FIRST EXPERIMENTAL OBSERVATIONS WITH CROSSED BEAMS FOR THE Sc + NO \rightarrow ScO + N REACTION AND AB INITIO POTENTIAL ENERGY SURFACES

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The experiment involved a subsonic/supersonic beam of scandium atoms, an effusive beam of NO molecules and a cw tunable dye laser to probe ScO reaction product via laser-induced fluorescence. It is expected to determine the shape of ScO absorption profiles which reflects the angular probability of scattering in the center-of-mass and to measure the area of the profiles which leads to the reaction cross section. By seeding the scandium beam by various rare gases, it is possible to vary the kinetic energy of the system and to estimate the height of the reaction barrier and the energy balance of the reaction. Ab initio calculation has been done for a limited domain of the reaction coordinates to obtain the exothermicity and the reaction barrier. The calculation also shows there are many ScNO intermediate states.