Ab initio calculation of the photoabsorption cross section of NO_2 by the two-dimensional reflection method.

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The C_{2v} potential energy surfaces of the X^2A_1, A^2B_2 and B^2B_1 states of NO_2 are calculated at a high level of theory (CASSCF/CMRCI/cc-pVTZ), together with the corresponding dipole moment surfaces for the transitions $X-A$ and $X-B$. All surfaces are fitted to a quadratic polynomial form in the symmetric stretching and bending coordinates, around the equilibrium geometry of the ground state. These *ab initio* data are used to calculate the relative and absolute photoabsorption cross sections by applying the two-dimensional reflection method [a], modified for taking the quadratic form of the potential energy surfaces into account. The theoretical cross section is found in good agreement with the experimental spectrum. The sensitivity of the calculated cross section with the level of *ab initio* theory will be discussed.

[a] see R. Schinke, "Photodissociation dynamics", Cambridge University Press (1993).