Electronic Supporting Information

Rotationally Inelastic Scattering of Quantum-State Selected ND_3 with Ar

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1. Density-to-Flux Transformation

The density-to-flux conversion was carried out using two separate and independent computer programs to compute instrument functions by which the experimental images are divided. The IMSIM program of McBane[1] employs an iterative correction to the raw experimental images, whereas our adapted version of the program of Eyles and Brouard[2] uses a Monte Carlo method to simulate the effects of the experimental design on the preferential detection of certain subsets of the scattered ND_3.

In both cases, careful characterization of several features of the experiment was necessary to provide precise input parameters to the computer code. Fig. S1 shows that DCSs extracted by the Monte Carlo and IMSIM method are in very good agreement for all final levels shown. Such comparisons were also made for scattering of ND_3 into several other final levels and good agreement in all cases imparts confidence in the process for extraction of DCSs from the experimental images.

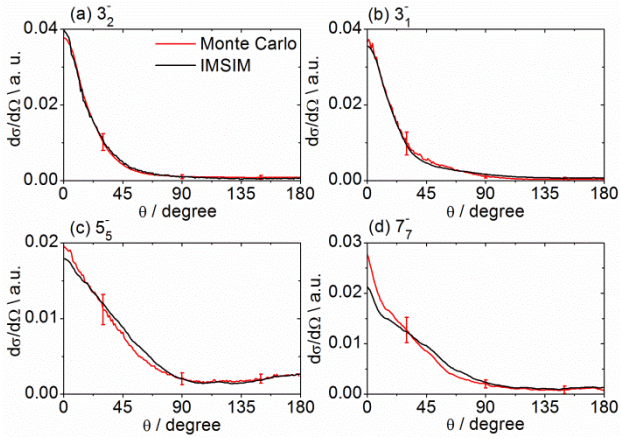

FIG. S1. Comparison of the DCSs extracted by the Monte Carlo and the IMSIM methods for inelastic scattering of initial-state selected (by a hexapole) ND_3 (1_1^-) with argon into several selected final states.

In addition, we verified that various measurements of images for a single final level yielded the same DCSs. Fig. S2 shows separately measured and uncorrected (for density to flux transformation) angular scattering distributions extracted directly from three different images measured for inelastic scattering of ND_3 with argon into the final level $j'^{\pm}_{k'} = 4_4^-$ under the same experimental conditions. The excellent agreement between these angular distributions indicates stable and reproducible measurement of images.

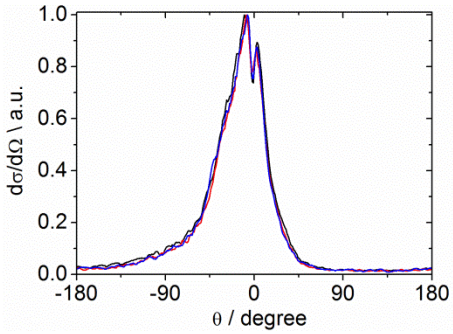

FIG. S2. Uncorrected angular scattering distributions extracted directly from three different images measured for inelastic scattering of ND_3 with Ar into the $j'^{\pm}_{k'} = 4^-_4$ final state under the same experimental conditions.

2. Velocity Map Images

Fig. S3 shows velocity map images for ND_3 – Ar collision experiments with hexapole state selection to prepare ND_3 (1^-_1) molecules seeded in Kr. The collision energy is 310 ± 30 cm^{-1}. Velocity map images were also measured for ND_3 – Ar collisions without use of the hexapole filter. Images for scattering into final levels with j' = 2 and 3 are shown in Fig. S4.

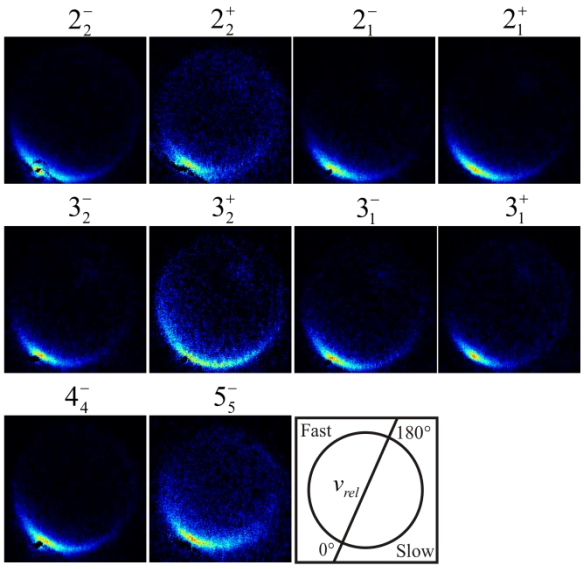

FIG. S3. Velocity map images for inelastic scattering of $ND_3(1^-_1)$ with Ar. The ND_3 was prepared by supersonic expansion of a dilute mixture in Kr and state selected using a hexapole filter prior to collision with the Ar beam. The collision energy was 310 ± 30 cm^{-1}.

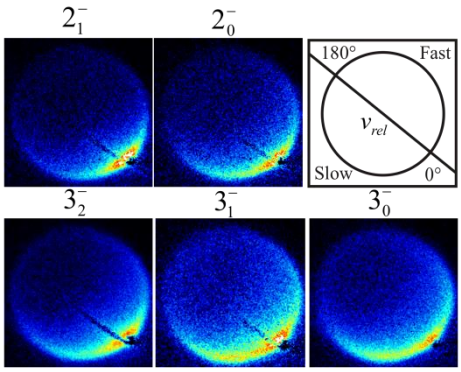

FIG. S4. Experimental velocity map images for the crossed molecular beam scattering of ND_3 (seeded in Ar) with Ar. The ND_3 was cooled in a supersonic expansion prior to collision with Ar, but was not further state-selected by a hexapole filter. The collision energy was 415 ± 40 cm^{-1}.

References

1. McBane, G. C. *Simulation of Crossed Beam Images (in Imaging in Chemical Dynamics)*. ACS Books: 2001.
2. Eyles, C. J. An Experimental and Theoretical Study of the Dynamics of Atom-Molecule Scattering. D. Phil., University of Oxford, 2010.