# Magnetically Tunable Feshbach Resonances in Ultracold Li-Yb Mixtures

Daniel A. Brue[*] and Jeremy M. Hutson[†]

*Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom*
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We investigate the possibility of forming Li + Yb ultracold molecules by magnetoassociation in mixtures of ultracold atoms. We find that magnetically tunable Feshbach resonances exist, but are extremely narrow for even-mass ytterbium isotopes, which all have zero spin. For odd-mass Yb isotopes, however, there is a new mechanism due to hyperfine coupling between the electron spin and the Yb nuclear magnetic moment. This mechanism produces Feshbach resonances for fermionic Yb isotopes that can be more than 2 orders of magnitude larger than for the bosonic counterparts.

It has recently become possible to convert gases of alkali-metal atoms coherently into molecules in their absolute ground state, by magnetoassociation followed by stimulated Raman adiabatic passage (STIRAP). This has so far been achieved for KRb [1] and $Cs_2$ [2], but other species are under active investigation. Other methods for producing ultracold ground-state molecules are also under development [3–8]. Ultracold polar molecules have important potential applications in quantum computing and quantum simulation, and dipolar quantum gases promise a rich new physics with many novel properties [9].

Even more new properties would be accessible for ultracold molecules with both electric and magnetic dipole moments [10]. However, alkali-metal dimers have singlet ground states, which cannot be tuned magnetically except through the very small magnetic moments of the constituent nuclei. There is therefore great interest in producing ultracold polar molecules with doublet or triplet ground states. Among the most promising candidates for this are molecules formed from an alkali-metal atom and a $^1S$ atom such as an alkaline earth or Yb. A number of experimental groups are studying ultracold mixtures in which such molecules might be formed, including Rb + Yb [11] and Li + Yb [12–14].

It was originally believed that systems of this type would not have Feshbach resonances suitable for magnetoassociation, because the bound-state channels (correlating with the upper hyperfine state of the alkali-metal atom) are uncoupled to the entrance channel by the conventional collision Hamiltonian. However, we have recently shown that a coupling does exist, due to the modification of the alkali-metal hyperfine coupling by the singlet atom at short range [15]. For the prototype system Rb + Sr, we showed that, under favorable circumstances, this mechanism could produce magnetically tunable Feshbach resonances with widths up to 100 mG, which might be used for magnetoassociation.

In the present Letter we consider the topical system Li + Yb, which is under experimental investigation by at least two groups and has also been investigated using

electronic structure calculations [16,17]. We show that the mechanism we previously proposed does produce Feshbach resonances in this system, but that for bosonic (spin-zero) isotopes of Yb they are extremely narrow. However, for fermionic isotopes of Yb there is a different mechanism that can produce resonances that are *more than 2 orders of magnitude* wider. Furthermore, the recent measurements of the scattering length for $^6$Li-$^{174}$Yb [13,14] allow us to estimate the magnetic fields at which these Feshbach resonances will occur.

The collision Hamiltonian for a pair of atoms $a$ and $b$ is

$$\frac{\hbar^2}{2\mu}\left[-R^{-1}\frac{d^2}{dR^2}R + \frac{\hat{L}^2}{R^2}\right] + \hat{H}_a + \hat{H}_b + \hat{V}(R), \quad (1)$$

where $R$ is the internuclear distance, $\mu$ is the reduced mass, $\hat{L}^2$ is the angular momentum operator for mechanical rotation of the atoms about one another, $\hat{H}_a$ and $\hat{H}_b$ are the Hamiltonians for the free atoms (in an applied field) and $\hat{V}(R)$ is the interaction operator. For collision of an alkali-metal atom $a$ with a closed-shell ($^1S$) atom $b$,

$$\hat{H}_a = \zeta_a\hat{i}_a \cdot \hat{s} + (g_a^e\mu_B\hat{s}_z + g_a^{nuc}\mu_N\hat{i}_{a,z})B,$$
$$\hat{H}_b = g_b^{nuc}\mu_N\hat{i}_{b,z}B, \quad (2)$$

where $\zeta_a$ is the hyperfine coupling constant for atom $a$, $\hat{s}$, $\hat{i}_a$, and $\hat{i}_b$ are the electron and nuclear spin operators, $g_a^e$, $g_a^{nuc}$, and $g_b^{nuc}$ are the corresponding $g$ factors, and $B$ is the magnetic field, whose direction defines the $z$ axis. There is only one electronic state, of symmetry $^2\Sigma^+$, arising from interaction of atoms in $^2S$ and $^1S$ states. As described in Ref. [15], the hyperfine coupling constant of the alkali metal is modified by the presence of the closed-shell atom, $\zeta_a(R) = \zeta_a + \Delta\zeta_a(R)$. However, if the closed-shell atom has nonzero nuclear spin $i_b$, there may also be a coupling $\zeta_b(R) = \Delta\zeta_b(R)$ between $i_b$ and the electron spin; this term has not been considered previously. The interaction operator is therefore

$$\hat{V}(R) = V(R) + \Delta\zeta_a(R)\hat{i}_a \cdot \hat{s} + \Delta\zeta_b(R)\hat{i}_b \cdot \hat{s}. \quad (3)$$

There are additional small contributions to $\hat{V}(R)$ from nuclear quadrupole coupling, electron-nuclear dipolar coupling and spin-rotation interactions, but the $\Delta\zeta$ terms have by far the largest effect [15].

In the present work, we obtained the quantities $\zeta_{\text{Li}}(R)$ and $\zeta_{\text{Yb}}(R)$ with the relativistic density-functional theory (DFT) approach [18] implemented in the ADF program [19], using the PBE0 functional [20] with a QZ4P quadruple-zeta relativistic basis set [21]. The asymptotic value of $\zeta_{\text{Li}}$ for $^7$Li was underestimated by 5.8% in the DFT calculations, so we scaled $\zeta_{\text{Li}}(R)$ to reproduce the experimental atomic value. The resulting quantities $\Delta\zeta(R)$ are shown in Fig. 1; they were fitted to Gaussian forms $\zeta_0 e^{-a(R-R_c)^2}$, with parameters $\zeta_0 = -129$ MHz, $a = 0.101$ Å$^{-2}$ and $R_c = 2.60$ Å for $^7$Li and $\zeta_0 = -406$ MHz, $a = 0.31$ Å$^{-2}$ and $R_c = 3.39$ Å for $^{173}$Yb. This corresponds to a 32% maximum reduction in $\zeta$ for $^7$Li (and also for $^6$Li). The values for $^7$Li and $^{171}$Yb are obtained by scaling according to the nuclear magnetic moments, giving $\zeta_0 = -48$ MHz and $-1500$ MHz respectively.

Zhang *et al.* [17] have carried out detailed studies of the potential curves of the ground and excited states of LiYb. In the present work, we used their CCSD(T)/ECP potential points [22], obtained from large-basis coupled-cluster calculations using a fully relativistic effective core potential for Yb and including counterpoise corrections. These were extrapolated at long range using the form $V(R) = -C_6 R^{-6}$, with coefficient $C_6 = 1594\ E_h a_0^6$ [17]. The short- and long-range parts of the potential were smoothly connected between 20 and 25 $a_0$ with the switching function used by Janssen *et al.* [23].

For a potential with known long-range behavior, both the energies of high-lying bound states [24] and the scattering
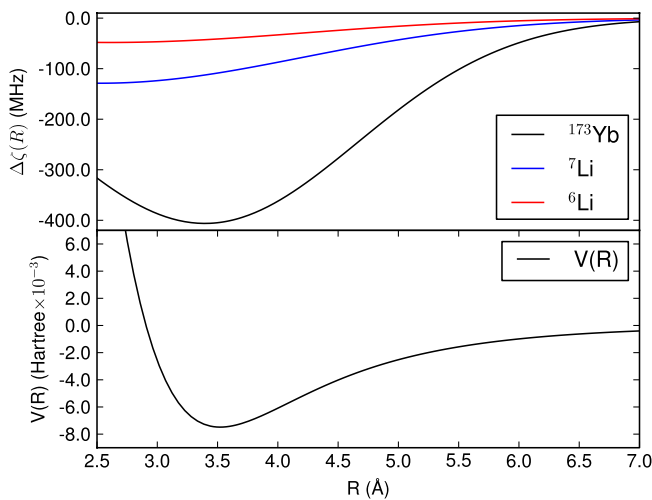
length [25] may be expressed in terms of the fractional part of the quantum number at dissociation, or equivalently in terms of a semiclassical phase integral, $\Phi = \int k(R)dR$, where $k^2(R) = 2\mu V(R)/\hbar^2$. The potential curve of Zhang *et al.* [17] supports 24 bound states for $^6$LiYb. However, it is probably accurate to only a few percent, and variations within this uncertainty are enough to span the entire range of scattering length $a$ from $+\infty$ to $-\infty$. However, Ivanov *et al.* [13] and Hara *et al.* [14] have recently measured values of the scattering length to be $|a| = 13 \pm 3a_0$ ($0.69 \pm 0.16$ nm) and $1.0 \pm 0.2$ nm, respectively. Because the sign of $a$ is unknown, we have scaled the potential of Zhang *et al.* to give two potentials, $V_+$ and $V_-$, with scattering lengths $a = +0.8$ nm and $-0.8$ nm, each within the error bars of both measurements.

Zero-energy Feshbach resonances of the type that might be suitable for magnetoassociation occur at magnetic fields where molecular levels cross atomic thresholds. In a molecule such as LiYb, the entire molecular Hamiltonian is nearly diagonal in a basis set of field-dressed atomic functions, so that the molecular levels lie parallel to the atomic thresholds as a function of magnetic field. This is shown in Fig. 2: for the $V_+$ potential, there is a group of crossings around 1000 G that might in principle cause Feshbach resonances, whereas for $V_-$ the corresponding crossings occur around 1600 G.

In the present work, we characterize resonances by carrying out coupled-channel scattering calculations using the MOLSCAT program [26], modified to handle collisions of atoms in magnetic fields [27,28]. The molecular wave
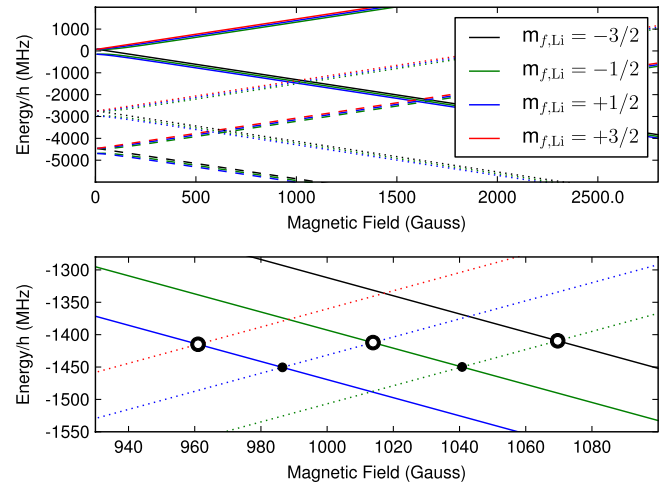


FIG. 1 (color online). Interaction potential $V(R)$ for LiYb (lower panel) [17] and $R$ dependence of hyperfine coupling constants $\Delta\zeta(R)$ (upper panel).



FIG. 2 (color online). Upper panel: Molecular levels (dotted and dashed) that cross atomic thresholds (solid) for $^6$LiYb, calculated for potentials $V_+$ (dotted lines) and $V_-$ (dashed lines) as a function of magnetic field. The Yb isotope chosen makes little difference on the scale of the Figure. The lower panel shows an expanded view of the crossing region for potential $V_+$. Filled circles show positions where narrow resonances occur for all isotopes and open circles show where wider resonances occur for Yb isotopes with nonzero spin.

functions are conveniently expanded in an uncoupled basis set $|sm_s\rangle|i_{\text{Li}}m_{i,\text{Li}}\rangle|i_{\text{Yb}}m_{i,\text{Yb}}\rangle|LM_L\rangle$. The Hamiltonian is diagonal in the total projection quantum number $M_{\text{tot}} = M_F + M_L$, where $M_F = m_s + m_{i,\text{Li}} + m_{i,\text{Yb}}$. The coupled-channel calculations provide the scattering length $a(B)$, which (in the absence of inelastic scattering [29]) follows the functional form $a(B) = a_{\text{bg}}[1 + \Delta/(B - B_{\text{res}})]$. The width $\Delta$ is conveniently obtained from the difference between the positions of the pole and zero in $a(B)$. In the present work, we extended MOLSCAT to provide an option to *converge* on poles and zeroes of $a(B)$, instead of extracting them from a fit to a grid of points.

There are only very small terms in the collision Hamiltonian that couple states of different $L$ or $M_L$. For mixtures containing spin-zero isotopes of Yb (mass numbers 168, 170, 172, 174, and 176), conservation of $M_{\text{tot}}$ and $M_L$ requires that the Li projection quantum number $m_{f,\text{Li}} = m_s + m_{i,\text{Li}}$ is also conserved. Because of this, Feshbach resonances can occur only where states of the LiYb molecule cross atomic thresholds with the same value of $m_{f,\text{Li}}$, as shown by solid circles in Fig. 2. The lowest-field resonances for the $V_+$ and $V_-$ potentials for $^6$Li$^{174}$Yb are shown in Table I. However, in both cases the resonances are extremely narrow ($\Delta < 10$ $\mu$G) and would be very challenging to observe experimentally. This arises

TABLE I. Calculated properties of LiYb Feshbach resonances caused by low-field-seeking bound states ($m_s^{\text{bound}} = +\frac{1}{2}$) crossing the lowest $m_s = -1/2$ threshold state. The bound states are labeled by the total angular momentum projection of the lithium atom alone, $m_{f,\text{Li}}^{\text{bound}}$. The results for Li$^{174}$Yb are for $M_{\text{tot}} = m_{f,\text{Li}}$ and those for $^6$Li$^{173}$Yb and $^7$Li$^{173}$Yb are for $M_{\text{tot}} = 1$ and $+3/2$, respectively.

| system | $B_{\text{res}}$ (G) | $a_{\text{bg}}$ (nm) | $\Delta$ ($\mu$G) | $m_{f,\text{Li}}^{\text{bound}}$ |
|---|---|---|---|---|
| | | $V_+$ potential | | |
| $^6$Li$^{174}$Yb | 996 | +0.80 | 1.89 | +1/2 |
| $^7$Li$^{174}$Yb | 261 | +1.74 | 1.64 | +1 |
| L$^6$i$^{173}$Yb | 961 | +0.82 | 824 | +3/2 |
| | 986 | +0.82 | 1.03 | +1/2 |
| | 1013 | +0.82 | <0.1 | −1/2 |
| $^7$Li$^{173}$Yb | 213 | +1.80 | 178 | +2 |
| | 253 | +1.80 | 38.5 | +1 |
| | 307 | +1.80 | 1.17 | 0 |
| | 388 | +1.80 | <0.1 | −1 |
| | | $V_-$ potential | | |
| $^6$Li$^{174}$Yb | 1648 | −0.80 | −6.13 | +1/2 |
| $^7$Li$^{174}$Yb | 679 | +0.73 | 14.9 | +1 |
| $^6$Li$^{173}$Yb | 1608 | −0.76 | −2790 | +3/2 |
| | 1634 | −0.76 | −4.59 | +1/2 |
| | 1661 | −0.76 | <|−0.1| | −1/2 |
| $^7$Li$^{173}$Yb | 615 | +0.76 | 857 | +2 |
| | 669 | +0.76 | 31.1 | +1 |
| | 733 | +0.76 | 0.52 | 0 |
| | 810 | +0.76 | <0.1 | −1 |

mostly because the $^6$Li hyperfine coupling constant is only 152 MHz in the free atom, so that even a 32% modification of it causes only very weak coupling.

The resonance positions for $^6$LiYb depend only very weakly on the Yb isotope, because changing the Yb isotopic mass has very little effect on the reduced mass for collisions with a light atom such as Li. The $^6$LiYb resonance positions are also quite insensitive to the quality of the potential curve. They do depend somewhat on the value of $C_6$: for example, increasing $C_6$ by 1% shifts the calculated resonance positions to higher field by 0.5 G for fixed $a$. However, the main source of uncertainty in the $^6$LiYb resonance positions comes from the uncertainty in the measured scattering length for $^6$Li$^{174}$Yb, and hence on the potential scaling, as described below.

Table I also includes predictions for $^7$LiYb, where the resonances are a little wider because of the larger value of $\zeta_0$. However, in this case the 17% mass scaling increases the number of bound states from 24 to 26: the scattering length obtained for $^7$LiYb, and the positions of the resonances, are far more sensitive to the depth of the potential. For $^7$LiYb, the predicted resonance positions could easily be in error by several hundred Gauss. An experimental measurement of the scattering length for $^7$LiYb would be needed to pin this down more accurately. Nevertheless, it is clear from Table I that the Feshbach resonances are very narrow for mixtures of $^7$Li with even-mass Yb isotopes, and this conclusion will not be altered by changes in the potential curve.

There is, however, a different mechanism that can create Feshbach resonances for Yb isotopes with nonzero spin ($^{171}$Yb, $i = 1/2$ and $^{173}$Yb, $i = 5/2$). Figure 1 shows that, as Li approaches Yb, it polarizes the spin density of Yb and creates a hyperfine coupling between the molecular spin and the nuclear magnetic moment of Yb. The hyperfine coupling produced in this way is substantially larger than the change in the Li hyperfine coupling. The operator $\Delta\zeta_{\text{Yb}}(R)\hat{i}_{\text{Yb}} \cdot \hat{s}$ has matrix elements that connect basis functions with $\Delta m_s = \pm 1$ and $\Delta m_{i,\text{Yb}} = \mp 1$. This coupling creates Feshbach resonances where states of the LiYb molecule cross atomic thresholds with values of $m_{f,\text{Li}}$ that differ by $\pm 1$, as shown by open circles in Fig. 2.

We have further extended MOLSCAT to handle the additional basis sets and couplings required for the $\Delta\zeta_{\text{Yb}}(R)$ coupling term, and have carried out coupled-channel calculations of the resonance positions and widths for $^6$Li$^{173}$Yb and $^7$Li$^{173}$Yb. The results are given in Table I. It may be seen that there are now resonances *more than 2 orders of magnitude wider* than for Li$^{174}$Yb, driven by a direct coupling involving $\Delta\zeta_{\text{Yb}}(R)\hat{i}_{\text{Yb}} \cdot \hat{s}$. The calculated widths range from 0.8 to 2.8 mG in width for $^6$Li$^{173}$Yb.

The criterion for producing molecules at a narrow resonance is that the field must vary smoothly enough to achieve adiabatic passage. Field calibration and field inhomogeneity are not necessarily a problem; it is high-frequency field
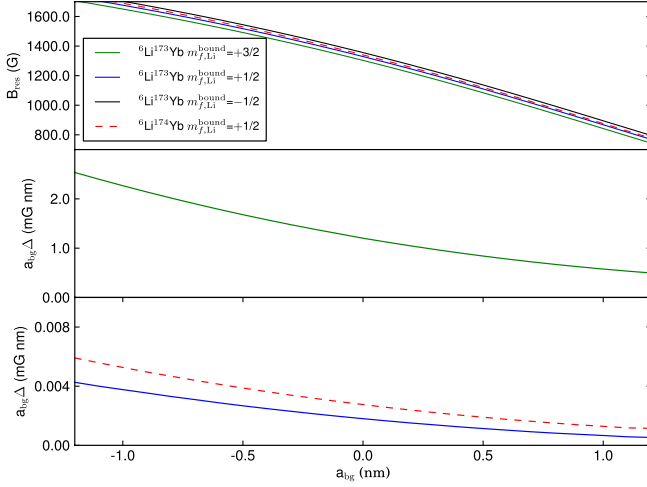
FIG. 3 (color online).   Positions and widths of the resonances at the lowest $M_{tot}(m_s = -1/2)$ threshold for $^6\text{Li}^{174}\text{Yb}$ (dashed) and $^6\text{Li}^{173}\text{Yb}$ (solid), as a function of the background scattering length produced by scaling the potential. The width is not shown for the very narrow $m_{f,\text{Li}}^{\text{bound}} = -1/2$ resonance of the $^6\text{Li}^{173}\text{Yb}$ system. The widths are shown as $a_{bg}\Delta$ because the product varies smoothly whereas $\Delta$ itself has a pole at $a_{bg} = 0$.

noise that must be reduced to well below the resonance width.

The main uncertainty in the resonance positions for $^6\text{LiYb}$ comes from the uncertainty in the measured scattering length. Figure 3 shows how the resonance positions and widths for $^6\text{Li}^{174}\text{Yb}$ and $^6\text{Li}^{173}\text{Yb}$ vary with the scattering length used to scale the potential. For $^7\text{Li}^{173}\text{Yb}$, as for $^7\text{Li}^{174}\text{Yb}$, the resonance positions depend quite strongly on the quality of the potential curve. However, the resonance widths for all isotopes depend mainly on the $\Delta\zeta(R)$ functions, obtained here from DFT calculations as described above, and are fairly insensitive to the depth of the potential.

At the fields where resonances occur for $^6\text{Li}^{173}\text{Yb}$, $m_s$ and $m_{i,\text{Yb}}$ are both reasonably good quantum numbers. For $^6\text{Li}^{173}\text{Yb}$, each line in Fig. 3 represents several levels with different values of $m_{i,\text{Yb}}$ and thus $M_{tot}$. These produce resonances very close together (within 0.2 G), but with different widths, because the matrix element of $\hat{i}_{\text{Yb}} \cdot \hat{s}$ between the spin functions $(m_s = +1/2, m_{i,\text{Yb}})$ and $(m_s = -1/2, m_{i,\text{Yb}} + 1)$ is $\frac{1}{2}[i_{\text{Yb}}(i_{\text{Yb}} + 1) - m_{i,\text{Yb}}(m_{i,\text{Yb}} + 1)]^{1/2}$. The resonance widths are proportional to the square of this. An experiment is likely to use Yb trapped in a single magnetic sublevel and would therefore sample only one of these resonances; for the lowest threshold ($m_{f,\text{Li}} = +1/2$), the different possible values for $m_{i,\text{Yb}}$ of $-5/2$, $-3/2$, $-1/2$, $+1/2$ and $+3/2$ lead to ratios in the resonance widths of 5:8:9:8:5, respectively. These ratios are confirmed by the numerical results. The resonance widths given for $^6\text{Li}^{173}\text{Yb}$ in Table I, for $M_{tot} = 0$, are for the widest of the group. There is no wide (Yb-driven)

resonance at this threshold for $m_{i,\text{Yb}} = +5/2$. The Yb-driven resonances for $^{171}\text{Yb}$ are substantially narrower than those for $^{173}\text{Yb}$, partly because $^{171}\text{Yb}$ has a smaller nuclear magnetic moment but mostly because the matrix element of $\hat{i}_{\text{Yb}} \cdot \hat{s}$ is much smaller (1 on the scale of the ratios above).

Resonances can also occur for Li atoms in magnetically excited states ($m_{f,\text{Li}} = -1/2$ and $-3/2$) at the crossing points shown in Fig. 2. However, the molecular states that are produced at these resonances are quasibound at energies above the lowest threshold. We have characterized these states by carrying out scattering calculations immediately below the $m_{f,\text{Li}} = -1/2$ threshold and fitting them to obtain Breit-Wigner widths $\Gamma$ [30]. For the $V_+$ potential, the states with $m_{f,\text{Li}}^{\text{bound}} = +3/2$ and $+1/2$ have calculated widths $\Gamma/h = 715$ and 2.9 Hz, corresponding to lifetimes $\tau = \hbar/\Gamma = 0.22$ and 55 ms, respectively, while the state with $m_{f,\text{Li}}^{\text{bound}} = -1/2$ is too narrow to characterise. At decaying resonances of this type, the real part $\alpha(B)$ of the complex scattering length $a(B)$ exhibits an oscillation of magnitude $a_{\text{res}}$ rather than an actual pole [29]. We obtain $a_{\text{res}} = 3.4$ fm, 1.3 $\mu$m and 4.0 $\mu$m, respectively, for these three resonances. For the two higher-field resonances the behavior is sufficiently polelike to extract values of $\Delta$, which are 824 and 1.2 $\mu$G, respectively.

In conclusion, we have investigated the possibility of using Feshbach resonances to produce ultracold LiYb molecules by magnetoassociation of ultracold atoms. The mechanism that we previously identified for RbSr [15] exists for LiYb, but produces only extremely narrow Feshbach resonances in this case. However, we have identified a new mechanism, which occurs only for Yb isotopes with nonzero nuclear spin ($^{171}\text{Yb}$, $^{173}\text{Yb}$) that can produce Feshbach resonances that are orders of magnitude wider. However, even for $^6\text{Li}^{173}\text{Yb}$ the largest calculated resonance width is 2.8 mG. Achieving the field stability to produce molecules at such a narrow resonance will be experimentally challenging.

*daniel.brue@durham.ac.uk
†J.M.Hutson@durham.ac.uk

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