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Fine-structure Excitation of O(^{3}P) Induced by Collisions with Atomic Hydrogen

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Abstract

The utility of the far-infrared lines of oxygen as diagnostics of gas outflows and for other applications depends on accurate descriptions of the rate coefficients for excitation (and relaxation) through collisions with electrons and with hydrogen atoms. For O and H collisions, earlier calculations of rate coefficients show discrepancies leading to ambiguity in astrophysical applications. In this note we introduce a methodology that yields consistent sets of rate coefficients for a number of cases. We then apply our method to the O–H system in order to investigate the discrepancies. The present rate coefficients will be of particular interest for modeling observations of astrophysical environments in the far-infrared.

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1. Introduction

The spectral lines of oxygen atoms OI at wavelengths of 63 and 145 μm are of particular interest for observation in the far-infrared, where they serve as probes of warm gas in, for example, outflows from protostars. Fine structure changing collisions between atomic hydrogen and oxygen may lead to excitation, which becomes an important cooling process through the subsequent photon emission. There is an outstanding discrepancy between prior calculations on the inelastic collisional processes

$$\mathrm{O}(^3\mathrm{P}_j) + \mathrm{H}(^2\mathrm{S}) \rightarrow O(^3\mathrm{P}_{j'}) + \mathrm{H}(^2\mathrm{S}), \qquad (1)$$

where (j, j') can be (2,1), (2,0), or (1,0), which has led to some ambiguity in the choice of sets of rate coefficients to use for astrophysical applications, see for example, Lebouteiller et al. (2017, footnote 7). Launay & Roueff (1977) used a quantum close-coupling method

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to obtain the fine-structure excitation transition rate coefficients though the interaction potentials used were unrefined by today's standards. Now, the interaction potentials are known accurately so it is significant that discrepancies remain. The rate coefficients were revisited by Abrahamsson et al. (2007) and Vieira & Krems (2017) who used the more accurate interaction potentials computed by Parlant & Yarkony (1999). More recently, with the potentials that were reported by Dagdigian et al. (2016), Lique et al. (2018) gave calculations of the relaxation rate coefficients. In this note we argue that the differences cannot arise from the potential energies nor from the different formulations of the scattering theory.

2. Scattering Calculations

Here we present our calculations on the rate coefficients of fine-structure excitation for the O–H system. The scattering calculations were performed using a Python code, which we wrote based partially on the Molcol FORTRAN code (Flower et al. 2019) utilizing Johnsons multichannel logarithmic derivative algorithm. The calculations were based on the theoretical quantum description of a collision between two open-shell atoms in arbitrary angular momentum states derived by Krems et al. (2006). The present Python code was used to calculate the rate coefficients for the C^+–H, the Si^+–H and the C–H systems; in all three cases the results were in very good agreement with the preceding calculations when we used the potential energy data of the original sources. Moreover, where cross sections were available for comparison the agreement was also excellent.

Having established the reliability of our theory and code, the cross-sections for process(1) were computed for total energies up to 10,000K. The corresponding excitation rate coefficients were computed for temperatures up to 1000K by averaging over a Maxwellian velocity distribution. Figure 1 presents the rate coefficients for the fine-structure excitation of O in collisions with H as a function of temperature; the different colors label the different transitions $(j \rightarrow j')$. The dots are the published data of Launay & Roueff (1977). Although not shown on the figure, we reproduced almost exactly their results with the present code and their potentials. The dashed lines are the corrected results of Lique et al. (M.Wolfire, private communication), which are available as relaxation rate coefficients in the Moldata https://home.strw.leidenuniv.nl/~moldata/datafiles/oatom@lique.dat database(Schöier et al. 2005). We used detailed balance to obtain excitation rate coefficients. The solid lines

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are the present calculations using the same potentials as Liqueet al. The present calculations are generally in harmony with the other results; the differences between our calculations and those of Liqueet al. may arise from their inclusion of off-diagonal fine structure couplings(Parlant & Yarkony 1999), which we omit. In turn, the discordance between the rate coefficients of Liqueet al. and of Vieira & Krems (2017), see for example (Lique et al. 2018, Table 2), may arise from their specific treatments of the off-diagonal couplings. A detailed analysis is being carried out.

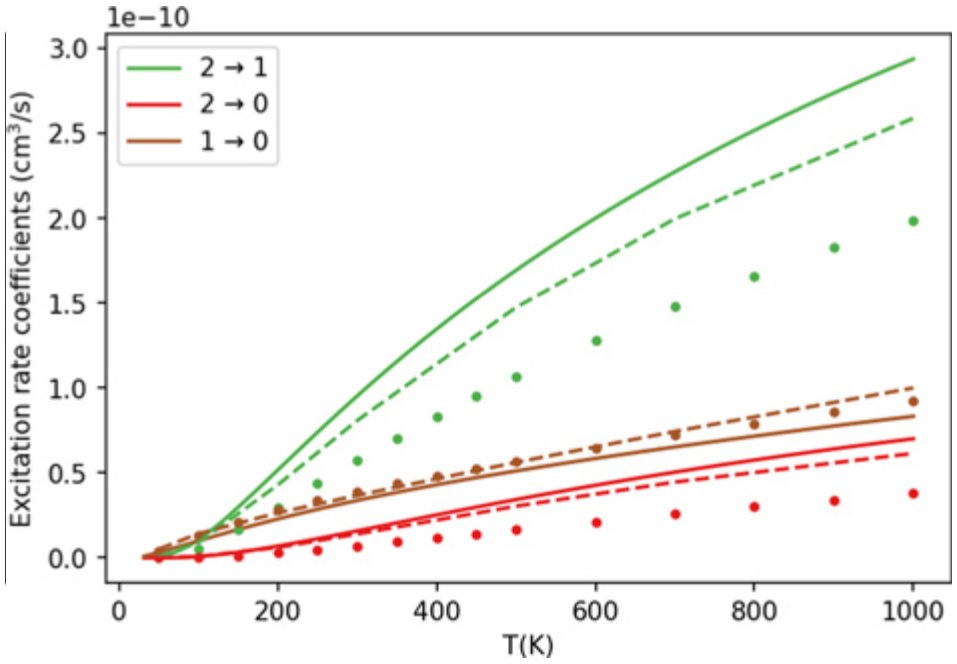

Figure 1. Temperature dependent rate coefficients for fine-structure excitation of O in collision with H. The dots are the results of Launay & Roueff (1977). The dashed lines are the rate coefficients reported by Lique et al. in the Moldata https://home.strw.leidenuniv.nl/~moldata/datafiles/oatom@lique.dat database. The solid lines are the present calculations. The three transitions $(j \rightarrow j')$ are labeled with different colors.

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Software: Molcol (Flower et al. 2019), NumPy (van der Walt et al. 2011), SciPy (Virtanen et al. 2020), Matplotlib (Hunter 2007).

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