

# 1 Memo: D/XB

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The  $D/XB$  values printed at the end of a HYDKIN job represent the ratio of influx density to the intensity of light emission from a particular line or band.

HYDKIN provides as primary output concentrations  $n_A(t)$  for specified influx, loss rates, initial conditions and database choices. Using these results some processed (secondary) quantities such as so called  $D/XB$ -values are also printed. These latter depend, additionally, on choices of excitation rates and branching ratios not taken from the Hydrocarbon database but from spectroscopic literature [1, 2, 3].

**The excitation rates and branching ratios to be employed depend upon experimental details (spectral range, ro-vibrational distribution of emitter molecule, etc.) Only certain “reference excitation rates” are utilized in HYDKIN.**

See below for a definition for the individual bands. Hence  $D/XB$  values obtained from HYDKIN using these reference excitation rates have to be scaled to the particular experimental conditions, again: see below.

$D/XB$  values are defined as follows [1]:

$$\begin{aligned} \frac{D}{XB} \Big|_A^B &= \frac{\Gamma_{in}^B}{\underbrace{n_A(t = t_{max})}_{\text{HYDKIN}}} \cdot \frac{1}{n_e \langle \sigma_{emm} v \rangle (T_e)} \\ &= \frac{\Gamma_{in}^B}{n_A(t = t_{max})} \cdot \frac{1}{n_e \langle \sigma_{exc} v \rangle (T_e) \cdot R} \end{aligned} \quad (1)$$

$\Gamma_{in}$  is the sum of all influx components, i.e.,  $\Gamma_{in} = \sum_i b_i$ ,  $b_i$  the vector of external influxes as specified for any particular HYDKIN case, and the sum is over all components for which a non-zero influx has been specified. In most cases there will be only one entry for this vector, say for species  $B$ .  $n_e$  is the electron density ( $1/cm^3$ ).

The emission rate coefficient  $\langle \sigma_{emm} v \rangle (T_e)$  (units:  $cm^3/s$ ) for light in a specific frequency range is approximated by the product  $\langle \sigma_{exc} v \rangle (T_e) \cdot R$  of excitation rate coefficient and branching ratio (“Corona approximation”).

The branching ratio  $R$  is taken to be one here:  $R=1$ , because in all bands mentioned here the diagonal transitions  $v - v'$  with  $v = v'$  are by far dominant. Hence:  $\langle \sigma_{emm} v \rangle (T_e) = \langle \sigma_{exc} v \rangle (T_e)$ , and, by abuse of language, we sometimes use “excitation rate coefficient” rather than the more correct term “emission rate coefficient”.

A HYDKIN run provides the density  $n_A(t)$  of species  $A$  vs. time. The value  $t = t_{max}$  should be chosen such that stationary conditions result for species  $A$ . E.g. for Gerö band:  $A = CH$ , and for Swan band:  $A = C_2$ .

Graphs and fits of excitation rate coefficients  $\langle \sigma_{exc} v \rangle$  vs.  $T_e (= \langle \sigma_{emm} v \rangle)$  for some frequently used molecular bands are available under

## [⟨ex⟩](#), **Examples**

at the bottom of the HYDKIN output page. The rate coefficient  $\langle\sigma_{exc}v\rangle$  used in Eq. (1) is directly linked to the spectral range, for which a given  $D/XB$  value is applicable. Currently the following excitation rates are used (see [1, 2])

- **Gerö-Band**

The full band of the CD (or CH) A - X transition, i.e., from around 420 to 435 nm. But, as can be seen on the figure  $\langle\sigma_{exc}v\rangle(T_e)$  by clicking [⟨ex⟩](#) near the printout of the  $D/XB$  value, or [⟨ex⟩](#), **Examples**, this excitation rate is calculated for the diagonal “reference band”  $v' - v'' = 0 - 0$  only [2]. Other important contributions (1 - 1 and 2 - 2) are in the same spectral range but are NOT included in this reference excitation rate. Depending upon the spectral range in a particular measurement, a scaling factor must be applied to account for this.

For example it was recently recommended (S. Brezinsek, U. Fantz, private communication, May 2006) to use 1.46 as factor to scale up the 0 - 0 excitation rate for this band to the full  $v' - v'' = 0 - 0$ , 1 - 1, 2 - 2 band. See Figure on page 4 (kindly provided by U. Fantz, IPP-Garching, 2006).

Often this Gerö band also contains a component of CII light. Therefore one often only measures the frequency range 430 - 431.5 (CH), and 429 - 431 (CD), respectively (the “band head”). The appropriate scaling factors from this 15 Angström wide range to the full reference ( $v' - v'' = 0 - 0$ ) band, for which  $D/XB$  values are evaluated in HYDKIN and in [1, 2], depend upon the rotational temperature. Experimentally determined factors are given in [2].

Strictly speaking, the scaling factor depends upon the spectral range and the ro-vibrational distribution of the CH molecule, hence e.g. on  $T_e, n_e, \dots$ . It can therefore only be accurately computed from a full collisional radiative model for the CH molecule, including also the rates for directly populating excited states of CH from dissociative excitation of larger hydrocarbon molecules or from dissociative recombination from larger hydrocarbon molecular ions. To our knowledge such a model is presently not available.

- **The B-X band at 390 nm**

Again the excitation rate is for the full band, 386 - 396 nm, but again for the 0 - 0 transition only. From experimental spectra in this range one has to subtract the CII and  $H_\epsilon$  lines, which also fall into this frequency range. Scaling to other spectral ranges or contributions from other vibrational states has to be carried out as needed, see remarks for the Gerö band.

- **Swan-Band**

Excitation rate for full band, 509 - 516.6 nm, 0 – 0 transitions only. Recommended procedure: only integrate over the band head 515.4 - 516.6 and use scaling factor given in [2] for the excitation rates (and D/XB values) given there and in HYDKIN.

The same general remarks as for the Gerö band apply: here a collisional radiative model for C<sub>2</sub> would be needed.

- **Mulliken band**

Excitation rate refers to full band width, from 229.5 - 233 nm. There are no perturbing lines in this range. The excitation rate here includes  $v' - v'' = 0 - 3$  transitions (i.e.: the 0 – 0, 1 – 1, 2 – 2 and the 3 – 3 transitions).

The same general remarks as for the Gerö band apply: here a collisional radiative model for C<sub>2</sub> would be needed.

At present all excitation rates accessible to us have been calculated with the IPProg code, A. Burgess, H.P. Summers, Mon. Not. R. Astr. Soc. 174 (1976) 345, which is based upon Bethe-Born approximations (calculations are kindly provided by Ursel Fantz, IPP Garching). We suspect that in particular at energies below the energy where the maximum values of the related cross sections are located, the validity of this approach is limited and should be checked by independent more sophisticated calculations.

## References

- [1] D. Naujoks et. al. J. Nucl. Mat. 266-269 (1999) p360 - 364
- [2] U. Fantz J. Nucl. Mat. 337-339 (2005) p1087 - 1091, and: U. Fantz priv. comm. 2005
- [3] S. Brezinsek et al., Physica Scripta Vol 111, 42- 48 (2004)

