THE $\widetilde{X}\,^2A_1 - \widetilde{A}\,^2B_2$ CONICAL INTERSECTION IN NO_2, OR HOW EXPERIMENTS AND THEORY INTERPLAY TOGETHER

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We present a comparison between experimental results (vibronic energies, absorption and LIDFS intensity ratios, rotational constants) and ab-initio calculations (diabatic and adiabatic energies, vibronic matrix elements). The three main inputs required in the analysis of the $\widetilde{X}\,^2A_1 - \widetilde{A}\,^2B_2$ conical intersection are: i) the diabatic levels of the $\widetilde{X}\,^2A_1$ state (*i.e.*, the complete set of approximatively 200 low lying levels of the $\widetilde{X}\,^2A_1$ observed by LIDFS), ii) the diabatic levels of the $\widetilde{A}\,^2B_2$ state (they are approximately predicted by the ab-initio calculations), iii) the matrix elements of the vibronic interaction, V_{12}, between the $\widetilde{X}\,^2A_1$ and $\widetilde{A}\,^2B_2$ electronic states. The validity of the simplified form proposed for V_{12}, namely "λQ_3", will be discussed. The comparison allows to assign some observed vibronic levels, which in return can be used to improve some parameters of the initial ab-initio PESurfaces. Up to now, our analysis is limited to the four lowest polyads of the $\widetilde{A}\,^2B_2$ state ranging from $9700\,\mathrm{cm}^{-1}$ to $12300\,\mathrm{cm}^{-1}$. At higher energy the interactions are stronger, leading to vibronic chaos above $\sim 17000\,\mathrm{cm}^{-1}$.