

Line-Mixing Relaxation Matrix model for spectroscopic and radiative transfer studies

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We present a generic model to compute the Relaxation Matrix easily adaptable to any molecule and type of spectroscopic lines or bands in non-reactive molecule collisions regimes. It also provides the dipole moment of every transition and level population of the selected molecule. The model is based on the Energy-Corrected Sudden (ECS) approximation/theory introduced by DePristo (1980), and on previous Relaxation Matrix studies for the interaction between molecular ro-vibrational levels (Ben-Rueven, 1966), atoms (Rosenkranz, 1975), linear molecules (Strow and Reuter, 1994; Niro, Boulet and Hartmann, 2004), and symmetric but not linear molecules (Tran et al., 2006).

The model is open source, and it is user-friendly. To the point that the user only has to select the wished molecule and vibrational band to perform the calculations. It reads the needed spectroscopic data from the HIGH-resolution TRANsmission molecular absorption (HITRAN) (Rothman et al., 2013) and ExoMol (Tennyson and Yurchenko, 2012).

In this work we present an example of the calculations with our model for the case of the $2\nu_3$ band of methane (CH₄), and a comparison with a previous work (Tran et al., 2010).

The data produced by our model can be used to characterise the line-mixing effects on ro-vibrational lines of the infrared emitters of any atmosphere, to calculate accurate absorption spectra, that are needed in the interpretation of atmospheric spectra, radiative transfer modelling and General Circulation Models (GCM).

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