AN INVESTIGATION ON THE ROLE OF ROTATIONAL MECHANISMS IN ELECTRON SWARMS AT LOW REDUCED ELECTRIC FIELD IN N_2, O_2 AND H_2

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INTRODUCTION

In molecular gas discharges running at very-low *E/N* (*E* is the electric field and *N* is the gas density) electron-neutral rotational and vibrational collisions are competitive enough to become important energy-transfer channels, influencing the electron energy distribution function and the corresponding swarm parameters.

In this work, the homogeneous electron Boltzmann equation, written under the classical two-term approximation, is solved in N_2, O_2 and H_2 for ***E/N* = 10⁻⁴ − 10 Td**. A code is especially developed for this purpose [1], adopting three different approaches to describe electron-neutral rotational excitations / de-excitations: (i) using the discrete inelastic / superelastic collisional operator for rotations **(DCOR)**, written for a number of levels that depends on the molecular gas and the specific rotational cross sections considered; (ii) replacing the discrete collisional operator for rotations by a continuous approximation for rotations **(CAR)**, deduced for the set of rotational cross sections derived by Gerjuoy and Stein [2] from the Born approximation (BA); (iii) generalizing the CAR expression to include a "Chapman-Cowling term" proportional to the gas temperature T_g [3] **(CC-CAR)**, similarly to what is usually adopted for the elastic collision operator [4], trying to bridge the gap between approaches (i) and (ii) for low / intermediate *E/N* values at various T_g.

To assess the validity of these approaches and of the rotational cross sections adopted for the different gases [2,5], calculation results are compared with measurements for the available swarm parameters, namely the electron mobility and the electron characteristic energy.

THE HOMOGENEOUS ELECTRON BOLTZMANN EQUATION

$$-N\sqrt{\frac{2e}{m}}\frac{d}{du}\left[\frac{u\,(E/N)^2}{3\,\sigma_t}\frac{df}{du}+\frac{2m}{M}u^2\sigma_m\left(f+\frac{k_BT_g}{e}\frac{df}{du}\right)\right]=\mathfrak{J}_{\rm rot}^{\rm inel}+\mathfrak{J}_{\rm rot}^{\rm sup}+\mathfrak{J}_{\rm vib}$$

The discrete collisional operator for rotations (DCOR)

$$\mathfrak{J}_{\rm rot}^{\rm inel}=N\sqrt{\frac{2e}{m}}\sum_J\delta_J\left[(u+u_{J,J+2})\sigma_{J,J+2}(u+u_{J,J+2})f(u+u_{J,J+2})-u\sigma_{J,J+2}(u)f(u)\right]$$

$$\mathfrak{J}_{\rm rot}^{\rm sup}=N\sqrt{\frac{2e}{m}}\sum_J\delta_J\left[(u-u_{J-2,J})\sigma_{J,J-2}(u-u_{J-2,J})f(u-u_{J-2,J})-u\sigma_{J,J-2}(u)f(u)\right]$$

The continuous approximation for rotations (CAR)

$$\mathfrak{J}_{\rm rot}\equiv\mathfrak{J}_{\rm rot}^{\rm inel}+\mathfrak{J}_{\rm rot}^{\rm sup}\simeq N\sqrt{\frac{2e}{m}}\frac{d}{du}(4\sigma_0Buf)$$

The Chapman-Cowling correction to CAR (CC-CAR)

$$\mathfrak{J}_{\rm rot}\equiv\mathfrak{J}_{\rm rot}^{\rm inel}+\mathfrak{J}_{\rm rot}^{\rm sup}\simeq N\sqrt{\frac{2e}{m}}\frac{d}{du}\left[4\sigma_0Bu\left(f+\frac{k_BT_g}{e}\frac{df}{du}\right)\right]$$

The Gerjuoy and Stein cs

$$\sigma_{J,J+2}(u)=\alpha(J)\left(1-\frac{u_{J,J+2}}{u}\right)^{1/2}$$

$$\alpha(J)\equiv\sigma_0\frac{(J+2)(J+1)}{(2J+3)(2J+1)}$$

[1] M A Ridenti, L L Alves, V Guerra and J Amorim, *Plasma Sources Sci. Technol.* **24** (2015) 035002

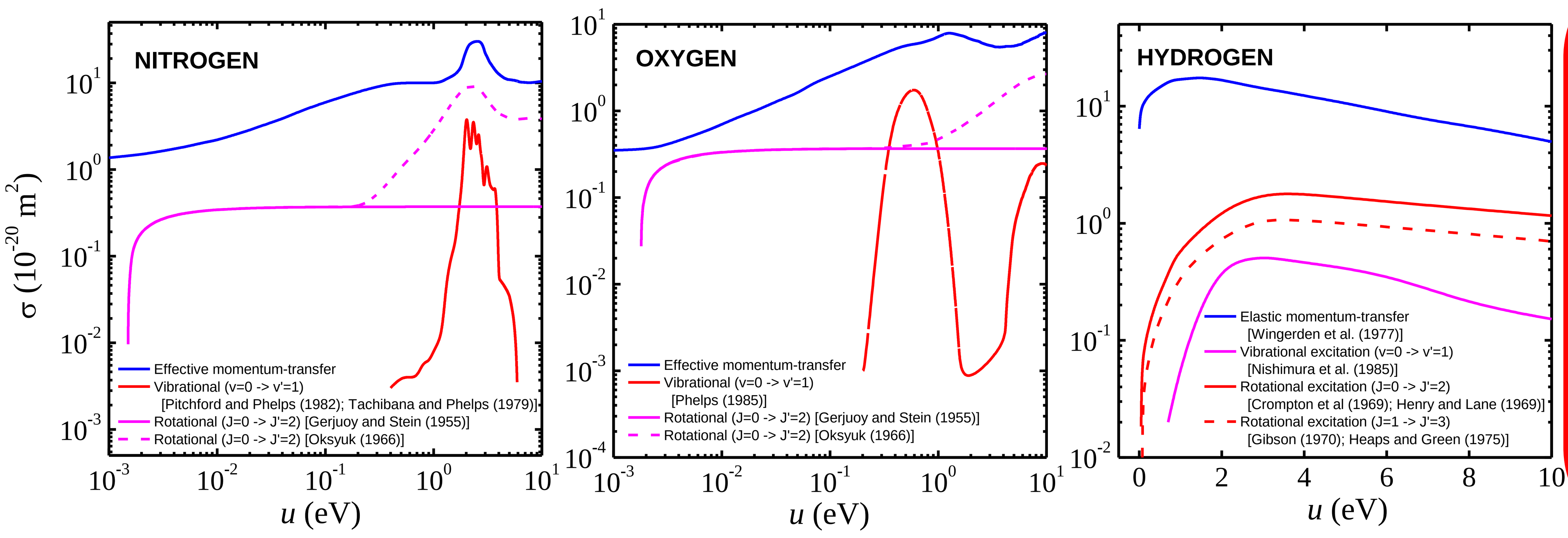
[2] E Gerjuoy and S Stein *Phys. Rev.* **97** (1954) 1671

[3] N A Dyatko, I V Kochetov and A P Napartovich, *J. Phys. D: Appl. Phys.* **26** (1993) 418

[4] I P Shkarofsky, T W Johnston and N P Bachynski (1966) *The particle kinetics of plasma* (Addison-Wesley)

[5] Yu D Oksyuk, *Sov. Phys. JETP* **22** (1966) 873

CROSS SECTIONS



Cross sections from the **IST-LISBON database** with LXCat (www.lxcat.net).

Relative densities of the rotational levels J assumed to follow a Boltzmann distribution at gas temperature $n_J/N=p_J\exp\left[-eBJ(J+1)/(k_BT_g)\right]/Z$

Summary:

- vibrational excitations v = 0 → v' (10 transitions for N_2 ; 4 for O_2 ; 3 for H_2)
- rotational excitations/de-excitations J ↔ J+2

N_2: J=0,1,2…,30 (*B* ~ 2.5x10⁻⁴ eV); cross sections of Gerjuoy and Stein (1955)

O_2: J=1,3,5…,30 (*B* ~ 1.8x10⁻⁴ eV); cross sections of Gerjuoy and Stein (1955)

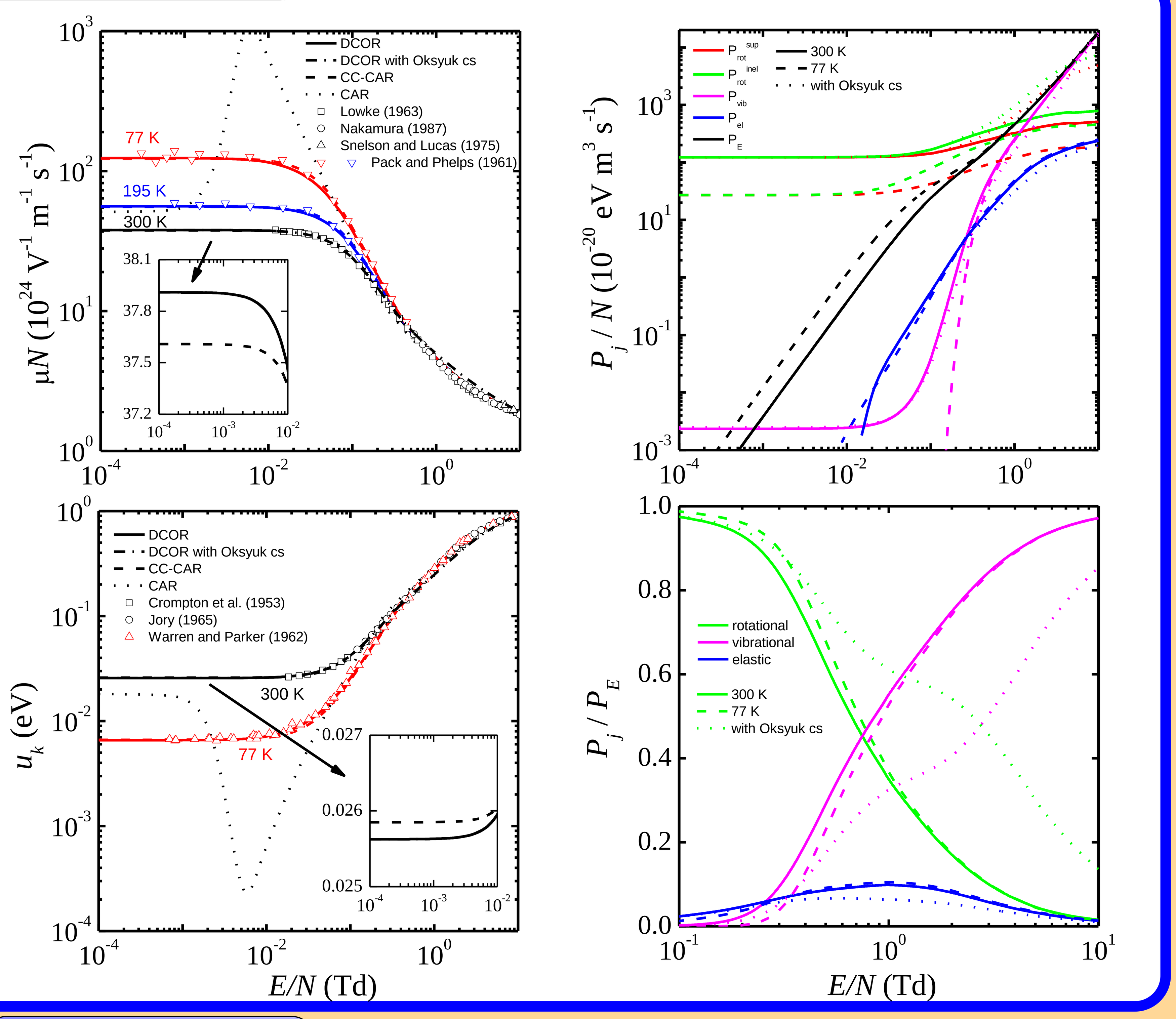
H_2: J=0,1,2…,20 (*B* ~ 7.3x10⁻³ eV); cross sections are as follows

J=0,1 – see figure; 2 ↔ 4 and 3 ↔ 5, Lane and Geltman (1967)

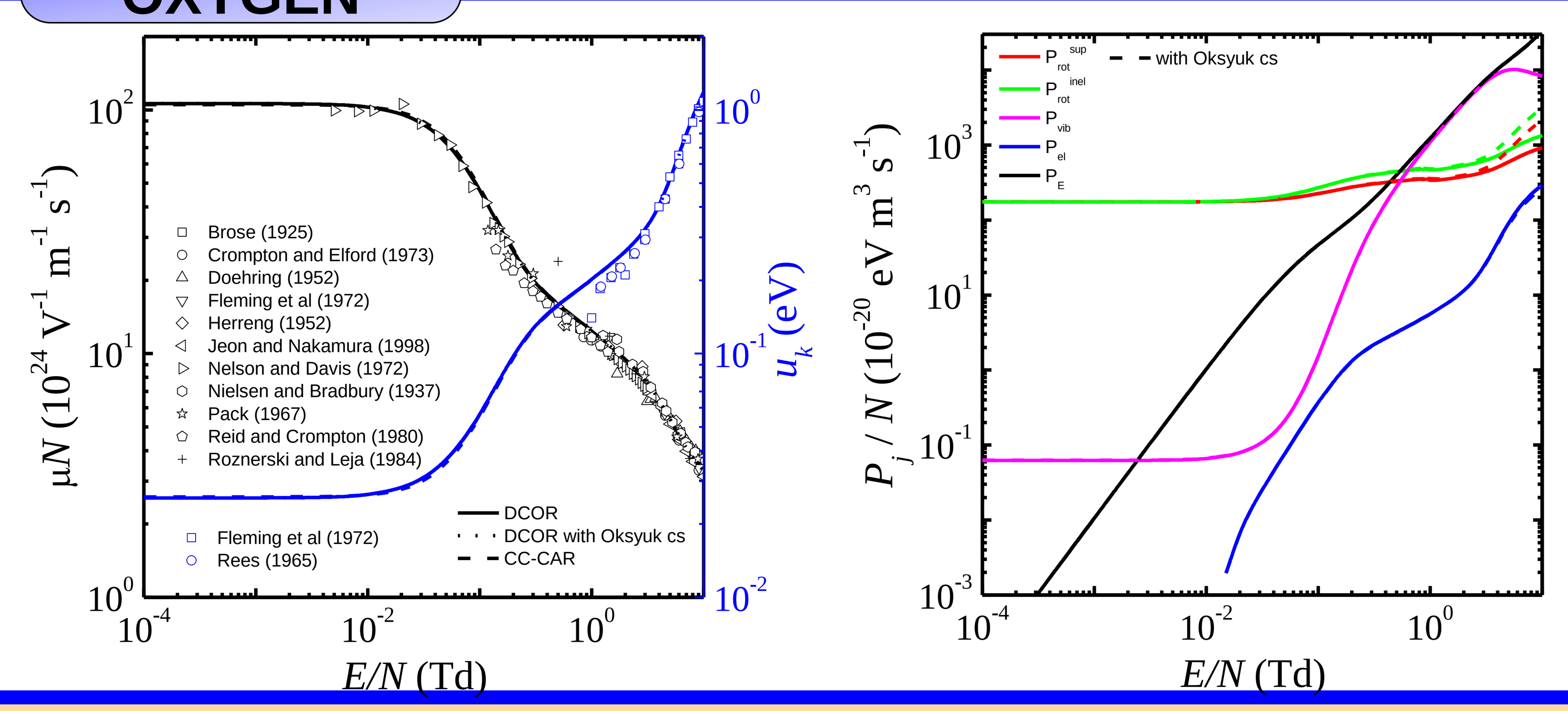
J ↔ J + 2 transitions (J > 4), Gerjuoy and Stein (1955)

We have considered separate density distributions for the para- and the ortho-systems of hydrogen, behaving as two independent components of a non-equilibrium mixture, taking $Z_{\rm ortho}$ = 3 $Z_{\rm para}$.

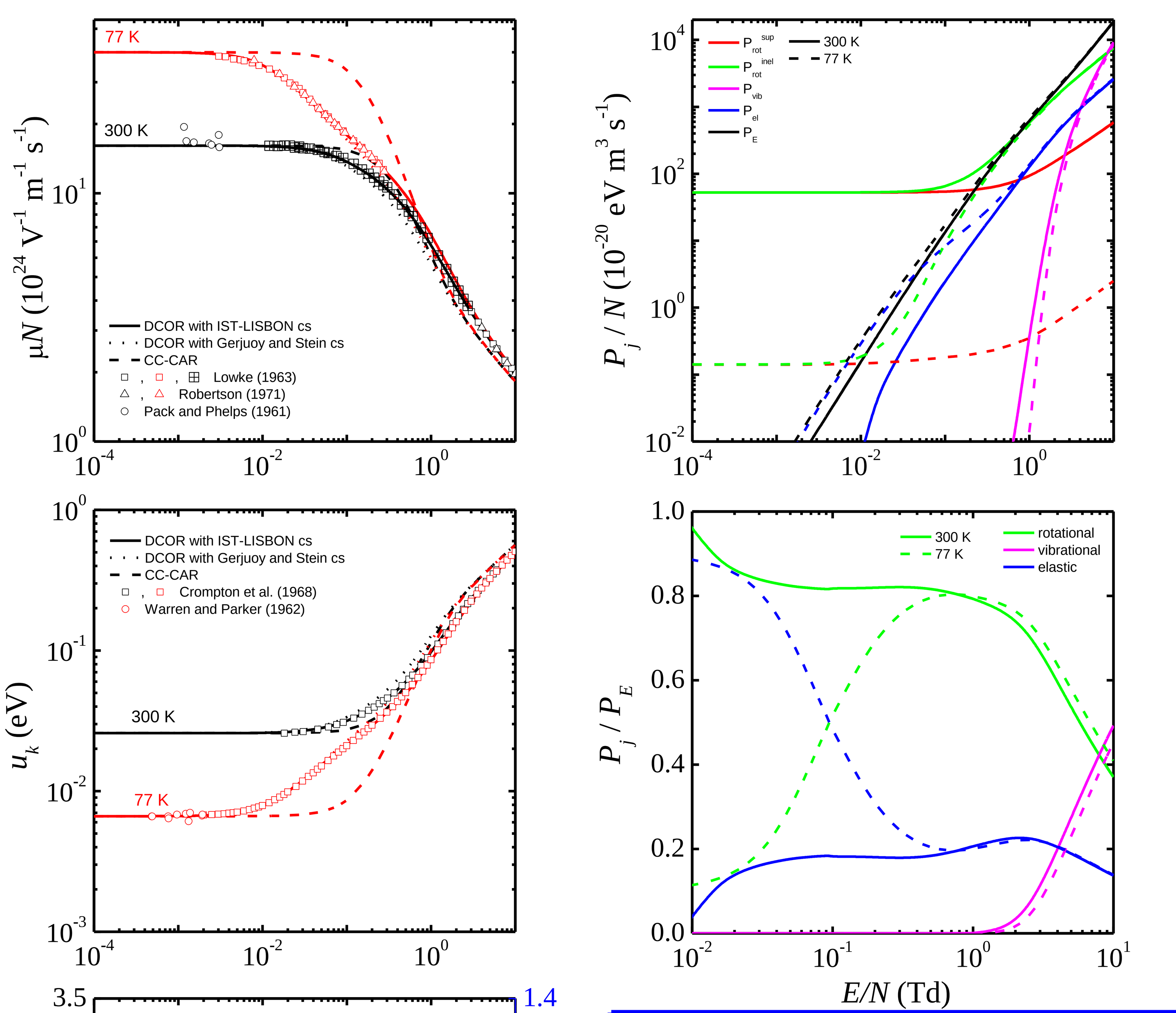
NITROGEN

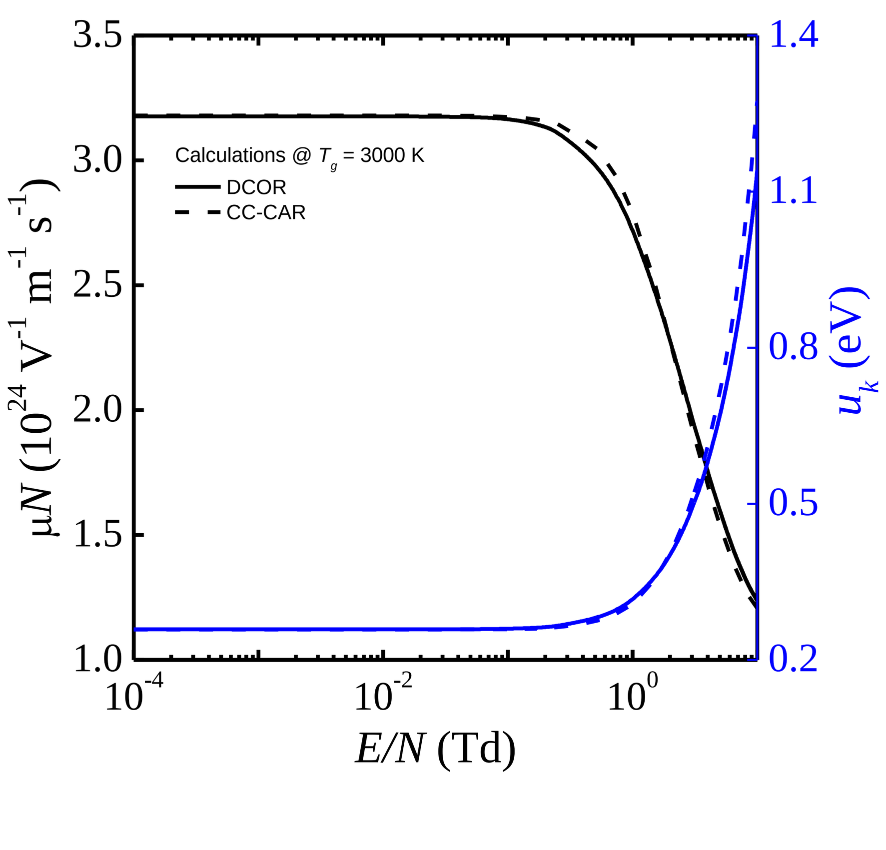


OXYGEN



HYDROGEN





CONCLUSIONS

For N_2 and O_2 very good swarm predictions (within experimental uncertainty) are obtained using both DCOR, with BA cross sections, and CC-CAR. For N_2, the BA cross sections fail to correctly describe the energy exchanges. For H_2, only DCOR with accurate cross sections gives satisfactory results. Moreover, CC-CAR fails below 1 Td, though yielding correct limiting values at zero field.

Results confirm that CC-CAR works only in cases where many rotational levels are populated.

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