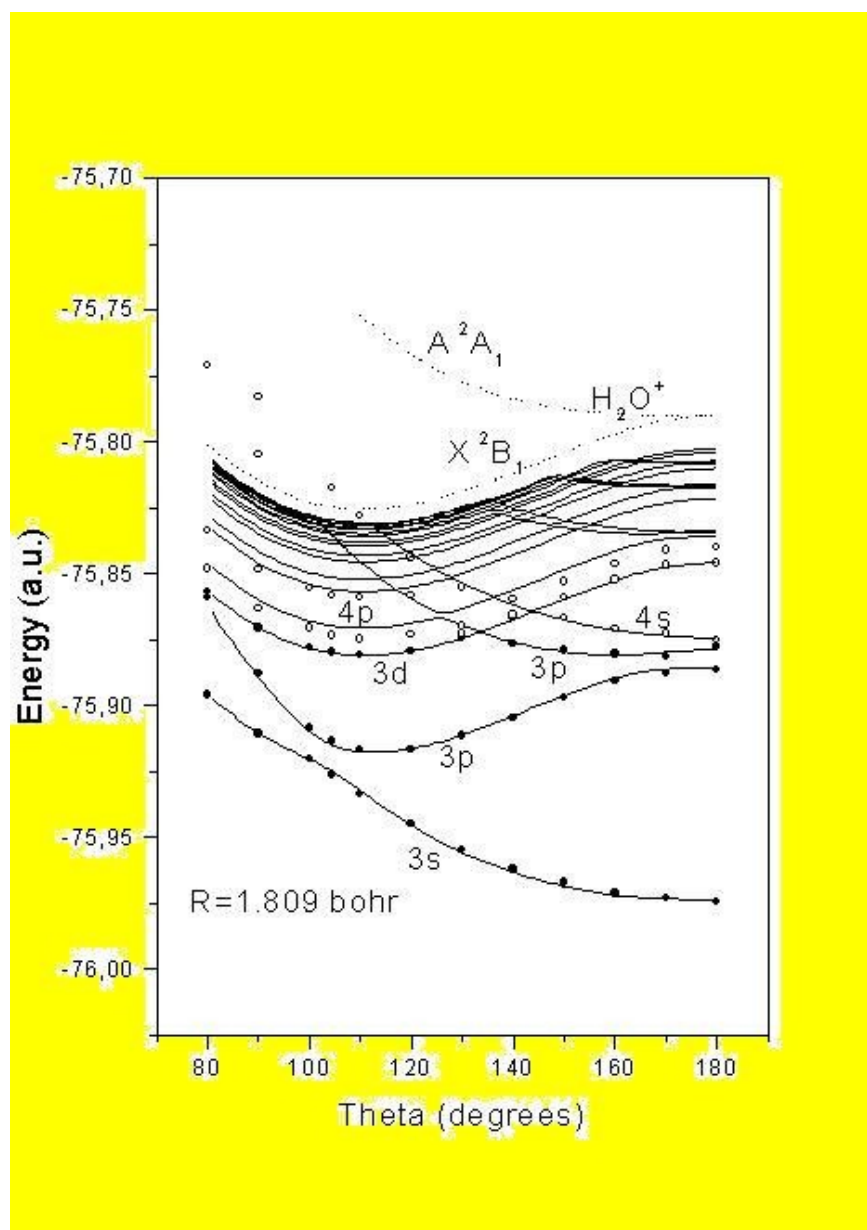


MQDT calculations- highly excited Rydberg states, vibrational autoionization

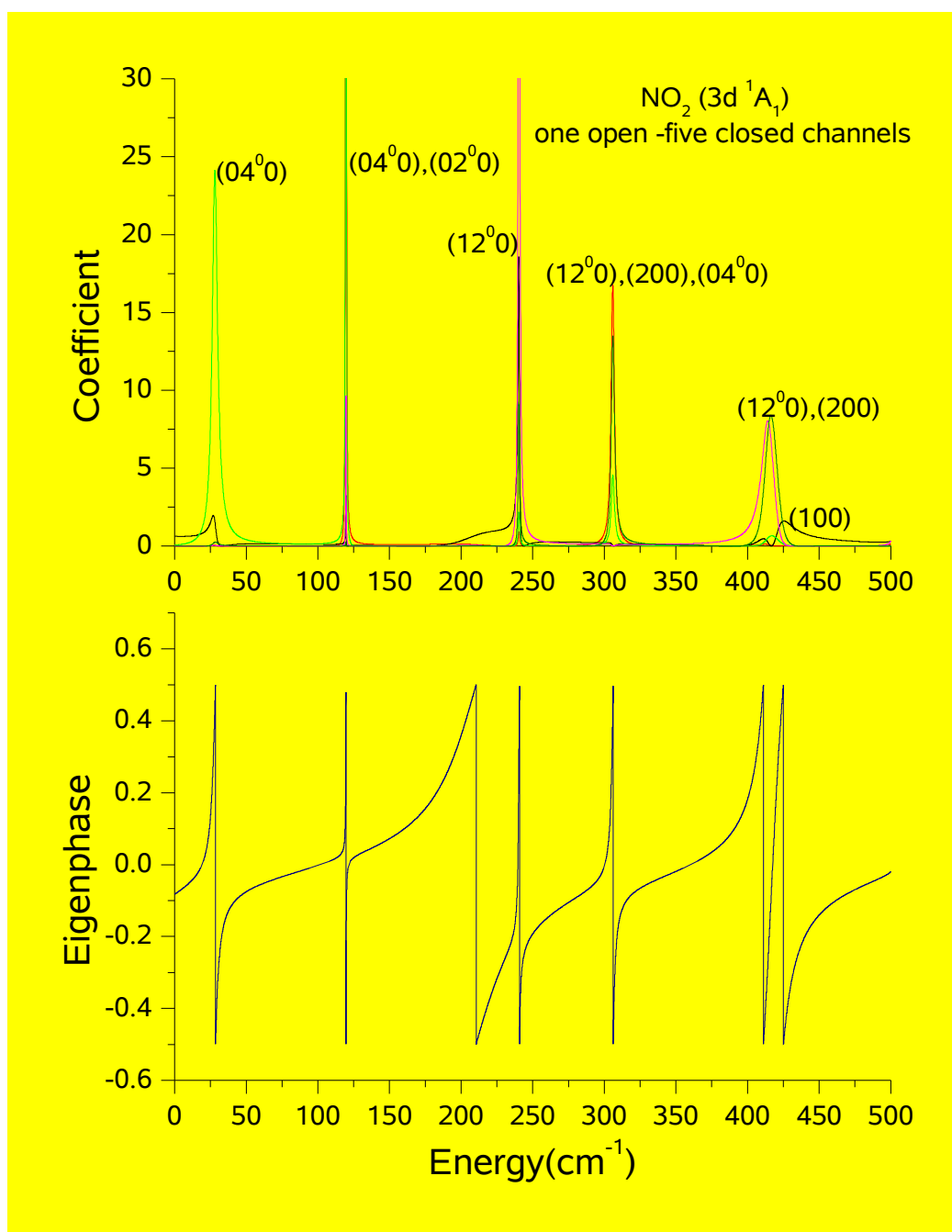
It is virtually impossible to calculate highly excited electronic states of molecules by ab initio methods. However, the ab initio data can form the basis for an extrapolation to the entire Rydberg spectrum of a molecule via Multi Channel quantum Defect Theory (MQDT). The scaling features of the MQDT theory lead to good approximations for the potentials of the whole manifold of states, from the lowest-lying ab initio potential energy surfaces,[1-5].

Rydberg states of 1A_1 symmetry generated from MQDT functions (solid lines) and from ab initio calculations (solid (for data employed in the fit) and open circles)



Vibrational perturbations in the Rydberg spectra as well as vibrational autoionization widths of levels of Rydberg states lying above vibrational levels of the ion, can be calculated from the quantum defect functions[6].

Autoionization of vibrational levels of the nd states of NO_2 , lying above the 000 level of NO_2^+



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