerkhoven-Bosscha Fond for financial support for their participation in the conference. This research was supported by the Netherlands Organization for Scientific Research (NWO) grant 614.041.004, the Netherlands Research School for Astronomy (NOVA) and a NWO Spinoza grant.

References
Black, J. H. 2000, in Astrochemistry: From Molecular Clouds to Planetary Systems, ed. Y. C. Minh & E. F. van Dishoeck, Vol. 197 (Astronomical Society of the Pacific), 81
Blake, G. A., Sutton, E. C., Masson, C. R., & Phillips, T. G. 1987, ApJ 315, 621
Flower, D. R. 1990, Molecular collisions in the interstellar medium (Cambridge Astrophysics Series, Cambridge: University Press, 1990)
Flower, D. R. 2001, MNRAS 328, 147
Flower, D. R. & Launay, J. M. 1985, MNRAS 214, 271
Goldsmith, P. F. & Langer, W. D. 1999, ApJ 517, 209
Green, S. 1975, in Atomic and molecular physics and the interstellar matter (North-Holland Publishing Co., Amsterdam), 83
Lindqvist, M., Schöier, F. L., Lucas, R., & Olofsson, H. 2000, A&A 361, 1036
Schinke, R., Engel, V., Buck, U., Meyer, H., & Diercksen, G. H. F. 1985, ApJ 299, 939
Schöier, F. L. 2000, Ph.D. Thesis, Stockholm Observatory
Schöier, F. L., Jørgensen, J. K., van Dishoeck, E. F., & Blake, G. A. 2002, A&A 390, 1001

are used. The output is compared both to an optically thin LTE analysis (rotation diagram method) and a full radiative transfer analysis using a sophisticated non-LTE code based on the Monte-Carlo method (MCC; Schöier 2000). The molecular data used in this example are the collisional rate coefficients for CO collisions with para-H$_2$ from Flower (2001). Levels up to $J = 29$ are included. The excitation temperatures of the lines vary from nearly thermalized, for transitions involving low $J$-levels, to sub-thermally excited for the higher-lying lines. The optical depth in the lines is moderate ($\sim 1 - 2$) to low. It is seen that the expressions of the escape probability for a sphere and the mean $[(1 - e^{-\tau})/\tau]$ give almost identical solutions and close to that obtained from the full radiative transfer. However, the slab geometry gives quite different results, in particular for high lying lines. The optically thin approximation, where the gas is assumed to be in LTE at 50K produces the largest discrepancy and only gives the correct answer for the $J = 1 \rightarrow 0$ line, where the requirements are fulfilled.
van Zadelhoff, G.-J., Dullemond, C. P., van der Tak, F. F. S.,
Yates, J. A., Doty, S. D., et al. 2002, A&A 395, 373
Wyrowski, F., Schilke, P., Walmsley, C. M. 1999, A&A 341, 882