FIRST EXPERIMENTAL OBSERVATIONS WITH CROSSED BEAMS FOR THE Ti + NO → TiO + N AND Ti + O₂ → TiO + N REACTIONS AND AB INITIO POTENTIAL ENERGY SURFACES

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The experiment involved a pulsed supersonic beam of titanium atoms, pulsed effusive beam of NO and O₂ molecules and a pulsed tunable dye laser to probe TiO reaction product via laser-induced fluorescence and chemiluminescence. By seeding the titanium beam and by varying the angle of scattering, we have measured the height of reaction barriers with the ground state titanium atoms. In contrast, we did not observe any reaction barrier with the titanium atoms in the first excited state. Ab initio calculation has been done for a limited domain of the reaction coordinates to obtain the energy levels and the reaction barriers. The calculation also shows there are many intermediate states for the TiNO and TiO₂ molecules.