Fringe fields are important when examining molecular orientation in a cold ammonia beam

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Abstract
External fields have been widely adopted to control and manipulate the properties of gas-phase molecular species. In particular, electric fields have been shown to focus, filter and decelerate beams of polar molecules. While there are several well-established approaches for controlling the velocity and quantum-state distribution of reactant molecules, very few of these methods have examined the orientation of molecules in the resulting beam. Here we show that a buffer gas cell and three-bend electrostatic guide (coupled to a time-of-flight set-up) can be configured such that 70% of ammonia molecules in the cold molecular beam are oriented to an external electric field at the point of detection. With a minor alteration to the set-up, an approximately statistical distribution of molecular orientation is seen. These observations are explained by simulations of the electric field in the vicinity of the mesh separating the quadrupole guide and the repeller plate. The combined experimental apparatus therefore offers control over three key properties of a molecular beam: the rotational state distribution, the beam velocity, and the molecular orientation. Exerting this level of control over the properties of a molecular beam opens up exciting prospects for our ability to understand what role each parameter plays in reaction studies.

Keywords: cold molecules, orientation, quadrupole guide, alignment, stereodynamics, ammonia

(Some figures may appear in colour only in the online journal)

1. Introduction
The development of new experimental techniques, accompanied by new combinations of well-established methods, has seen the emergence of cold and controlled chemistry as an active field of research. The last decade, in particular, has seen exceptional progress made in the range of reactant species that can be carefully manipulated and studied [1–3]. Reac-

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The influence that orientation effects have on molecular reactivity has been a topic of active investigation for many decades. Measurements undertaken in the mid-1960s controlled the polarisation of CH₃I molecules using an electrostatic hexapole followed by a uniform electric field region [4, 5]. The polar CH₃I molecules were found to orientate to the (inhomogeneous) field within the hexapole, and were able to maintain orientation to the external field axis by adiabatically following the field through to the (homogeneous) detection region. By changing the polarity of the uniform field, the authors found that the collision dynamics showed a dependence on the orientation of the reactants. In the subsequent decades, the field of stereodynamics has evolved—with a number of methods introduced to study polarisation effects on chemical reaction dynamics. Widely-adopted techniques used to polarise molecules for collision studies include the use of external electric, magnetic or optical fields, as detailed in a 2014 review article [6].

The ability to monitor the effects of molecular orientation on the outcome of collision events has provided stringent tests for theories of reactivity and for the accuracy of calculated potential energy surfaces. For example, the measurement of vector correlations in the collision of (optically prepared) NO(A 2Σ⁺) molecules with Ne atoms revealed ‘non-intuitive’ rotational reorientation effects—allowing the accuracy of high-level electronic-structure calculations to be tested more sensitively than had been possible in any previous study [7]. In the ultracold regime, bimolecular reactions between two KRb molecules have been observed to occur readily in the presence of an external electric field (where the molecules are easily oriented and can undergo ‘head-on’ collisions), but are strongly suppressed when molecules are confined in an optical lattice trap and only allowed to undergo ‘side-by-side’ collisions [8].

Bringing together different experimental techniques offers the prospect of controlling a number of reaction parameters at once. For example, the combination of Stark deceleration, magnetic trapping, buffer-gas cooling and electrostatic guiding enabled state-selected trap loss cross sections to be measured for OH—ND₃ collisions at an average collision energy of 5 K [9]. Here, the set-up features a buffer gas cell and bent quadrupole electrostatic guide for the generation of an internal and translationally cold beam of polar molecules—with the option of adding an ion trap to the field through to the molecular beam for ion–molecule reaction studies [10]. The variable parameters that can be controlled include the rotational state distribution [11], the velocity of the beam [11], and (as presented in this work) the orientation of molecules to an external field. The ability to independently control and manipulate these variables opens up the prospect of examining the role each parameter plays in reactive collisions, and could deepen our understanding of chemical reactivity at a fundamental level [3].

In this paper, we explore the extent to which orientation can be maintained in a beam of cold, deuterated ammonia molecules as they pass from a quadrupole guide, through a mesh, and into a linear field region. While a number of previous studies have successfully produced and manipulated state-selected beams of ammonia (see, for example, references [9, 11–14]), we are not aware of any previous work (aside from our own preliminary study [10]) that has focused on quantifying orientation effects in a cold ND₃ beam. As the quadrupole features three bends, only low-velocity ND₃ molecules in low-field-seeking states are present; all molecules are oriented to the local electric field. After the quadrupole, a mesh is in place to shield the interaction region from the inhomogeneous fields emanating from the quadrupole. A number of different mesh configurations are explored, to examine the extent to which orientation can be retained in the beam with minor alterations to the setup.

A repeller plate, situated on the other side of (and parallel to) the mesh, creates a linear electric field region between the repeller and the mesh. By altering the extent to which fringe fields from the repeller plate can penetrate the mesh, the ease with which ND₃ molecules can adiabatically follow the field is affected. When fringe fields are present at the mesh, approximately 70% of ND₃ molecules are oriented to the external field at the point of detection. As the mesh is permeable, the fields created by the repeller can pass a short distance through the pores of the mesh. This results in a smooth transition between the different field regions and ensures that molecules do not pass through a near-zero field region. In contrast, when the configuration of the mesh and mesh holder is altered slightly, an approximately statistical redistribution of population is observed. When the fields from the repeller plate are more effectively shielded, fringe fields are absent and an extended near-zero field region is present in the vicinity of the mesh. Hence, through careful design and simulation of the mesh region, it is possible to control and vary the orientation of ammonia molecules—using an apparatus that also offers control over the rotational state distribution and beam velocity.

2. Methods

2.1. Experimental apparatus

The experimental set-up has been described in some detail in previous publications [10–12]. In summary, a cold beam of deuterated ammonia is formed through the combination of buffer gas cooling and quadrupole velocity selection, as illustrated schematically in figure 1. The buffer gas cell is attached to the second stage of a two-stage pulse-tube cryocooler. Helium buffer gas thermalises with each stage and enters the cell at a temperature of approximately 6 K. Room temperature ND₃ is subsequently admitted to the buffer gas cell through a leak valve. The ammonia molecules are cooled by elastic and inelastic collisions with the helium buffer gas. On the opposite wall to the molecular inlet valve, there is an exit aperture that allows gas particles to leave the cell. Before reaching the exit aperture, ammonia molecules undergo multiple collisions with the buffer gas [15].

A three-bend, 2 m long electrostatic quadrupole guide is positioned at the exit aperture of the buffer gas cell to guide slow-moving ammonia molecules in low-field-seeking quantum states through to the detection region. Voltages of
±5 kV are applied to the quadrupole electrodes, creating a zero-field region in the centre of the quadrupole and high fields close to the electrode surfaces (of maximum strength 90 kV cm$^{-1}$). Each of the three bends in the quadrupole act as a low-pass velocity filter: only low-field-seeking molecules with a velocity below a certain threshold value are confined by the guide, with all other species overshooting the bend and lost from the beam. Previous characterisation studies reported a translational temperature of 10 K, with the majority of ammonia molecules in the $J = 1$ rotational state [11]. Only molecules in $J = 1$ are considered in this work. The Stark splitting induced by the application of an electric field is shown for the $J = 1$ rotational state of ND$_3$ in figure 2. Note that $J$ is the total angular momentum quantum number (excluding nuclear spin), $K$ is the projection of $J$ onto the molecular axis, and $M$ is the projection of $J$ onto the external field axis [16].

At the exit of the quadrupole, a grounded mesh is positioned to shield the detection region from the fields emanating from the quadrupole electrodes. The mesh is composed of nickel wires, each 12.7 μm thick, with a pore area of 0.042 mm$^2$—corresponding to a geometric (or optical) transmittance of 88%. In the detection region, transmitted ammonia
molecules are probed using \((2 + 1)\) resonance-enhanced multi-photon ionisation (REMPI), exciting the \(B(v^2_J = 5) \leftrightarrow X(v^2_J = 0)\) transition. Molecules are ionised between a pair of repeller and extractor plates, with the resulting ions accelerated into a field-free flight tube and onto a microchannel plate (MCP) detector.

### 2.2. Measurement of the ammonia alignment

The orientation of a polar molecule can be controlled by the application of an external electric field. For a symmetric top molecule (such as ammonia), one can calculate the angle \(\theta\) between the dipole moment, \(\mu\), and the axis of the external field, \(E\). The magnitude of the interaction energy between the dipole moment and the electric field is given by 
\[-\mu E \cos(\theta),\]

where \((\cos \theta) = KM/J(J + 1)\). The molecular beam is deemed to be fully aligned if all molecules can be described as \([J = 1, MK = \pm 1]\). Complete orientation of the beam is achieved if all molecules have the same \(MK\) value (i.e., if all molecules are pointing in the same direction).

As set out in the preceding subsection, REMPI measurements are undertaken to examine the properties of the cold molecular beam. Uniform conditions can only be achieved for a short window of time; after a few hours of operation, ammonia ice forms on the exit aperture of the buffer gas cell, causing fluctuations in the beam properties. As such, a small spectral region of interest is chosen, spanning from 63 008 cm\(^{-1}\) to 63 026 cm\(^{-1}\) (corresponding to the two-photon transition frequencies, see figure 3), to ensure that the experimental conditions are as consistent as possible.

The PGOPHER spectral fitting and simulation software package [17] is used to fit the experimental spectra and to calculate the population of each state. With our method of measurement, \(MK = 1\) and \(MK = -1\) are indistinguishable as the transition energy is the same (irrespective of the laser polarisation direction). As such, only the alignment of the ammonia molecular beam can be established in these experiments; the orientation cannot be directly measured, but can be deduced from simulations (see the following subsection).

Measurements are made under a range of slightly different experimental conditions, with the properties of the mesh (and mesh holder) separating the quadrupole guide and detection region modified. In all configurations, the mesh is either grounded (by connecting it to the chamber) or has a small bias voltage applied to it. For each set of parameters chosen, up to 30 repeat spectra are measured and the relative populations extracted—with the mean values and their associated standard error reported in tables 1–3. No dependence is found on the laser power under the range of experimental conditions explored. Quantum state populations extracted from spectra recorded using linearly polarised light, with the polarisation axis either parallel or perpendicular to the time-of-flight axis, are in agreement (as seen in previous work [10]). To explore the effect of the grounded mesh on the orientation of ammonia molecules emerging from the guide and entering the detection region, the properties of the mesh are varied experimentally and examined using simulations.

### 2.3. Simulations

The field between the wires that make up the mesh—the region inside the mesh pores—is rarely uniform. These so-called fringe effects can cause a beam of particles to focus
(or diverge) as they fly through the mesh. In this work, the mesh has a pitch of 0.2 mm and the mesh wires have a circular cross-section, with a diameter of 0.0127 mm. While it has been known for some time that meshes can give rise to fringe effects and local field distortions [18–24], it is still rare to see the mesh region of an experimental set-up explicitly described in simulations. While the optical transmission of a mesh is often considered, it is otherwise usually treated as a featureless plane or ideal grid in simulations carried out using software packages such as SIMION. As this work illustrates, the field in the vicinity of the mesh is critical as it affects the trajectories of the molecules (and their orientation) as they pass through the mesh region. To accurately simulate and account for these effects, it is important to include the mesh region in simulations. However, the components of the mesh are typically several orders of magnitude smaller than other elements in the experimental set-up—and, as such, explicitly simulating the mesh can take up a huge amount of additional calculation power.

SIMION, a widely used software package for calculating electric fields and ion trajectories, has identified a number of methods that can be used to overcome the challenges associated with modelling a mesh or grid accurately. One such example is the trajectory and square jump method [25]. The field generated within one pore is calculated and extended (using boundary condition interpolation) to reproduce the global behaviour of the mesh. An alternative approach to modelling a mesh is to run three different simulations: one before the mesh, one in the immediate vicinity of the mesh, and one after the mesh. Other hybrid approaches have also been proposed [25], where only a small region of the mesh is explicitly described while the majority of the mesh is treated as an ideal grid. However, there are known discontinuities that often arise at the transitions between separate simulations and when adopting hybrid approaches. These discontinuities can affect the particle trajectories and impede the accurate modelling of fringe effects.

In this work, the presence of symmetry in the relevant components of the experimental set-up means that the mesh and the surrounding electrodes can be explicitly modelled in a single simulation. In contrast to the usual approach of accurately describing the large components of an experimental set-up and approximating the mesh, an alternative method is explored. The mesh is explicitly described in the simulations while the dimensions of the surrounding electrodes are reduced. To ensure that the different electric field regions are accurately represented, the voltages applied to the different electrodes are adapted such that the electric field strength in the regions of interest are consistent with the experimental conditions.

The mesh is simulated as follows. The wire diameter is kept at the experimental value of 12.7 μm, with this choice of wire diameter influencing the scale at which other components of the apparatus can be represented. The simulated pore dimensions are as close to the experimental dimensions as possible, at 0.17 mm × 0.17 mm. The distances between the quadrupole, the mesh and the repeller are reduced (compared to the experimental parameters), with the voltages applied to each component adapted to create the same local field environment around the mesh. On the detection side of the mesh—the side with the repeller and extractor plates—the field is linear, \( E = V/r \) (where \( E \) is the electric field, \( V \) the applied voltage and \( r \) distance). The same field strength can therefore be achieved by reducing \( V \) and \( r \) proportionally. The repeller plate is treated in different ways (with and without a mesh-covered circular hole in the centre), to ensure that scaling down the dimensions of the experimental repeller plate in the simulations does not affect the fields emanating from it. As expected, due to the linearity of the field, no difference is observed. On the source side of the mesh, where the field is due to the high voltages applied to the electrostatic quadrupole guide rods, the electric field is not linear. The field around the quadrupole is proportional to \( 1/r_0^2 \), where \( r_0 \) is the distance between the central quadrupole axis and the quadrupole rods. As such, \( r_0, d \) (the distance between the quadrupole and the mesh), and the potential applied to the quadrupole are all reduced accordingly in the SIMION simulations.

A variety of different scenarios are explored by calculating the electric field regions around the mesh using SIMION, complemented by experimental measurements to verify the accuracy of the simulations. The parameters that are varied include the material and design of the mesh holder, the application of a bias voltage to the mesh, and the region over which the mesh extends (i.e., the diameter of the hole in the mesh holder). In all cases, the electric fields are calculated using SIMION and then exported and plotted using Python. The corresponding experimental measurements are carried out as described in the preceding subsection.

3. Results and discussion

3.1. Peek mesh holder, grounded

In the first set of measurements, the effect of holding the mesh in place with an insulating material (namely Peek) is explored. By using an insulator in place of a metal mesh holder, it was expected that the extent of the near-zero field region around the grounded mesh would be reduced [10]. The hole in the mesh holder (i.e., the area covered by the mesh) has a diameter of 2 mm, and the mesh holder thickness is 1 mm. The average of all measured spectra recorded with the mesh grounded and held in place with Peek is shown in blue in figure 3. The corresponding quantum state populations, established from PGOPHER fits to the spectra, are shown in table 1. With parallel light and the mesh grounded, approximately 72% of ammonia molecules are in the \( |1, ±1⟩ \) states. As expected, this is in agreement with a complementary set of measurements undertaken with a bias field of 0 V applied to the mesh, where approximately 74% of population is found to be in \( |1, ±1⟩ \) states, with 25% in \( |1, 0⟩ \) [10]. The findings from these two studies are in excellent agreement. Analysis of the composition of the molecules in the \( |1, ±1⟩ \) states from [10] indicate that almost all molecules are in the \( |1, −1⟩ \) state, as expected when considering the presence of an external field that preferentially orients the dipoles of the
ammonia molecules; as few as 5% of molecules are in the $|1, 1\rangle$ state [10].

At the end of the quadrupole guide, all ammonia molecules will be in the $|1, -1\rangle$ state—as only slow-moving molecules in low-field-seeking states are transmitted by the guide. However, it can be difficult for molecules to adiabatically follow the field once they exit the quadrupole guide, due to the rapid rotation of the field axis (from radial to axial) and the low field region induced by the grounded mesh (see [10] for further details). As expected from the Stark energy diagram (figure 2), molecules can rotate into the $|1, 0\rangle$ state if they enter a region of zero (or near-zero) field, with a small subset of molecules inverting into the $|1, 1\rangle$ state. By simply using an insulating material to hold the grounded mesh, approximately 70% of orientation can be maintained in the beam, confirming earlier predictions [10].

3.2. Peek mesh holder and bias voltage

In previous work [10], it was proposed that applying a small bias voltage to the mesh would further reduce the size of the low-field region, and thereby enable more of the beam orientation to be maintained. The quantum state populations recorded following the application of a small bias voltage to the mesh (in a Peek mesh holder) are shown in table 1. Surprisingly, no statistically significant difference is observed when a bias voltage of 36 V is applied compared to when a bias voltage of 0 V is applied (or with the mesh grounded). To explore why this is the case, the electric field strength in and around the mesh must be considered in more detail.

The SIMION simulations related to this experimental configuration are shown in figure 4, where the electric field strength calculated around the mesh region is shown both when the mesh is grounded and when a bias voltage of 36 V is applied. As can be seen in the two plots on the left, the two sets of conditions give rise to similar fields around the mesh. In both cases, there is a low field region in the centre of the quadrupole and in front of the mesh (i.e., at around $-150 < r < 0 \mu m$). Between the mesh and the repeller (i.e., for $r > 0 \mu m$), as expected, the field is uniform. When zooming in to examine the mesh region in more detail, it can be seen that the field in front of the mesh is a little higher when a bias voltage is applied to the mesh. However, there is not as much difference between the magnitude of the field under the two sets of conditions as might have been expected. The mesh is permeable, and the repeller field successfully extends a short distance beyond the mesh, giving rise to fringe effects. Even when no bias field is applied, it can be seen that the field from the repeller penetrates the pores of the mesh; in both cases, a field on the order of a few hundred V cm$^{-1}$ is present in front of the mesh. Applying a small bias voltage of 36 V to the mesh does not significantly change the properties of the field in this region—as, even without the bias field, there is sufficient field strength to maintain the orientation of most molecules as they pass through the region.

3.3. Metallic mesh holder wide

To explore whether any boundary effects are at play, and to test the agreement between the simulations and experimental measurements in another configuration, a different mesh holder can be used. In this case, the mesh holder is made of metal and has a very wide opening of 20 mm, meaning that the mesh extends over a much larger area and the mesh holder is less important (as it is much further away from the molecular beam). Spectra are recorded with the mesh (and mesh holder) at 0 V and when a bias voltage of 36 V is applied. The resulting quantum state populations are shown in table 2. Again, there are no statistical differences between the populations recorded with and without the bias voltage applied to the mesh. With 75% of ammonia molecules in the $|1, \pm 1\rangle$ states, the findings are consistent with the results seen using a narrower Peek mesh holder. Again, inspection of the electric fields in the vicinity of the mesh indicates that the electric field emanating from the repeller plate successfully penetrates through the mesh in this experimental configuration. The presence of an electric field on the order of several hundred V cm$^{-1}$ is sufficient to again retain orientation in the majority of molecules in the beam.

3.4. Metallic mesh holder narrow

To verify the importance of fringe fields from the repeller in maintaining orientation in the beam, the area covered by the mesh is reduced. With the mesh only covering a narrow opening (2 mm diameter) in the metal mesh holder, the repeller field can no longer penetrate through the mesh pores. While the position of the mesh is also altered slightly, placing it further from the repeller and closer to the exit of the quadrupole, this small change does not appear to affect the fringe fields. The quantum state populations recorded under these conditions are provided in table 3. This time, 35% of the molecules are in the $|1, 0\rangle$ state, with only 65% in the $|1, \pm 1\rangle$ states. While the experimental spectra measure alignment and not orientation, with the assistance of simulations we can predict the relative populations of the $MK = 1$ and $MK = -1$ states. In the scenarios explored in the preceding subsections, almost all of the population in $|1, \pm 1\rangle$ is attributed to the $|1, -1\rangle$ low-field-seeking state. The conclusion that orientation is maintained in the beam under these circumstances—with approximately 70% of ammonia molecules in the $|1, -1\rangle$ state—is based on both trajectory calculations (where orientation is explicitly examined [10]) and extensive simulations (performed as part of this work). In contrast, in the configuration described within this subsection—where the field from the repeller cannot penetrate the mesh—an almost completely statistical redistribution of population over the three levels is predicted. There is no preferential orientation of ammonia molecules by the time the beam reaches the detection region. This can be directly observed in the experimental measurements, with a significant increase in the population of the $|1, 0\rangle$ state; the $|1, 0\rangle$ state
accounted for 25 ± 2% of population in the earlier configurations, compared to 33%–35% of population here. The experimental populations set out in table 3 can be explained by considering the simulated electric fields in the region of the mesh, as shown in figure 4. Clearly, the modifications to the mesh holder impede the ability of the repeller field to penetrate the mesh. The field in the region of the mesh is on the order of tens of V cm\(^{-1}\), an order of magnitude lower than the fields calculated for the previous configurations. This is because the field from the repeller is unable to reach the mesh; within 200 μm of the mesh, on the repeller side, the field drops below 20 V cm\(^{-1}\) along the central beam axis. This occurs even when a bias field of 36 V is applied to the mesh and mesh holder. Without the repeller field penetrating the mesh, the molecular beam passes through an extended region with near-zero field magnitude and orientation effects are lost.

4. Discussion
The properties of the mesh and mesh holder are critical in determining whether or not orientation can be maintained in a beam of cold ammonia molecules as they pass from a quadrupole guide, through a mesh, and into a linear electric field region where they are detected. As the mesh that separates the two different electric field regions is permeable, the field from the repeller can extend a short distance through the pores of the mesh. When this occurs, the resulting fringe fields ensure that the electric field in the region of the mesh is on the order of a few hundred V cm\(^{-1}\) and approximately 70% of ammonia molecules are found in the \(|1, -1\rangle\) state. Most molecules in the beam adiabatically follow the electric field as it rotates from a radial to axial direction, retaining their orientation. When the properties of the mesh holder are altered so as to impede the penetration of the repeller field through the mesh pores (see figure 5), no orientation effects are seen and an approximately statistical population distribution is recorded.

The ability to control the orientation of a molecular beam is a powerful tool in the study of chemical reaction dynamics. This is especially true for the current set-up, where several other properties of the molecular beam can be concurrently manipulated and controlled. For example, the
Figure 5. 2D slices of the electric field strength with a metallic mesh holder in place. The mesh is located closer to the quadrupole, with an extended mesh holder; all other components are unchanged. Voltages of ±225.3 V are applied to the quadrupole, 36 V to the mesh and mesh holder, and 55.8 V to the repeller plate. The x-axis follows the molecular beam axis, and is plotted with respect to the position of the mesh (with the middle of the mesh at $r = 0 \mu m$). The lower panel provides a zoomed-in plot of the region immediately after the mesh (still within the mesh holder). The colour scale on the right of each plot gives the magnitude of the electric field strength in V cm$^{-1}$. Dark blue corresponds to regions of low field, and yellow indicates regions of high field.

rotational temperature of the beam can be adjusted by using a different buffer gas (swapping from H$_2$ to Ne), by modifying the temperature of He buffer gas, and by altering the relative flow rates of buffer gas and molecular gas into the cell [11]. The velocity of the beam can be adjusted by modifying the voltages applied to the quadrupole guide rods. With a minor alteration to the experimental set-up in the region of the mesh, this work clearly demonstrates that it is possible to also exert some control over the orientation of ammonia molecules in the beam—generating a beam where the majority of molecules are oriented to the external field, or where there is no preferential molecular orientation. Future work will look at whether other experimental parameters can be altered to achieve even more orientation in the beam.

It is the field generated by the repeller plate, and the ability of this repeller field to penetrate a small distance through the mesh, that enables most of the ammonia molecules to adiabatically follow the field and retain their orientation through to the detection region. The relative simplicity of the detection set-up, with a standard implementation of repeller and extractor
plates ahead of a flight tube and MCP detector, make the findings of this work broadly applicable. Furthermore, excellent optical access is maintained in the detection region, as demonstrated by the use of spectroscopic measurements to probe the properties of the beam in this work.

5. Conclusion

The findings reported in this work highlight the importance of considering the properties of the mesh when probing orientation (or alignment) effects. Contrary to convention, the mesh is explicitly included in the simulations with the dimensions of other components adjusted accordingly—ensuring that the electric field in the vicinity of the mesh is described as accurately as possible. By considering the ability of the repeller field to penetrate the mesh in the different experimental configurations explored, the retention (or loss) of alignment recorded in the experimental measurements can be understood. Through comparison with trajectory simulations, where ammonia molecules are propagated through the different electric field regions [10], the orientation of molecules in the beam can be accounted for. Careful selection of the appropriate mesh and mesh holder configuration can preserve the orientation of approximately 70% of ammonia molecules as the beam passes into the detection region. This work opens up exciting new possibilities for the study of reaction dynamics, providing a source of cold molecules where the rotational state, collision energy and orientation can be manipulated.

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Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: http://dx.doi.org/10.17638/datacat.liverpool.ac.uk/1495.

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