

Calculation of rate coefficients for electron capture in collisions of O^{2+} and N^{2+} ions with H.

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ABSTRACT

We present calculations of electron capture cross sections in collisions of O^{2+} and N^{2+} with $H(1s)$ for impact energies $0.001\text{eV} < E < 10\text{keV}$ and the corresponding rate coefficients for temperatures $10^2\text{K} < T < 10^5\text{K}$. Our molecular close-coupling treatment leads to significant differences with the capture rates usually employed in the modeling of astrophysical plasmas.

Subject headings: Atomic data, atomic processes

1. Introduction

Electron capture (EC) reactions are important processes in astrophysical plasmas (Pequignot 1980a). In particular, EC between low charge state ions and H is relevant in HII regions and planetary nebulae (Pequignot 1980b; Rodríguez-Gaspar and Tenorio-Tagle 1998; Aannestad and Emery 2001; Simpson et al. 2004; Wood et al. 2004), and has been proposed as a heating mechanism in photoionized nebulae (Kingdon and Ferland 1999). On the other hand, EC has been recently suggested as the source of X-ray and far-ultraviolet emission from cometary atmospheres (Lisse et al. 2001), where the emission is produced when multicharged ions of the solar wind capture electrons from atmospheric atoms or molecules, leading to excited states, which subsequently decay through photon emission. A similar mechanism explain the X-ray emission from planetary atmospheres (Liu and Schultz 1999).

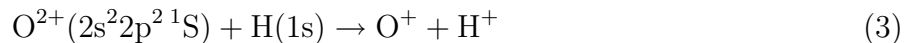
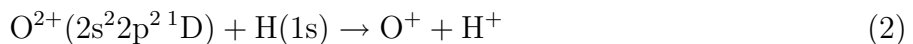
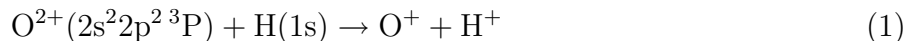
EC cross sections at low energies are currently measured by applying the merged beam technique (Havener 2003). At $E > 100\text{ eV/amu}$, crossed-beam photon emission spectroscopy or translational energy spectroscopy are used ((Bodewits et al. 2004a,b) and references therein). Rate coefficients for charge transfer between multiply charged ions and He have been measured in ion traps ((Fang and Kwong 1997) and references therein), but EC rate coefficients employed in Astrophysics are usually obtained theoretically. In particular, rate

coefficients for ion-H charge transfer reactions tabulated by Kingdon and Ferland (1996) were generally obtained by applying the Landau-Zener formula, although a few of them (Forster et al. 1991; Honvault et al. 1995; Herrero et al. 1995) were calculated by employing *ab initio* techniques to evaluate the potential energy curves and non-adiabatic couplings. The data of Kingdon and Ferland (1996) are currently included in the CLOUDY program (Ferland et al. 1998), which is widely employed for modeling astrophysical plasmas. More recently, cross sections and rate coefficients for charge transfer between singly charged ions and H have been evaluated by Stancil et al. (1998) and Stancil et al. (1999).

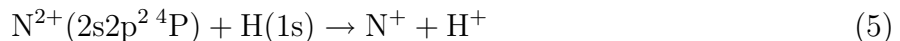
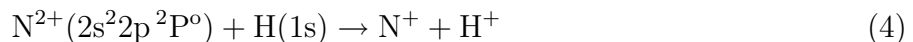
In this work, we present calculations of rate coefficients for EC in collisions of O^{2+} and N^{2+} with $H(1s)$. We employ the close-coupling expansions of Cabello et al. (2003) and Barragán et al. (2004) in terms of state-of-the-art (multireference configuration interaction) molecular wavefunctions. In those works significant differences were found with previous ones for EC cross sections at impact energies $E > 200$ eV/amu. In this paper we have extended our calculations to lower energies in order to obtain the corresponding rate coefficients. We have also evaluated the rate coefficients for EC from metastable species O^{2+} ($2s^2 2p^2 \ ^1D$), O^{2+} ($2s^2 2p^2 \ ^1S$) and N^{2+} ($2s 2p^2 \ ^4P$), since these processes might influence the populations of the excited levels, and the emission from these metastable states is often employed, in particular from O^{2+} metastable states, to determine temperature, density (Crawford et al. 2000) and abundances (see e.g. (Mathis and Liu 1999; Pilyugin 2000; Kwitter and Henry 2001)) of heavy elements in ionized nebulae. On the other hand, doubly charged ions are found inside the cometopause (Bodewits et al. 2004b), as a result of successive electron capture processes between ions and cometary atoms and molecules, where metastable ions can be formed.

2. Calculations

In the present work we report rate coefficients for the reactions



and



Details of the calculation procedure will be presented elsewhere Barragán et al. (2005); it involves the use of a molecular close-coupling expansion with a semiclassical eikonal approach

at impact energies $E > 250$ eV/amu, and a quantal treatment for lower energies. In the present work we have extended previous calculations to low energies that are critical in the evaluation of rate coefficients at $T < 10^5$ K. In general, the calculation of EC cross sections at low energies requires the use of very precise molecular wavefunctions, and a quantal treatment for the dynamics, including reaction coordinates (see Delos (1981) and references therein) to ensure that the expansion fulfills the collision boundary conditions. We have evaluated the molecular wavefunctions by applying a multireference configuration interaction treatment by means of the program MELD (Davidson 1990). In this method we construct a basis of configurations by allowing single and double excitations from a set of reference configurations; these are antisymmetrized products of molecular orbitals, which are linear combinations of Gaussian type orbitals. In short, our calculations have improved the previous ones in two aspects:

1. We have included a larger molecular set than previous calculations. In particular, for $O^{2+} + H$, our expansion includes all molecular states correlating to the 10 most important atomic states, while that of Honvault et al. (1994) included 5 atomic channels. In $N^{2+} + H$, Bienstock et al. (1986) used a two-state expansion and Herrero et al. (1995) only considered triplet states. This extension is critical for collision energies $E > 250$ eV/amu.
2. We have improved the electronic structure calculation in order to describe with similar accuracy ($\simeq 10^{-2}$ Hartree) all molecular states, which is crucial to ensure the accuracy of our results at low energies.

3. Discussion and conclusions.

In fig. 1 we compare our cross sections for reaction (1) with previous values of Heil et al. (1983) and Honvault et al. (1995). The shape of our cross section is different from that of Honvault et al. (1995) as a consequence of the different energy gap in the avoided crossing regions. In particular, for the $^4\Pi$ subsystem, we obtain a minimum energy difference of $\Delta E = 0.41$ eV at $R_0 = 4.57 a_0$, while the value of Honvault et al. (1995) is $\Delta E = 0.102$ eV at $R_0 = 4.5 a_0$. Our cross sections are closer to those reported by Heil et al. (1983) in the region $1 < E < 10$ eV, where we obtain a plateau that was not found in the calculation of Honvault et al. (1995). For $E < 0.1$ eV, our cross section rapidly increases, as expected from the Langevin model (see (Pieksma et al. 1996) and references therein). Sharp peaks are also noticeable that are due to shape resonances in the entrance channel potential.

Our rate coefficients for reaction (1) (fig.2 and table 1) show good agreement with

those of Butler et al. (1980) (based on the cross section reported by Heil et al. (1983)). On the other hand, the rate coefficients of Honvault et al. (1995) exhibit large values at $T < 2 \times 10^4\text{K}$, being a factor of two larger than ours at $T = 10^4\text{K}$. The comparison of our results with previous ones illustrates the sensitivity of the rate coefficients for reaction (1) to the potential energy curves. In particular, while Honvault et al. (1994) employed a larger molecular expansion than those of Heil et al. (1983), their potential energy curves were less accurate in the avoided crossing region. Our large-scale calculation supports the rate coefficients of Butler et al. (1980) for $T < 10^4\text{K}$, which is relevant, since the program CLOUDY currently includes the rate coefficients of Honvault et al. (1994). At higher T we have found some deviations from the results of Butler et al. (1980), which may be relevant in modeling the precipitation of ions in planetary atmospheres. At low energies, our calculation points to a significant contribution to the EC reactions of resonant processes, and therefore we expect that radiative EC becomes relevant ((Rittby et al. 1984), (Zygelman et al. 1989)), which probably limits the application of our rate coefficients at low temperatures.

In order to evaluate the rate coefficient for reaction (4), we have recalculated the corresponding cross section (figure 3), and we have found that the maximum at $E \simeq 0.3\text{ eV}$, reported by Herrero et al. (1995), and also found in our previous calculation (Barragán et al. 2004), has disappeared in our new calculation that yields a Langevin-type increase of the total cross section, previously found for other collisions (Pieksma et al. 1996; Lee et al. 2003) at $E < 0.2\text{ eV}$. As explained in (Barragán et al. 2005), the main difference between previous and new calculations is a more dense grid of molecular energy data at high internuclear separations, which in our previous calculation, and probably in that of Herrero et al. (1995), led, after interpolation and integration of radial couplings, to a spurious energy barrier of about 0.1 eV . The new calculation yields EC cross sections very similar to the two-state cross sections of Bienstock et al. (1986) for $E \lesssim 40\text{ eV}$, and accordingly, our rate coefficients (table 2 and fig. 4) agree with the values reported by Herrero et al. (1995) and evaluated from the cross sections for populating $\text{N}^+ (2s2p^3\ ^3\text{D}^\circ)$ of Bienstock et al. (1986).

With respect to collisions with metastable species, our cross sections for reactions (2)-(3) are of the same order of magnitude as those for reaction (1), while the calculations of Honvault et al. (1995) (not shown in fig. 1) yielded values smaller than 0.02 \AA^2 . These new results have led us to evaluate the rate coefficients for these two processes (see table 1 and fig.2), which are similar to those for reaction (1). We have also considered EC reactions with the metastable state $\text{N}^{2+}(2s2p^2\ ^4\text{P})$. In contrast with previous results, we have found that they are fast reactions in both systems. To gauge the importance of reactions involving ions in metastable states, we consider the particular case of reaction (2), with a rate constant of about $2 \times 10^{-9}\text{ cm}^3\text{ s}^{-1}$. Since the radiative emission coefficient for this state is $\simeq 2 \times 10^{-2}\text{ s}^{-1}$ (Physical Reference Data, National Institute of Standards and Technology; <http://physics.nist.gov>),

a hydrogen number density of 10^7cm^3 is required to make process (2) competitive. We conclude that, this reaction will not take place in ionized nebulae, but it might be significant in planetary atmospheres (Krasnopolsky and Gladstone 1996; Barabash et al. 2002; Gunell et al. 2005).

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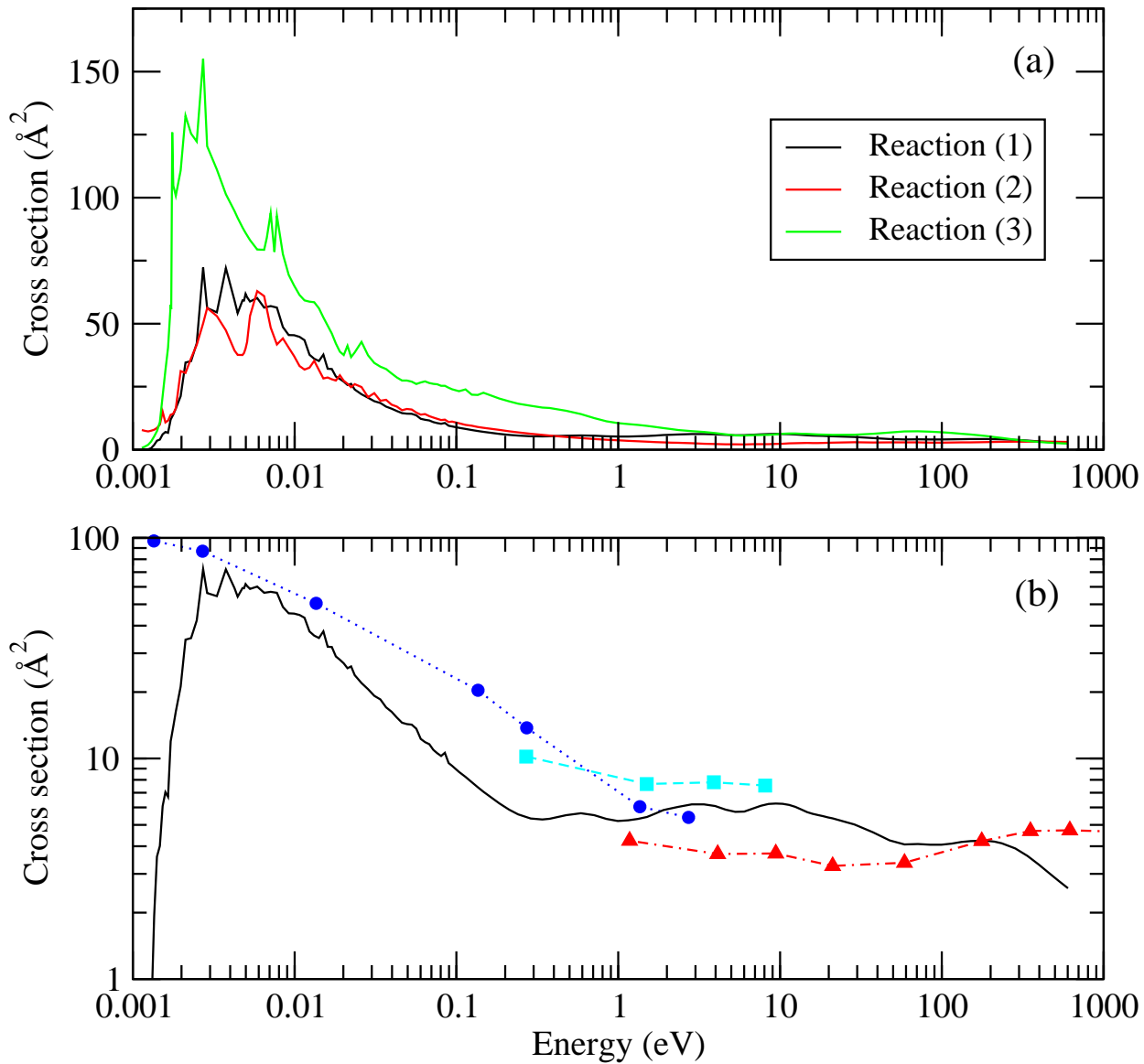


Fig. 1.— (a) Total cross sections for reactions (1)-(3) as indicated in the figure. (b) Comparison between total EC cross section for reaction (1) with previous results: Full line, present results; $\cdots\bullet\cdots$, (Honvault et al. 1995); $-\square--$, (Heil et al. 1983); $-\blacktriangle-$, (Honvault et al. 1994)

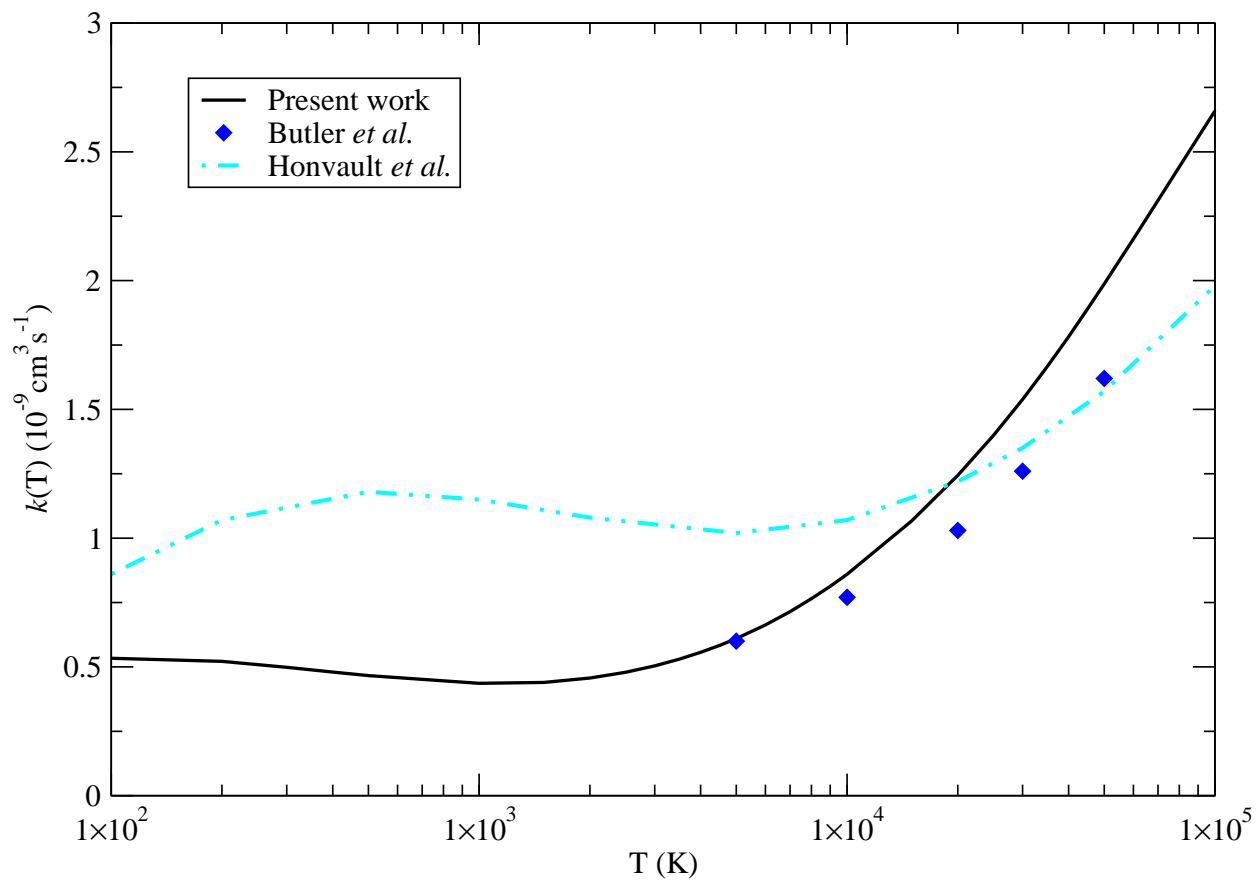


Fig. 2.— Rate coefficients for reaction (1) as functions of the temperature compared to previous results of , Butler et al. (1980) and Honvault et al. (1995) .

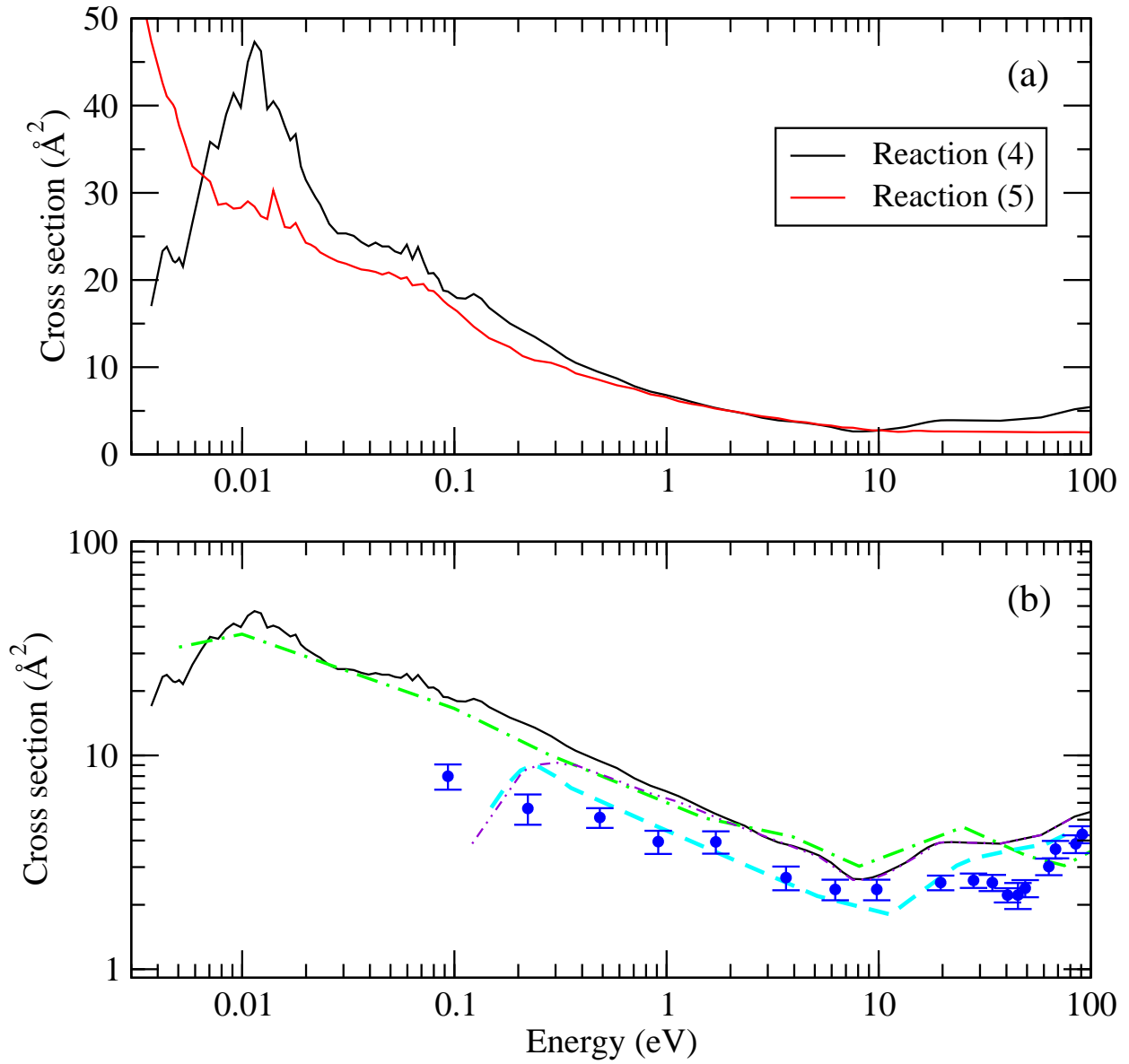


Fig. 3.— (a) Total cross sections for reactions (4) and (5) as indicated in the figure. (b) Comparison between total EC cross section for reaction (4) with previous results. Experimental results: \bullet , Pieksma et al. (1997). Theoretical values: $-\cdot-\cdot-$, (Herrero et al. 1995); $-\cdot-\cdot-$, (Bienstock et al. 1986); $-\cdot-\cdot-$, (Barragán et al. 2004).

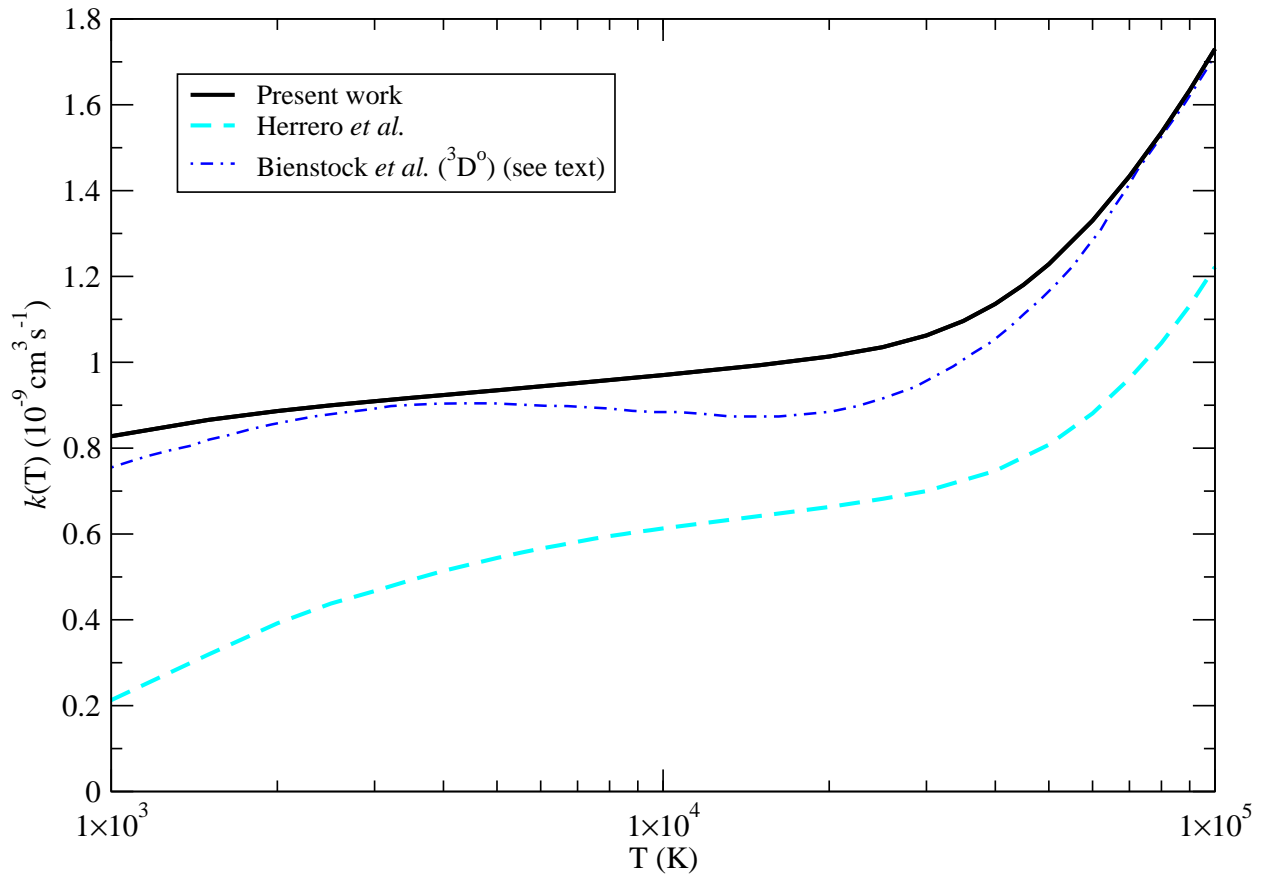


Fig. 4.— Rate coefficients for reaction (4) as functions of the temperature. Previous results: $-\cdot-$, Rate coefficients evaluated by Herrero et al. (1995) from the EC cross sections of Bienstock et al. (1986); $- - -$, Herrero et al. (1995).

Table 1: Rate coefficients in $10^{-9}\text{cm}^3\text{s}^{-1}$ for reactions (1)-(3).

T (K)	k_1	k_2	k_3
100	0.53362	0.47935	0.85536
200	0.52153	0.50734	0.88203
300	0.49852	0.50876	0.90861
400	0.48016	0.50603	0.93893
500	0.46613	0.50279	0.96914
1000	0.43607	0.49305	1.09377
1500	0.43975	0.49064	1.18063
2000	0.45679	0.49104	1.24293
2500	0.47931	0.49279	1.28948
3000	0.50418	0.49527	1.32588
4000	0.55659	0.50131	1.38078
5000	0.60995	0.50790	1.42213
6000	0.66288	0.51455	1.45569
7000	0.71464	0.52104	1.48417
8000	0.76481	0.52733	1.50904
9000	0.81319	0.53341	1.53125
10000	0.85973	0.53933	1.55146
20000	1.24359	0.59893	1.71265
30000	1.53854	0.67074	1.87392
40000	1.78217	0.75305	2.04607
50000	1.98734	0.83939	2.21775
60000	2.16168	0.92544	2.38288
70000	2.31143	1.00914	2.54045
80000	2.44169	1.08976	2.69159
90000	2.55653	1.16713	2.83780
100000	2.65907	1.24133	2.98038

Table 2: Rate coefficients in $10^{-9}\text{cm}^3\text{s}^{-1}$ for reactions (4) and (5).

T (K)	k_4	k_5
100	0.46312	0.41483
200	0.59312	0.50366
300	0.65966	0.56116
400	0.70483	0.60055
500	0.73830	0.62854
1000	0.82782	0.70016
1500	0.86587	0.73618
2000	0.88640	0.76151
2500	0.89963	0.78166
3000	0.90935	0.79863
4000	0.92378	0.82652
5000	0.93484	0.84914
6000	0.94395	0.86820
7000	0.95174	0.88465
8000	0.95857	0.89912
9000	0.96469	0.91202
10000	0.97027	0.92368
20000	1.01334	1.00425
30000	1.06250	1.06181
40000	1.13596	1.11869
50000	1.22873	1.17615
60000	1.33023	1.23110
70000	1.43343	1.28235
80000	1.53502	1.33028
90000	1.63390	1.37577
100000	1.73000	1.41968