AB INITIO CALCULATIONS OF QUANTUM SCATTERING AND LINE-SHAPE PARAMETERS IN O_2 PERTURBED BY N_2

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The study and modelling of the N_2-perturbed lines in O_2 is of great importance for Earth's atmosphere studies. However, collisional systems with the ground-state molecular oxygen, O_2 ($X^3\Sigma_g^-$), either as perturbing or active molecule, are difficult to handle because of its non-zero spin that needs to be taken into account in the description of quantum scattering. Here, we present the methodology as well as the results of our quantum scattering calculations and the line-shape parameters for the O_2 immersed in molecular nitrogen bath. It is the first theoretical *ab initio* investigation of this collisional system in the context of the shapes of molecular lines. The PES for this study was constructed automatically using the AUTOSURF code [a]. The data provided through this investigation is important for the terrestrial atmospheric measurements and can be used for populating the spectroscopic databases such as HITRAN or GEISA.

[a] Quintas-Sánchez, Ernesto, and Richard Dawes. "AUTOSURF: A freely available program to construct potential energy surfaces." Journal of chemical information and modeling 59, no. 1 (2018): 262-271