Magnetic Manipulation of Rotational Orientation Projection States in Ground State Molecules

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INTRODUCTION

Creating spatially anisotropic samples of gas phase molecules to study steric effects in gas-surface collisions has been typically limited to those that can be prepared by laser excitation1 or to paramagnetic molecules2. Here we present a recently developed technique3 which can be used to prepare and manipulate the rotational orientation and nuclear spin projection states of ground-state molecules. We will also show a summary of the results from the first application, the extraction of a scattering matrix for H2 scattering from LiF(100)4. These results will provide extremely stringent benchmarks which will help develop and benchmark accurate theoretical models.

EXPERIMENTAL SETUP

Hexapoles

The hexapoles create an inhomogeneous magnetic field that focusses low field seeking and defocusses high field seeking states. In the case of ortho-H2 (below), m1 = -1 is focussed and m1 = 1 defocussed.

Solenoids

The (H21) molecules precess in the applied homogeneous magnetic field at a frequency determined by the (Ramsey) Hamiltonian, given by3:

\[
\frac{\mathcal{H}}{\hbar} = -c \cdot \mathbf{I} \cdot \mathbf{B} - c \cdot \mathbf{J} \cdot \mathbf{B} - c \cdot \mathbf{J} \cdot J + d \left(3 \mathbf{I} \cdot \mathbf{J}^2 + \frac{3}{2} \mathbf{I} \cdot \mathbf{J} \cdot J - J^2 \mathbf{I}^2 \right)
\]

Signal calculation

The signal is the overlap integral of the wavefunction for each individual m1, m0 state at the detector with itself, weighted by the hexapole probabilities and summed over the velocity distribution of the molecular beam.

DETERMINING A SCATTERING MATRIX

H2 SCATTERING FROM LiF(100)4

The scattering matrix characterises how the wavefunction changes when the molecules scatter from the surface. The different elements give information about the rotational orientation states that scatter into and from the surface in different directions.

REFERENCES

5. N. F. Ramsey, Phys. Rev., 85, 60, (1952)