A reinvestigation on the energy levels of CO2 up to the dissociation limit

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The energy levels of the radiative states of CO2 have been extensively studied, and several very accurate databases such as HITRAN/HITEMP or CDSD exist in the literature. However, knowledge on the near-dissociation levels of CO2 is lacking due to the absence of experimental data, or the fact that transitions from these higher-lying levels are hidden by the strongest transitions of lower levels. This study proposes to achieve a better prediction of these states through potential reconstruction methods.

1. Introduction

State-to-state modelling of CO2 vibrational excitation processes is a current "hot-topic" in view of such diverse applications like plasma reforming of CO2 [1] and the modelling of atmospheric entries in Mars and Venus [2]. Typical modelling activities have thus far delved on the legacy from state-to-state modelling of atomic and molecular diatomic plasmas, with preliminary simulations being rather successful in reproducing experimental data. Indeed, the treatment of such a triatomic molecule like CO2 may be simplified with some baseline assumptions like the separability of its three internal modes and the determination of its levels up to dissociation through polynomial models [1]. However, if the accuracy of such approaches is to be increased, improved methods for the calculation of the overall manifold of vibrational levels needs to be achieved, based on potential reconstruction techniques.

2. Potential reconstruction methods

Lower-lying levels of CO2 are accurately described to the 10^{-2} cm^{-1} by such databases like HITRAN [3] or CDSD [4]. From these extensive databases of levels, potential reconstruction methods have been developed by Huang et al. at NASA Ames to determine an accurate potential curve up to 25,000 cm^{-1} [5]. Examples for the assymmetric stretch and bending modes of CO2 are fresented in Fig. 1. This potential curve serves as the baseline for this work. Here we will present an adequate extrapolation of the 3 modes of CO2 up to the dissociation limit by adequate long-range potentials. Near-dissociation levels will then be determined by solving the adequate radial Schrödinger equation on such potentials. The resulting extrapolated levels will follow a smoother and more realistic distribution up to the dissociation limit than the traditional polynomial expansions.

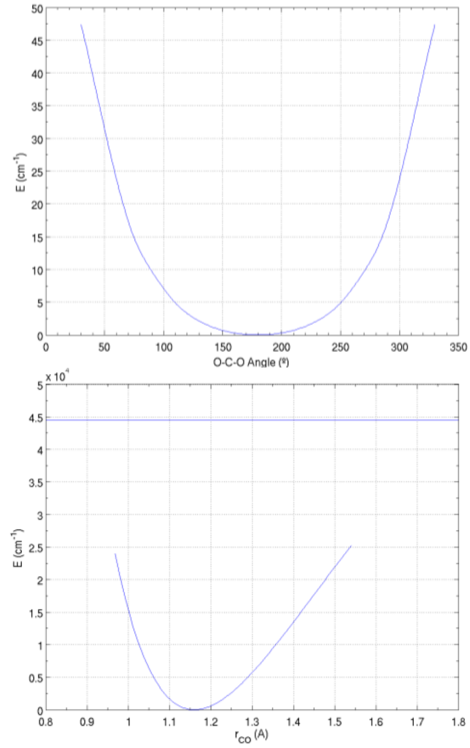

Fig 1: Asymmetric stretch and bending energies of CO2

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3. References

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