

Challenges in opacity modeling for planetary and stellar atmosphere studies: line widths

R.E.Lupu¹, R.S.Freedman¹, and M.S.Marley²

1.SETI Institute, Mountain View, CA; 2.NASA/Ames Research Center, Moffett Field, CA

Abstract

Opacity calculations play an essential role in planetary atmosphere modeling. One of the fundamental problems encountered by opacity calculations is the limited knowledge of line broadening, for which laboratory data is often lacking and theoretical models offer only coarse approximations in most cases. In addition, the spectral averaging methods employed in computing the atmospheric structure and radiative transfer can lead to additional discrepancies between models, and make on-the-fly changes to the atmospheric composition difficult. We present a brief comparison between our model and other current methods of opacity calculations for atmosphere modeling, show the line width variation as a function of temperature and pressure, and the possible implications of these variations for deriving rotational velocities.

VSTAR

- Molecular opacities include H₂, TiO, VO, H₂O, CO, CO₂, CH₄, NH₃, CaH, FeH, MgH, CrH, TiH, CH, CN, C₂, HCN/HNC (Bailey and Kedziora-Chudczer 2011).
- Line widths are taken from detailed calculations in the literature: e.g. CH₄ from HITRAN, Pine 1992, Pine and Gabard 2003; H₂O from Bailey 2009, Delays et al. 1989, Gamache et al. 1996; CO from Rothman et al. 2005, Regalia-Jarlot et al. 2005.
- Voigt profiles + van Vleck-Weisskopf profile for the line wings, with correction factors.
- Radiative transfer code DISORT (1D, plane-parallel, LTE).

Our model

- Molecular opacities include H₂, TiO, VO, H₂O, CO, CaH, FeH, OH, MgH, SiH, SiO, SO₂, SH, PH₃, O₂, O₃, NO, NO₂, NH₃, N₂, LiCl, HF, HCN, HCl, H₂S, CrH, CO₂, ClO, CH₄, depending on atmospheric composition.
- The line widths are taken from the literature or approximated using similarities with available measurements: e.g. CH₄ from L. Brown 1996 (priv. comm.); H₂O from Gamache et al. 1998, 2001; CO from Bulanin et al. 1984, Mannucci 1991, Le Moal and Severin 1986.
- Voigt profiles are computed for all lines. Turbulent broadening can be included, but not used by default.
- Custom radiative transfer code (1D, plane-parallel, LTE), same results as DISORT.

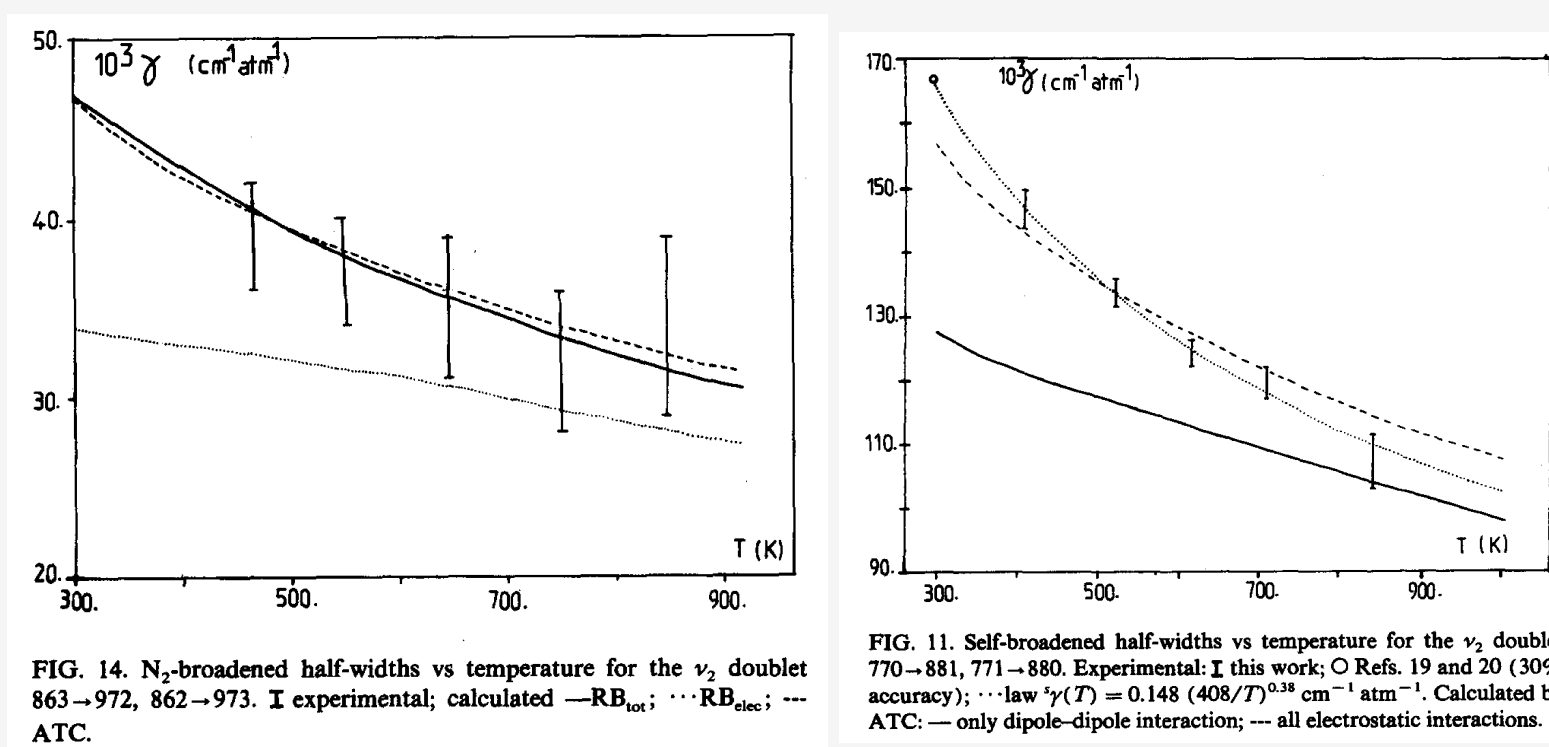
Phoenix

- Molecular opacities include H₂, TiO, VO, H₂O, CO, CaH, FeH, CH, NH, OH, MgH, SiH, C₂, CN, SiO (Allard et al. 1995).
- All line widths are computed in the van der Waals approximation, with corrections for non-alkali species. This does not take into account the dependence on molecular structure and energy levels. A comparison between this approach and other calculations has not been performed.
- Partial Voigt profiles, constant 2 km/s turbulent broadening.
- Phoenix radiative transfer code (1D and 3D, spherical and plane parallel, optional NLTE).

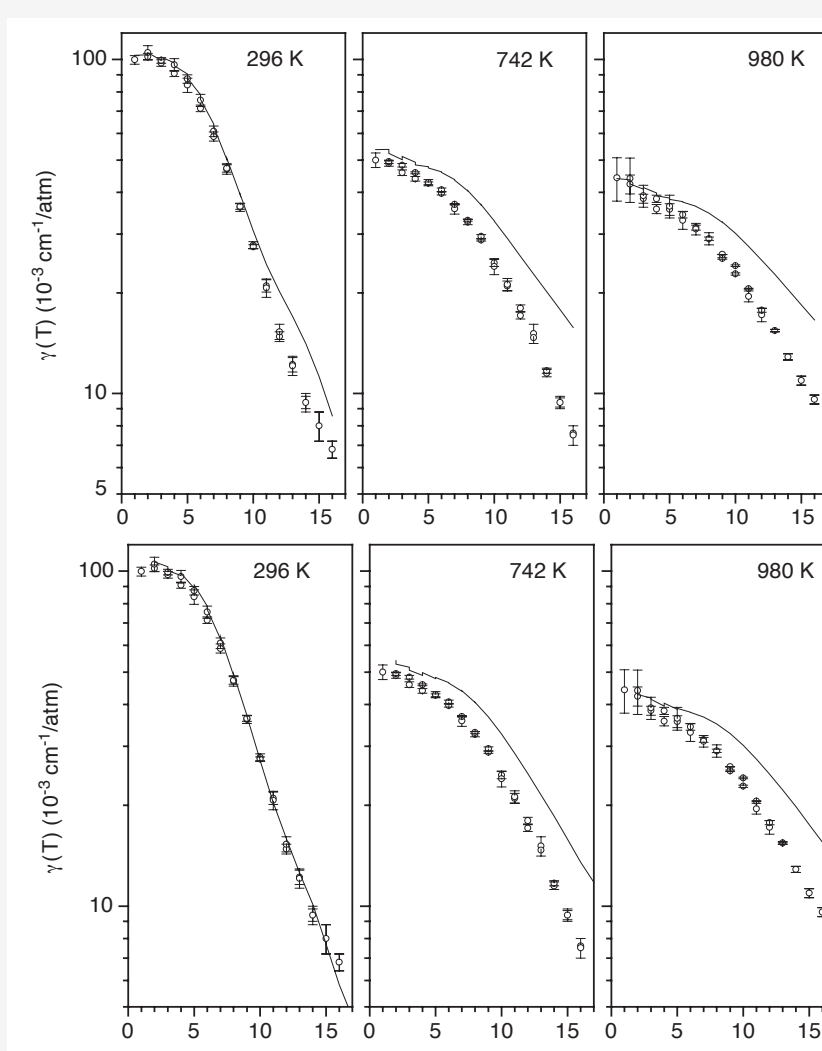
Line width overview

Molecular line width values are difficult to obtain, being determined by numerous factors, including: temperature, pressure, quantum numbers, energy levels, collisional partner, turbulent velocity, polarizability. These dependences are often poorly known due to the lack of experimental data.

Depending on the assumptions made and available data, differences by factors of a few can arise in the estimated line widths.



H₂O self- and N₂ line broadening. Models include dipole and higher order electrostatic interactions. Large variations are also present between low and high J levels (Hartmann et al. 1987).



Temperature dependence of water line widths, broadened by air. Even after corrections to the interaction potential, discrepancy factors of ~ a few remain at higher temperatures (Wagner et al. 2005).

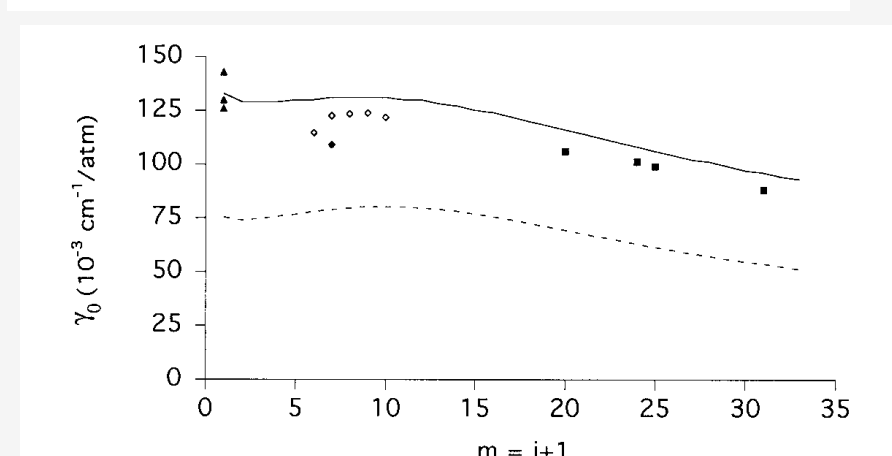


FIG. 2. H₂-induced broadening of HCN at room temperature. The experimental broadening parameter γ_0 (in 10^{-3} cm²/atm) is reported versus m for rovibrational transitions (■) R branch of the v₂ band (this work), for l-doubling transitions (●) v₂ state (L2, L3), and for rotational transitions (▲ ground state (L-3)). Calculated results obtained from the RB formation including electrostatic and atom-atom interactions (—), and electrostatic interactions only (---).

Line widths in our model

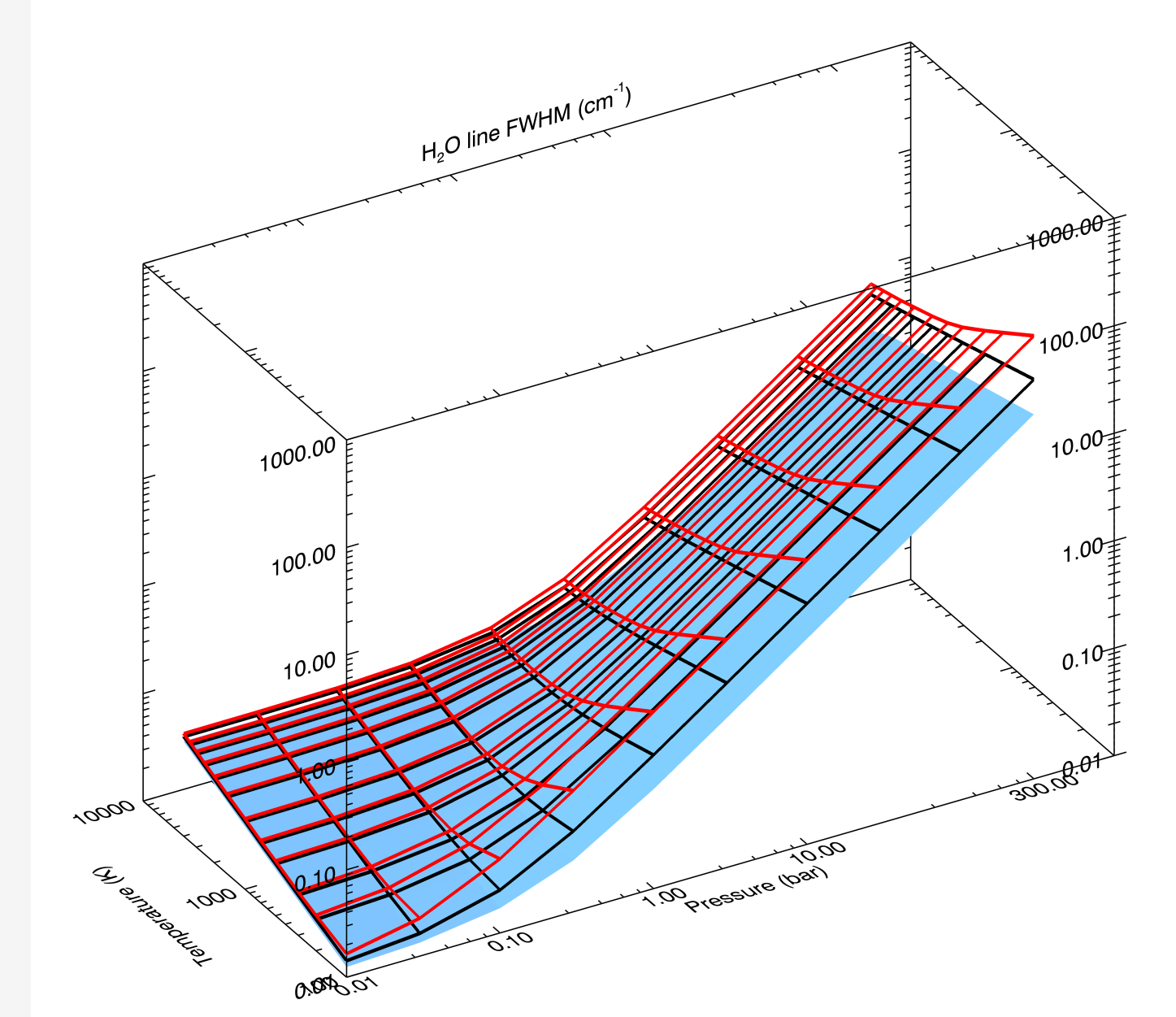
We use Voigt profiles, with the FWHM given by

$$F_v \approx F_D * (\sqrt{(F_L/F_D)^2 + 2.012(F_L/F_D) + 4.07} - 1.075)$$

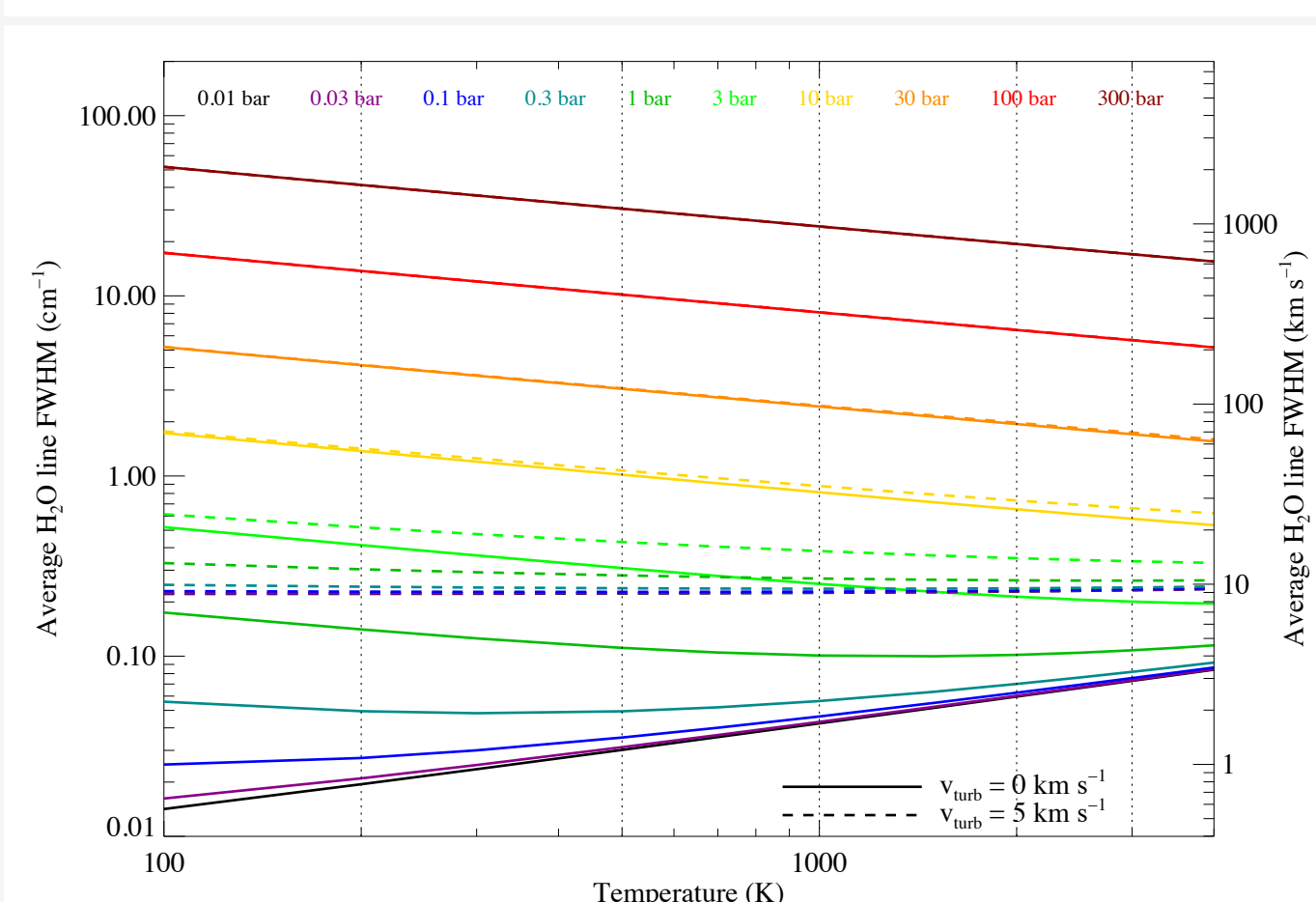
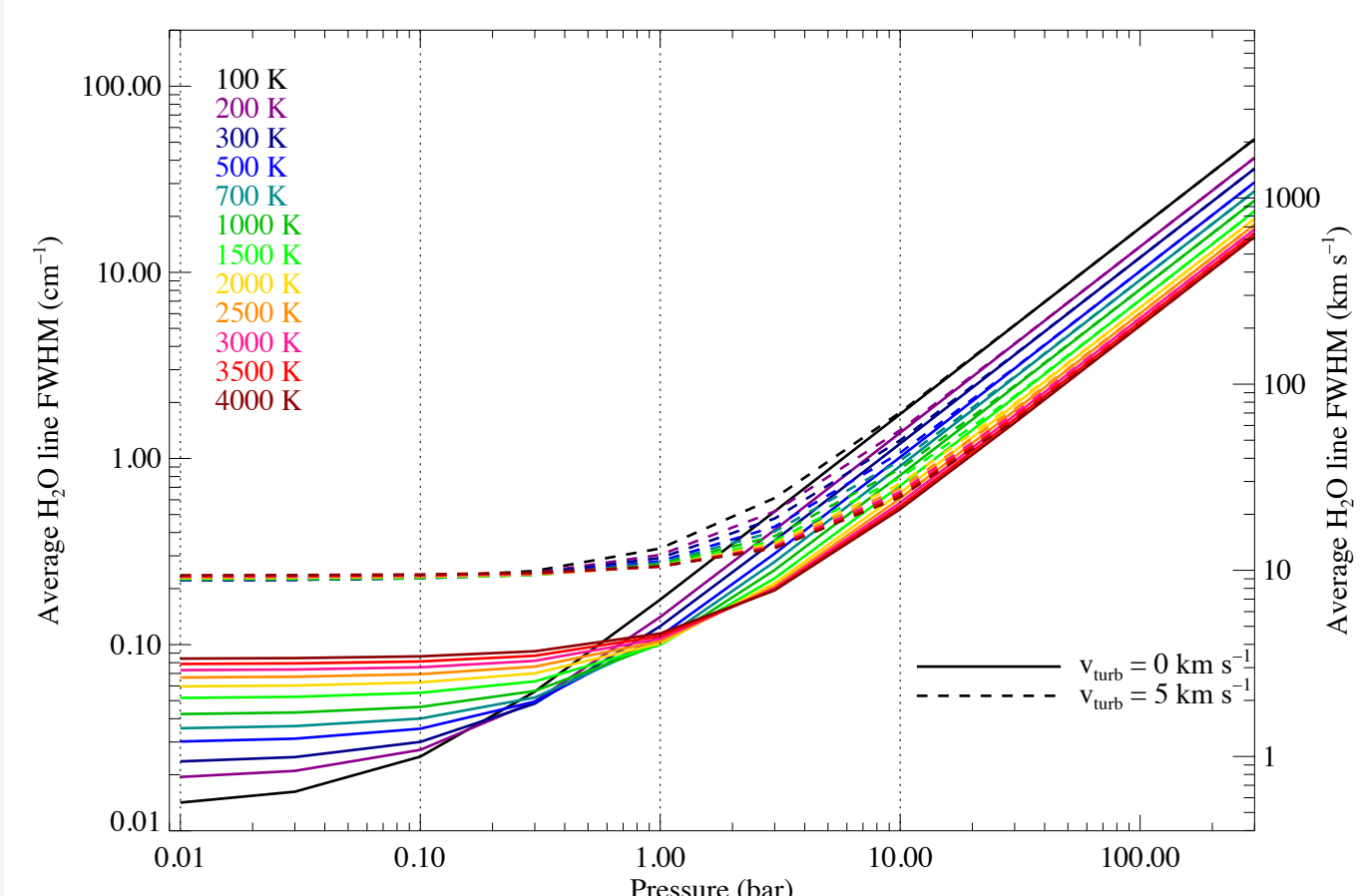
where the Doppler and Lorentz widths are

$$F_D = 2\sqrt{\ln 2} * \tilde{\nu}_0 / c * \sqrt{v_T^2 + v_{turb}^2}$$

$$F_L = 2 * \gamma_0 * (p / 1.01325) * (296/T)^n$$

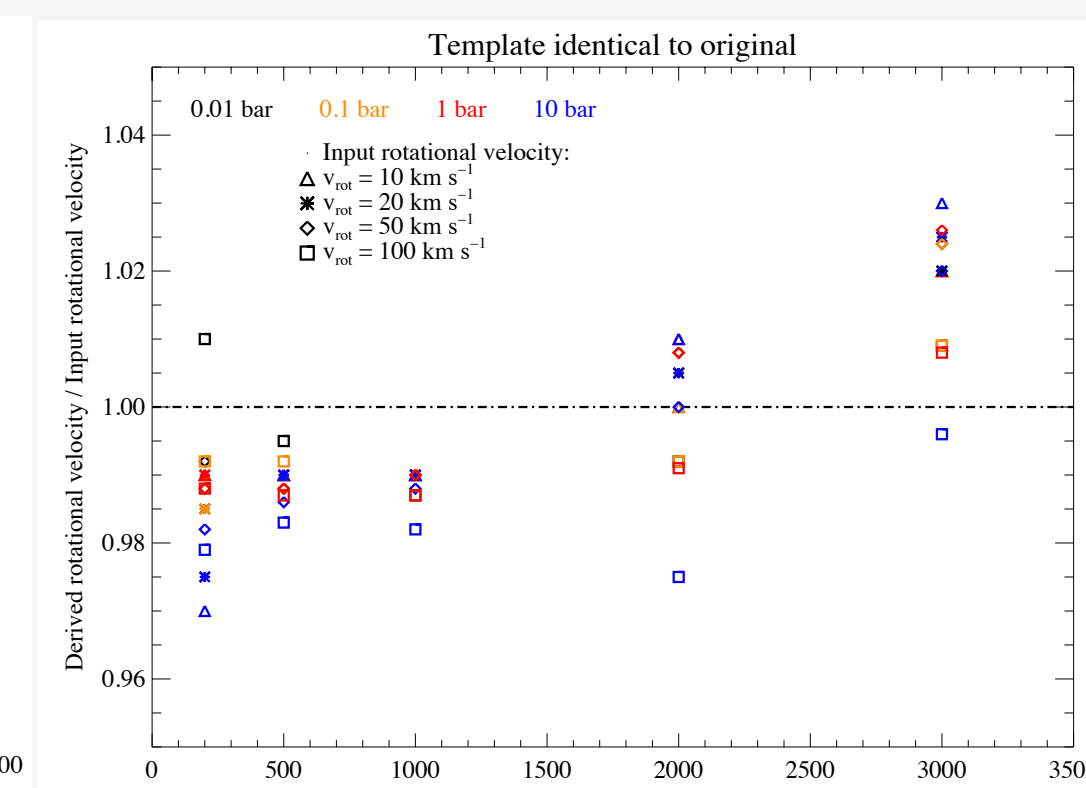
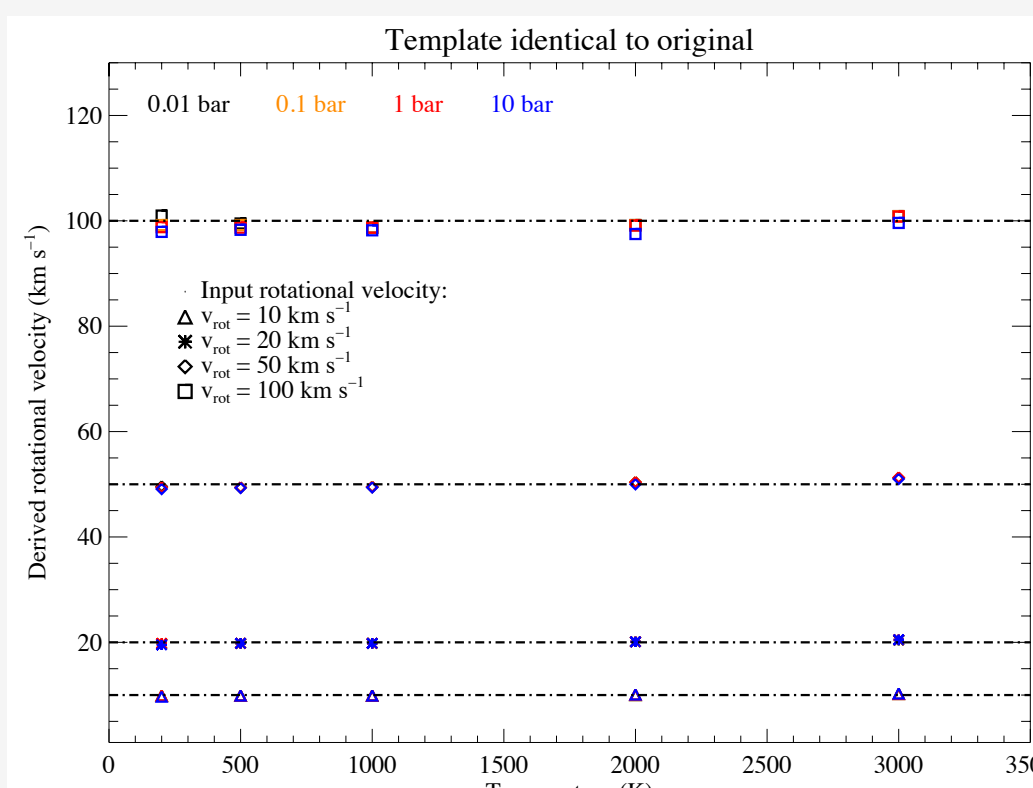


H₂O line widths as a function of (p,T), calculated over J-band at v_{turb}=0: average-black, minimum-blue, maximum-red.

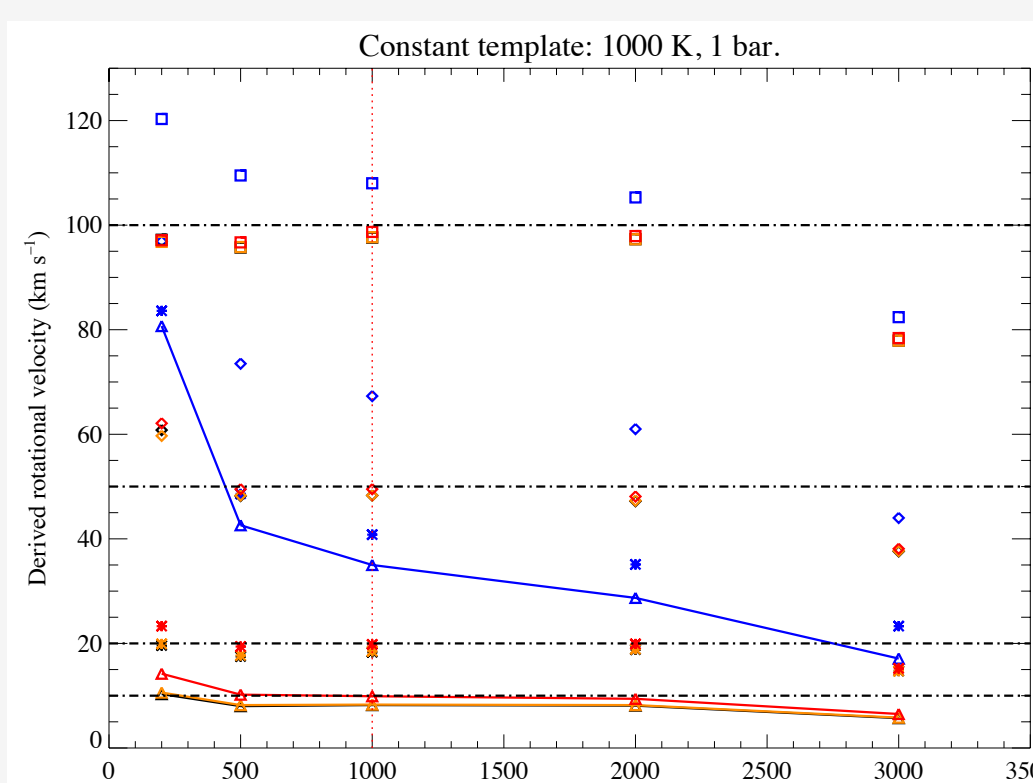


Rotational velocities

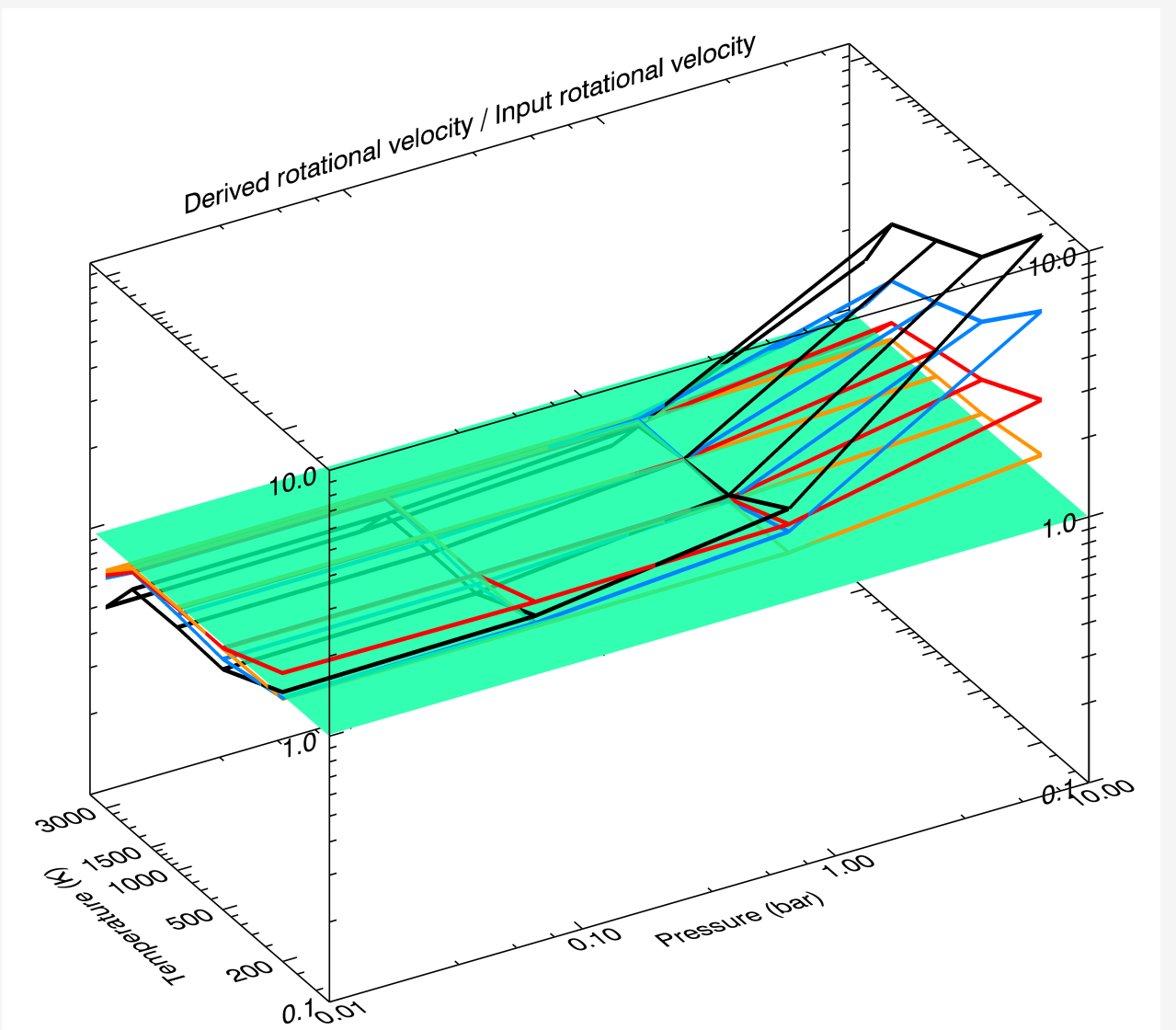
We construct H₂O absorption spectra for a set of (p,T) points and convolve them with the rotational profiles for velocities of 10, 20, 50 and 100 km/s. Each convolved spectrum is cross-correlated with the assumed input template spectrum, and the rotational velocity is derived by fitting the peak of the cross-correlation function using an MCMC algorithm.



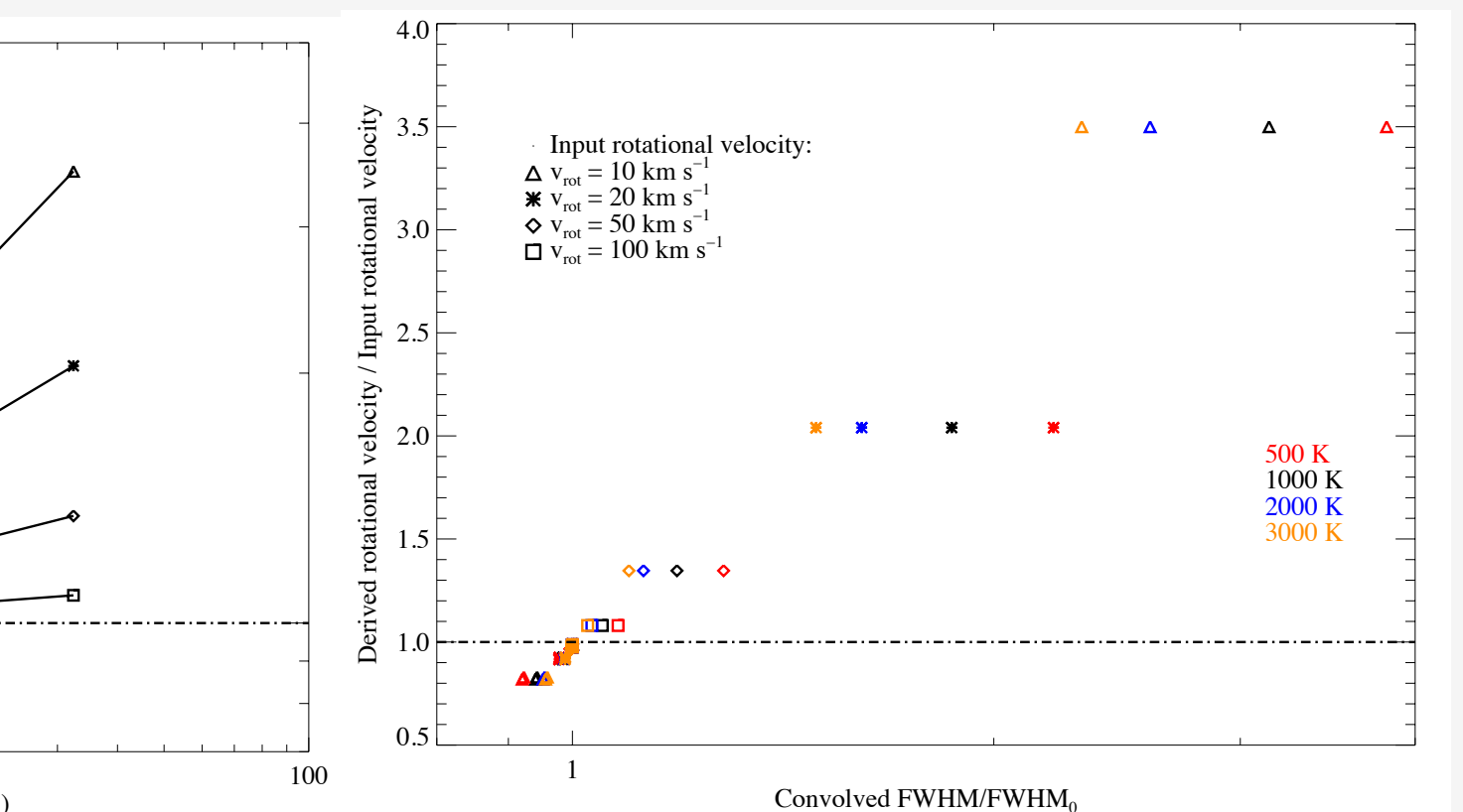
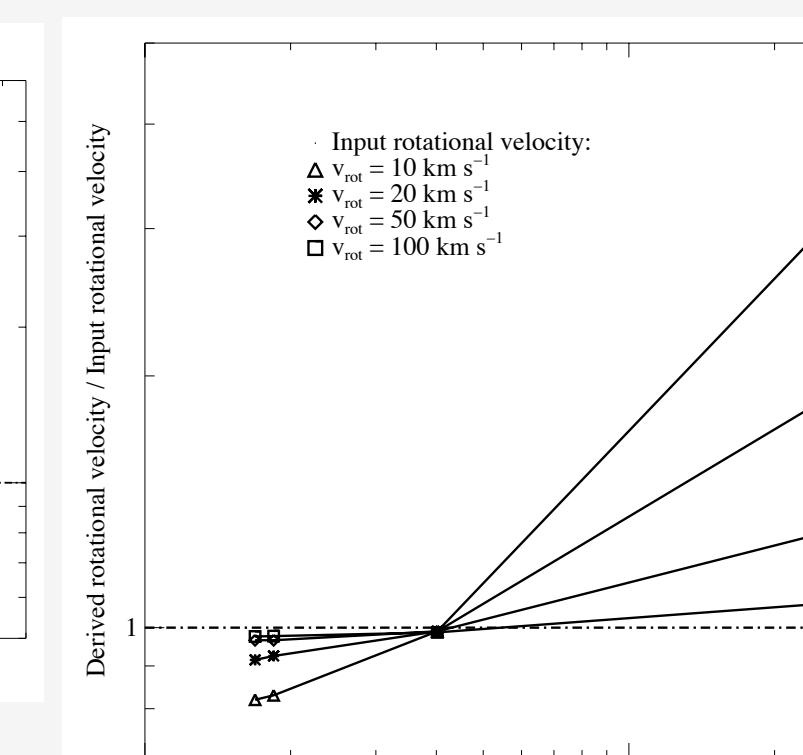
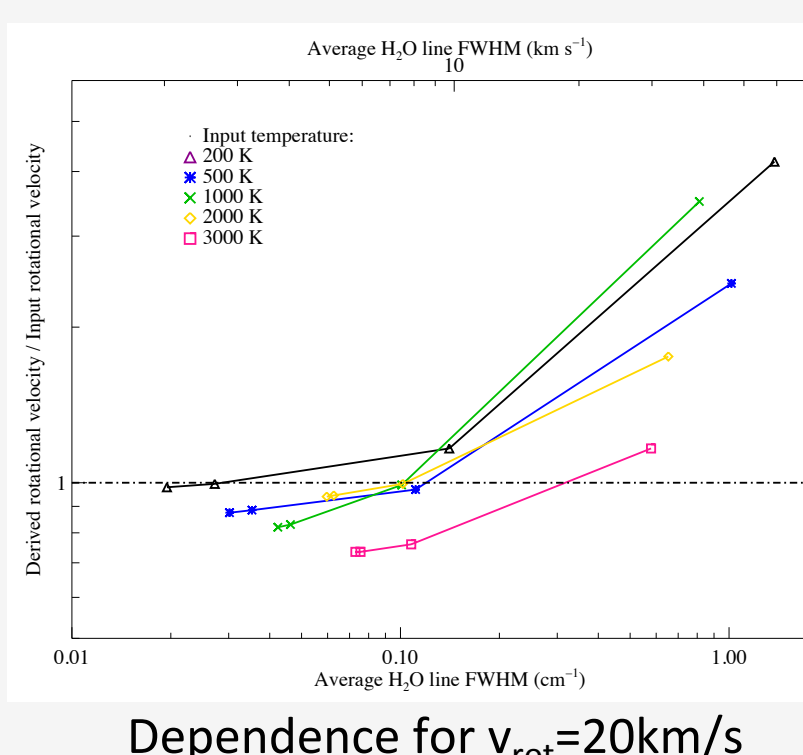
If the template used to derive the rotational velocity is identical to the original spectrum before convolution, the rotational velocity is recovered within ~4%.



Template mismatch relative to the original spectrum led to factors of up to ~8 difference in the derived rotational velocity relative to the true v_{rot} over the searched parameter space, depending on the original (p,T).



The v_{rot} discrepancy is caused not only by the variation of the line width with (p,T), but also by differences in the line list. For each temperature we limit the line list to the most important transitions. When the template is computed at the same temperature as the original, the results will show only the dependence of the derived rotational velocity on the line width.



When both the original and the template are calculated at the same T, the v_{rot} correction factor depends also on the value of v_{rot}. Over the chosen temperature range, this translates into a monotonic relationship between this correction factor and the total FWHM of the line, approximated as $FWHM = \sqrt{FWHM_0^2 + v_{rot}^2}$, where FWHM₀ matches the pressure of the original.