

## ARTICLE

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# Nuclear-spin dependent parity violation in optically trapped polyatomic molecules

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Improved nuclear spin-dependent parity violation measurements will enable experimental determination of poorly known electroweak coupling parameters. Here, we investigate the suitability of optically trapped linear polyatomic molecules as probes of nuclear spin-dependent parity violation. The presence of closely spaced, opposite-parity  $\ell$ -doublets is a general feature of such molecules, allowing parity-violation-sensitive pairs of levels to be brought to degeneracy in magnetic fields typically 100 times smaller than in diatomics. Assuming laser cooling and trapping of polyatomics at the current state-of-the-art for diatomics, we expect to measure nuclear spin-dependent parity-violating matrix elements  $iW$  with 70 times better sensitivity than the current best measurements. Our scheme should allow for 10% measurements of  $iW$  in nuclei as light as Be or as heavy as Yb, with averaging times on the order of 10 days and 1 s, respectively.

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Measurements of nuclear spin-independent (NSI) and nuclear spin-dependent (NSD) parity violation (PV) are a means to probe standard model (SM) electroweak interactions on a tabletop scale<sup>1</sup>. NSI-PV has been measured in protons and a number of heavy atoms<sup>2–9</sup> and found to be in good agreement with SM PV predictions due to the weak charge  $Q_W$ . However, the only non-zero measurement (14% relative uncertainty) of NSD-PV in an atomic system comes from Cs<sup>10</sup>, and this result implies constraints on SM meson-nucleon couplings which are in disagreement with other atomic PV measurements<sup>11,12</sup>. NSD-PV arises primarily from three interactions: vector electron-axial nucleon electroweak current coupling ( $V_e A_n$ ), the nuclear anapole moment, and the combined effects of nuclear weak charge and normal hyperfine structure. The  $V_e A_n$  effect is described by two parameters  $C_{2u}$  and  $C_{2d}$  relating to spin-dependent  $Z_0$  boson exchange between an electron and an up or down quark, respectively. These parameters are among the most poorly measured in the SM, with relative uncertainties 300 and 70%, respectively<sup>13</sup>. PV measurements may also probe beyond standard model physics<sup>14,15</sup>. Searches for oscillating PV signals have been proposed as a means to detect axion-like particles, a leading dark matter candidate<sup>16</sup>.

A beam of cold diatomic molecules has been demonstrated<sup>17–21</sup> to be a highly sensitive system for measuring NSD-PV effects. Mixing of opposite-parity quantum states from PV effects is amplified when the states have nearly the same energy<sup>6</sup>. The lowest two rotational states of diatomic molecules have opposite parity and may be brought to near degeneracy using a large magnetic field  $B$ . While this method is quite general, current systematic uncertainties are roughly 100 times too large to measure NSD-PV in the lightest nuclei where nuclear structure calculations are tractable<sup>22</sup>.

Recent advances in laser cooling have led to optically trapped diatomic molecules with sub-Doppler temperature and single-molecule detection efficiency<sup>23</sup>, while similar strides with polyatomic molecules have followed closely behind<sup>24–28</sup>. Moreover, polyatomic molecules have been proposed as exquisite systems for precision measurements of fundamental symmetries<sup>29–31</sup> and time variation of fundamental constants<sup>32,33</sup>.

Here, we show that linear asymmetric polyatomic molecules in an optical trap are well-suited for measurement of NSD-PV. Polyatomic molecules possess opposite-parity states 10–1000 times closer in energy than diatomics, requiring similarly smaller B-fields. Systematic uncertainties are reduced compared to beam experiments due to the lower magnetic field and a smaller interaction volume. Furthermore, these smaller fields may be produced without superconducting magnets, allowing trivial B-field reversal for detection and mitigation of systematic effects. We show that these molecules may be optically trapped using “magic” conditions where differential light shifts are small enough for a precise PV measurement. The obvious advantage of performing a precision measurement on trapped species compared to a beam is the increased interaction time  $\tau$ . The sensitivity to any PV matrix element  $iW$  is  $\delta W/W = 1/\tau\sqrt{N_m}$ , where  $N_m$  is the total number of measurements ( $iW$  is purely imaginary due to conservation of time-reversal symmetry). Assuming optical trapping of polyatomic molecules at the current state-of-the-art for diatomics<sup>23,34,35</sup>, we expect at least a factor of 70 increase in PV sensitivity over the state-of-the-art BaF measurement<sup>20,36</sup>. Our method is applicable to all laser-coolable polyatomic molecules with  $^2\Sigma$  ground states, and possibly others.

## Results

**Relevant properties of polyatomic molecules.** Consider the properties of linear asymmetric molecules with a  $^2\Sigma^+$  electronic

ground state. If a bending vibrational mode (with vibrational constant  $\omega_b$  and quantum number  $\nu_b$ ) is excited and all other vibrational modes are in their ground state, the molecule’s rotational angular momentum  $\mathbf{N}$  has a projection along the molecular axis  $\ell = \pm \nu_b, \pm(\nu_b - 2), \dots, \pm 1$  or 0. Within this vibrational manifold, the effective Hamiltonian is

$$H = B_e(\mathbf{N}^2 - \ell^2) \pm (-1)^N \frac{q_e}{2} \mathbf{N}^2 + \gamma \mathbf{N} \cdot \mathbf{S} + b \mathbf{I} \cdot \mathbf{S} + c I_z S_z - e \mathbf{T}^2(\nabla \mathbf{E}) \cdot \mathbf{T}^2(\mathbf{Q}) + (\mu_B g_S \mathbf{B} \cdot \mathbf{S} + \mu_B g_L \mathbf{B} \cdot \mathbf{L} + \mu_N g_I \mathbf{B} \cdot \mathbf{I}), \quad (1)$$

where  $B_e$  is the rotational constant,  $\gamma$  is the spin-rotation (SR) constant,  $b$  and  $c$  are hyperfine (HF) constants,  $e$  is the electron charge,  $\mathbf{T}^2(\nabla \mathbf{E}) \cdot \mathbf{T}^2(\mathbf{Q})$  is a scalar product of rank-2 spherical tensors describing the electric field gradient  $\nabla \mathbf{E}$  at the nucleus with quadrupole moment  $\mathbf{Q}$ ,  $\mathbf{S}$  is the electron spin,  $\mathbf{L}$  is the electron orbital angular momentum, and  $\mathbf{I}$  is the nuclear spin<sup>37,38</sup>. The upper (lower) sign corresponds to the parity  $P$  of the closely spaced “ $\ell$ -doublet” eigenstates  $|N, \nu_b^\ell, P = \pm\rangle = \frac{1}{\sqrt{2}} (|N, +\ell\rangle \pm (-1)^{N-\ell} |N, -\ell\rangle)$ . The  $\ell$ -doublet is the key property of polyatomic molecules absent from diatomics which we wish to exploit for a PV measurement. In linear modes, as well as diatomics, opposite-parity levels are spaced by roughly the rotational constant  $B_e/2\pi \sim 1$  GHz to 100 GHz. In an excited bending mode, opposite-parity states are spaced by only  $q_b \approx -2B_e^2/\omega_b$ , which is on the order of  $q_b/2\pi \sim 10$  MHz to 100 MHz. The relative spacing between levels may be tuned to degeneracy via the Zeeman interaction (last three terms of Eq. (1)), with  $\mu_B$ ,  $\mu_N$  the Bohr and nuclear magneton, respectively; and  $g_S$ ,  $g_L$ , and  $g_I$  the  $g$ -factors corresponding to  $\mathbf{S}$ ,  $\mathbf{L}$ , and  $\mathbf{I}$ , respectively). Examples are provided in Supplementary Note 1.

**Nuclear spin-dependent parity violation.** For a given electronic state of a molecule, the effective NSD-PV Hamiltonian is<sup>39</sup>

$$H_p^{\text{eff}} = \kappa W_p (\mathbf{S} \times \hat{\mathbf{I}}) \cdot \hat{\mathbf{n}}. \quad (2)$$

Here,  $W_p$  encodes the overlap of unpaired electrons with the nucleus and can be calculated with high accuracy by ab initio or semiempirical methods,  $\hat{\mathbf{n}}$  is a unit vector along the molecular axis, and  $\kappa$  is the measurable parameter of interest. In a given nucleus, various NSD-PV effects contribute to  $\kappa = \kappa_2 + \kappa_a + \kappa_Q$ .  $\kappa_2$  is proportional to the strength of the  $V_e A_n$  coupling, and is independent of nuclear mass  $A$  (for a typical nucleus,  $|\kappa_2| \simeq 0.05$ ).  $\kappa_a$  is proportional to the nuclear anapole moment and is proportional to  $A^{2/3}$ .  $\kappa_Q$  is due to the combined effects of nuclear weak charge and normal hyperfine structure, and is negligible compared to  $\kappa_2$  and  $\kappa_a$ <sup>40</sup>. Measurements in several nuclei are required to distinguish among the different NSD-PV effects.

Ultimately, the ability to precisely determine  $\kappa$  and its underlying contributions will be limited to the accuracy of theoretical values of  $W_p$ . Calculations of  $W_p$  have been performed on several diatomic molecules via Dirac-Hartree-Fock and relativistic density-functional<sup>41</sup>, quasirelativistic zero-order regular approximation<sup>29,42</sup>, and (with an estimated 1.5% accuracy) relativistic coupled-cluster<sup>43</sup> methods. While such calculations are beyond the scope of this proposal, a semiempirical method may be used to calculate  $W_p$  for any species to  $\sim 10\%$ , assuming the SR/HF constants in Eq. (1) are known<sup>17</sup>. The SR/HF constants relating to a typical metal atom  $M$  differ by a  $\sim 10\%$  between laser-coolable monofluorides  $MF$  and  $MX$  molecules, where  $X$  is a suitable ligand with charge state  $-1$  (e.g., OH, NC, or CCH). Thus, we expect similar 10% accuracy when estimating  $W_p$  for  $MX$ , using either  $MX$  SR/HF constants for a semiempirical calculation or a more detailed method described above for the

corresponding MF. This approximation is in line with available theoretical values  $W_p(\text{Ra})$  in  $\text{RaF}^{41,42}$  and  $\text{RaOH}^{29}$ . In Table 1, we give a list of laser-coolable polyatomic molecules MX, with  $W_p$  from calculations on MX where available or MF otherwise (see also Supplementary Note 2).

In general, Eq. (2) should be summed over all nuclei  $i$  with spin  $I_i \geq 1/2$  in a molecule. The PV signal is easiest to interpret when the unpaired electron is centered on one atom in the molecule, i.e.  $W_p^{(i)} \approx 0$  for all but one atom. A single-atom-centered unpaired electron is also a defining characteristic of laser-coolable molecules: this electron interacts negligibly with the nuclear vibration of the molecule, leading to electronic transitions which are highly diagonal in vibrational quantum number (and thus requires a small number of vibrational repump lasers for cooling)<sup>44</sup>. Laser cooling schemes have been proposed for molecules with an electron centered on atoms with a wide range of mass (as light as  $\text{Be}^{45}$  and  $\text{B}^{46}$ , and as heavy as  $\text{Yb}^{47}$  and  $\text{Tl}^{48,49}$ ), and extension to polyatomic species, while technically more complicated, is straightforward<sup>27</sup>.

$H_p^{\text{eff}}$  is a pseudoscalar interaction, which connects states with different parity  $P$  and the same lab frame angular momentum projection  $m_F$ . We dub such states  $|\tilde{\eta}; m_F, +\rangle, |\tilde{\eta}'; m_F, -\rangle$  a “PV pair”, with  $\tilde{\eta}$  denoting all other nominal quantum numbers when  $B=0$ . So long as the  $\ell$ -doublet splitting is not smaller than all SR/HF splittings, PV pairs of a given rotational manifold  $N$  cross in an applied B-field when  $\mu_B B \sim q_b$ . This situation is common for light molecules due to their typically smaller HF interactions and larger  $q_b$  arising from their larger rotational constant  $B_e$ . Typical values of  $q_b$  imply a modest field of  $B \sim 1$  mT to 10 mT will bring a PV pair to degeneracy. For instances where the  $\ell$ -doublet splitting is smaller than all SR and HF intervals, states  $|\tilde{\eta}; m_F, \pm\rangle$  remain split by  $\sim q_b$  for any applied B-field. In this case, the Zeeman interaction repels this  $\ell$ -doublet from a neighboring  $|\tilde{\eta}'; m_F, \pm\rangle$  doublet, preventing the crossing of PV pairs  $|\tilde{\eta}; m_F, \pm\rangle, |\tilde{\eta}'; m_F, \mp\rangle$ . Examples are provided in Supplementary Note 1. Regardless of the hierarchy of  $\ell$ -doubling, SR, and HF interactions, PV crossings always occur between neighboring rotational levels at  $\mu_B B \approx B_e$ , as in a diatomic molecule<sup>19</sup>, but require an experimentally more challenging  $B \sim 100$  mT to 1000 mT<sup>19</sup>.

In some cases, it may be advantageous to measure  $iW$  in a more highly-excited rotational or vibrational state. For example, consider  $^{171}\text{YbOH}$  ( $I(^{171}\text{Yb})=1/2$ ). We may estimate the relevant parameters in Eq. (1) by reduced-mass-scaling (where appropriate) the constants  $B_e, \omega_{b=2}, \gamma, b(\text{H})$ , and  $c(\text{H})$  from the  $^{174}\text{YbOH}$  isotopologue ( $I(^{174}\text{Yb})=0$ )<sup>50</sup>, by assuming constants  $b(\text{Yb})$  and  $c(\text{Yb})$  to be the same as in chemically similar  $^{171}\text{YbF}$ ; and by taking  $q_b = -2B_e^2/\omega_2$ . With these parameters, the  $\ell$ -doublet in  $|\nu_b^\ell = 1^1, N=1\rangle$  is smaller than the SR and Yb HF interactions. For all possible PV pairs, the value of  $\langle (\mathbf{S} \times \hat{\mathbf{I}}(\text{Yb})) \cdot \hat{\mathbf{n}} \rangle$  is only nonzero due to the small state mixing from the HF interaction with the H nucleus. However, in  $|\nu_b^\ell = 1^1, N=2, 3\rangle$ , the  $\ell$ -doublet is larger than the Yb HF splitting and multiple PV pairs with  $\langle (\mathbf{S} \times \hat{\mathbf{I}}(\text{Yb})) \cdot \hat{\mathbf{n}} \rangle \sim 0.1$  exist.

**Measurement procedure.** We now propose a procedure to trap polyatomic molecules and measure matrix elements  $iW$  of  $H_p^{\text{eff}}$ . A cryogenic buffer gas beam source creates a slow, cold beam of the desired molecule species<sup>51,52</sup>. Molecules are sequentially laser-slowed<sup>53</sup>, trapped using a magneto-optical trap (MOT)<sup>54</sup>, and loaded into a red-detuned optical dipole trap (ODT) while performing  $\Lambda$ -enhanced cooling<sup>35</sup>. Then, one of the cooling laser frequencies is turned off in order to optically pump molecules into a single, optically dark SR/HF state. Stimulated Raman

**Table 1 Parameters for parity violation measurement in polyatomic molecules**

Species	$I$	$100\kappa_a$	$100\kappa_2$	$W_p/2\pi$ (Hz)	$W^m/2\pi$ (Hz)
$^9\text{BeNC}$	3/2	-0.66	-5.0	0.46 <sup>43</sup>	0.010
$^{25}\text{MgNC}$	5/2	-1.4	-5.0	4.91 <sup>43</sup>	0.13
$^{43}\text{CaOH}$	7/2	-2.1	-5.0	10.8 <sup>43</sup>	0.31
$^{87}\text{SrOH}$	9/2	-3.4	-5.0	51 <sup>43</sup>	1.7
$^{137}\text{BaOH}$	3/2	4.1	3.0	147 <sup>43</sup>	4.2
$^{171}\text{YbOH}$	1/2	3.9	1.7	576 <sup>41</sup>	12.9
$^{225}\text{RaOH}$	1/2	-4.7	-5.0	1400 <sup>29</sup>	54

Values of  $W_p$  are taken to be equal to the value calculated for the corresponding metal-fluoride molecule<sup>41,43</sup>, except  $\text{RaOH}$  for which a calculation exists<sup>29</sup>. Values for  $\kappa_2$  assume  $C_{2N} = -0.05$ ; values for  $\kappa_a$  assume weak neutron-nucleus coupling  $g_N = -1$ .  $W^m$  is the value of  $W$  with typical maximal  $\langle (\mathbf{S} \times \hat{\mathbf{I}}) \cdot \hat{\mathbf{n}} \rangle = 0.4$  (see Supplementary Note 2 for further details)

adiabatic passage completes state preparation by efficiently transferring to the  $|\nu_b^\ell = 1^1, N, \eta, m_F, P = (-1)^N\rangle$  state<sup>55,56</sup>. Performing the measurement in an ODT allows for long interaction times while only requiring precise field control over a small volume.

The PV signal is measured by the Stark interference method, which has been examined in detail elsewhere<sup>6,7,19</sup>. We summarize the main points closely following the notation of Cahn et al.<sup>36</sup>. We apply a static magnetic field  $\mathbf{B} = B\hat{z}$  to shift a particular PV pair to near degeneracy. We denote the time-dependent probability amplitudes of these states  $c_\pm(t)$ , and assume an initial state  $c_-(0)=1, c_+(0)=0$ . An oscillating electric field  $\mathbf{E} = E_0 \cos(\omega_E t) \hat{z}$  is applied to drive the transition between the near-degenerate levels. The effective Hamiltonian  $H_\pm^{\text{eff}}$  for the two-level system can be written<sup>36</sup>

$$H_\pm^{\text{eff}} = \begin{pmatrix} \Delta & d E_0 \cos(\omega_E t) + i W \\ d E_0 \cos(\omega_E t) - i W & -\alpha' E_0^2 \cos^2(\omega_E t)/2 \end{pmatrix}. \quad (3)$$

Here  $\Delta$  is the small detuning from degeneracy,  $d$  is the transition dipole moment, and  $\alpha'$  is the differential polarizability of the two states. In the limit where  $W \ll d E_0, \Delta \ll \omega_E$ , and assuming for now that  $\alpha' = 0$ , the PV signal  $S = |c_+(t)|^2$  is

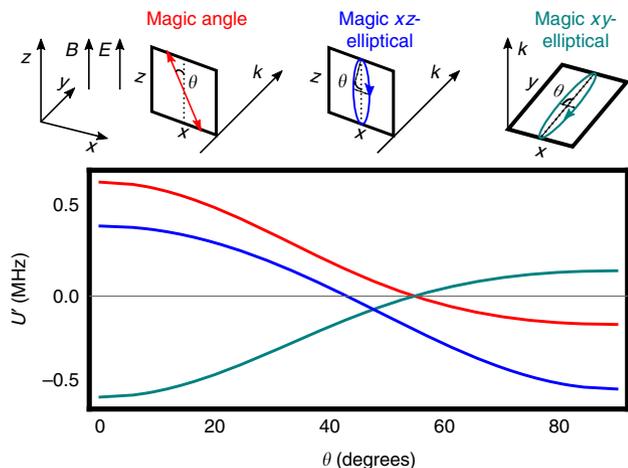
$$S \approx 4 \left[ 2 \frac{W d E_0}{\Delta \omega_E} + \left( \frac{d E_0}{\omega_E} \right)^2 \right] \sin^2 \left( \frac{\Delta t}{2} \right). \quad (4)$$

From Eq. (4), we see that the combined PV and electric dipole transition probability (first term in square brackets) interferes with the standard electric dipole transition probability (second term in square brackets). The interference term changes sign under a reversal of either  $\mathbf{E}, \mathbf{B}$ , or  $\Delta$ . The PV matrix element  $iW$  may be extracted through an asymmetry measurement<sup>19</sup>

$$\mathcal{A} = \frac{S(+E_0) - S(-E_0)}{S(+E_0) + S(-E_0)} = 2 \frac{W \omega_E}{\Delta d E_0} + \dots, \quad (5)$$

where the ellipse denotes higher order terms in  $W/\Delta$ . Detection using optical cycling should provide shot noise-limited readout<sup>57</sup>.

**Estimates of broadening and systematic uncertainties.** Sensitivity to  $iW$  is expected to be limited by inhomogeneous broadening of  $\Delta$ . For optically trapped molecules, the detuning uncertainty  $\delta\Delta$  is dominated by the differential Stark shift due to the optical trap. Employing certain “magic” polarization conditions in an ODT<sup>58–62</sup> will set  $\alpha' = 0, U' = 0$ , and  $\delta\Delta = \delta U' = \frac{\partial U'}{\partial \theta} \delta\theta$ , where  $U$  is the trap depth,  $U'$  is the differential trap depth, and  $\theta$  is an angle related to the polarization. We investigated three such magic conditions for PV pairs in  $\text{MgNC}$



**Fig. 1** Polarization sensitivity for magic optical trapping. The Differential ac Stark shift  $U'$  is plotted as a function of polarization angle  $\theta$  as defined in the figures for the nominal  $|N=1, J=1/2, F=3, m_F=3, P=+\rangle, |N=1, J=3/2, F=3, m_F=3, P=-\rangle$  parity violation (PV) pair in  $^{25}\text{MgNC}$ . For each configuration  $U=1.2$  MHz for the PV pair when  $U'=0$  at  $\theta_{\text{magic}}$ . The calculation is performed with  $B \approx 8.072$  mT such that the PV pair is degenerate in the absence of the trapping field. (Red) linear polarization in the  $x, z$ -plane, (blue) elliptical polarization in  $x, z$ -plane, (green) elliptical polarization in  $x, y$ -plane

and  $\text{YbOH}$  and find  $\frac{\partial U'}{\partial \theta} = U/(\theta - \theta_{\text{magic}})$  is typical. Figure 1 demonstrates magic conditions for one PV pair in  $\text{MgNC}$ . In producing magic conditions with a general elliptical polarization, we estimate  $\delta\theta/\theta \sim 10^{-361}$ , while for linear polarized light,  $\delta\theta/\theta < 10^{-4}$  is possible using high-quality Glan-type polarizers. We, therefore, expect  $\delta U'/U \sim 10^{-4}$  using a magic angle trap<sup>58,59</sup>, where the ODT linear polarization is rotated by  $\theta_{\text{magic}} = \cos^{-1}(\frac{1}{\sqrt{3}}) \approx 54.7^\circ$  with respect to the quantization axis. For  $U = 2\pi \times 1$  MHz,  $\delta\Delta = 2\pi \times 100$  Hz.

An inhomogeneous  $\mathbf{B}$ -field will also produce broadening; typically  $\delta\Delta \approx \mu_B \delta B$ <sup>21</sup>. We require  $\delta B \ll 1/\delta U \mu_B \lesssim 1$  nT for  $\mathbf{B}$ -field inhomogeneity to not limit sensitivity. This implies  $\delta B/B = 10^{-7}$  for the largest fields we may require,  $B = 10$  mT. For comparison, the recent BaF NSD-PV measurement demonstrated  $\delta B/B = 10^{-8}$ , even with the much more experimentally challenging  $B \approx 460$  mT<sup>20,21</sup>. We expect that the ability to easily reverse a smaller field will further aid in detecting and eliminating  $\mathbf{B}$ -field inhomogeneities. Moreover, the field must only be homogenous over a small, fixed interaction volume for an ODT. For measurements in a molecular beam, the interaction volume grows proportional to the interaction time; in a fountain or free fall configuration, the interaction volume grows proportional to the square of the interaction time. The smaller interaction volume in an ODT implies that systematic uncertainties involving field gradients should also be reduced. In order to prevent temporal fluctuations from limiting sensitivity, we will require fluctuations  $\delta B \lesssim 1$  nT for all timescales longer than  $1/\omega_E$ , the shortest relevant timescale in the experiment.

From Eq. (3), we see that electric dipole and NSD-PV transition amplitudes are  $\pi/2$  out of phase, and there is no interference in a static  $\mathbf{E}$ -field. However, the presence of a non-reversing  $\mathbf{E}$ -field  $E_{\text{nr}}$  still poses an issue. In the molecule frame, a static  $E_{\text{nr}}$  has significant frequency components at axial and radial ODT frequencies  $\omega_z, \omega_r$ , and multiples, sums, and differences thereof. Assuming uncorrelated trap oscillations, this effect will lead to an inhomogeneous broadening much smaller than that of

the differential ac Stark shift. Accurate measurement of  $E_{\text{nr}}$  is possible by Stark interference with a reversible pulsed dc field  $E_r$ <sup>21</sup>, or by microwave depletion spectroscopy<sup>63</sup>. Finally, investigating multiple PV pairs in the same molecule provides strong systematic error rejection by varying the ratio  $\langle (\mathbf{S} \times \hat{\mathbf{I}}) \cdot \hat{\mathbf{n}} \rangle/d$  by a calculable, possibly large, amount<sup>19</sup> (see Supplementary Note 3). For example, in PV pairs with different signs of  $\langle (\mathbf{S} \times \hat{\mathbf{I}}) \cdot \hat{\mathbf{n}} \rangle/d$ , contributions to  $\mathcal{A}$  from actual NSD-PV will switch sign, but contributions from  $E_{\text{nr}}$  will not.

Other relaxation mechanisms are expected to lead to negligible broadening compared to differential ac Stark shifts. For example, in a beam experiment,  $\delta\Delta$  is typically limited by interaction time  $\tau$ , with  $\tau \sim 100 \mu\text{s}$ <sup>20</sup>. In an ODT,  $\tau$  may easily exceed 1 s. Trapped molecule lifetimes  $\tau_{\text{trap}} = 0.5$  s to 25 s have been reported in a variety of traps<sup>23,55,64,65</sup>. With near-ideal vacuum conditions, we expect trap lifetimes  $\tau_{\text{trap}} \sim 10$  s, limited by vibrational decay. The loss rate due to off-resonant scattering from the trapping laser can typically be made  $R_{\text{sc}} \lesssim 1 \text{ s}^{-1}$  by using standard mid-infrared wavelength fiber lasers. Typical inelastic collision cross sections are expected to be  $\sigma_{\text{in}} \lesssim 10^{-9} \text{ cm}^2/\text{s}$ . Comparing with the trapping conditions of Cheuk et al.<sup>35</sup>, with  $N = 1300$  molecules at density  $n = 6 \times 10^8 \text{ cm}^{-3}$ , we estimate an inelastic molecule-molecule collision rate of  $R_{\text{in}} \approx 0.5 \text{ s}^{-1}$ . Therefore, collisions will become important when trapped molecule number  $N \gtrsim 10^5$ , or with additional cooling.

**Estimated sensitivity to parity violating effects.** We now estimate the sensitivity of our method to NSD-PV matrix elements,  $\delta W = 1/\tau \sqrt{RNT}$ , where  $R$  is the repetition rate,  $N$  the number of trapped molecules per measurement, and  $T$  the total measurement time. We assume molecules are trapped in a  $U = 2\pi \times 1$  MHz deep magic angle trap, with  $\delta\theta/\theta = 10^{-4}$ . The combined effects of all relaxation times considered should allow for interaction times of  $\tau \lesssim 1$  s, but optimum sensitivity is achieved by setting the interaction time equal to the coherence time of the system:  $\tau = \frac{1}{\delta\Delta} \approx \frac{1}{U} \frac{\partial U'}{\partial \theta} \approx 1.6$  ms. Allowing  $t_{\text{MOT}} = 50$  ms to load the MOT and  $t_{\text{trans}} = 40$  ms for state transfer, repetition rates  $R = 10 \text{ s}^{-1}$  should be possible. We expect that with molecules produced from an isotopically enriched source,  $N \approx 1000$  for all species; this would be equivalent to the best to-date sample of directly cooled molecules in an ODT<sup>35</sup>. Under these conditions, our expected experimental sensitivity is  $\delta W \approx 2\pi \times 1 \text{ Hz}/\sqrt{\text{Hz}}$ . This represents a factor of 70 improvement over the best to-date NSD-PV measurement in BaF<sup>20,21,36</sup>. More ambitiously, one could plausibly expect  $N = 10^5$  to  $10^6$  could be achieved with improved loading and cooling efficiency<sup>31,66</sup>.

## Discussion

With the proposed sensitivity, it should be possible to separate contributions to  $\kappa$  from nuclear anapole ( $\kappa_a \propto A^{2/3}$ ) and  $V_e A_n$  ( $\kappa_2$   $A$ -independent) effects by measuring NSD-PV in a variety of nuclei. With the only non-zero NSD-PV measurement to-date in the heavy  $^{133}\text{Cs}$ <sup>10</sup>, a precise measurement of PV in a light system would be especially illuminating. In light nuclei,  $\kappa \approx \kappa_2$ . As stated,  $\kappa_2$  depends upon  $C_{2u,d}$  which are among the most poorly known SM parameters and are suppressed at tree level. Thus, a precise measurement of NSD-PV in light systems could potentially be sensitive to beyond SM physics above the 1 TeV scale<sup>14</sup>. In molecules such as BeNC and MgNC, the nuclear and molecular calculations are highly tractable. Furthermore,  $W_p(N) \sim W_p(C) \sim 2\pi \times 10$  mHz in these systems; a single species could provide a 10% measurement of  $\kappa$  for three nuclei ( $^{13}\text{C}$ ,  $^{14}\text{N}$ , and either  $^9\text{Be}$ ,  $^{10}\text{Be}$ , or  $^{25}\text{Mg}$ ) with  $T \lesssim 100$  hours per nucleus. The nuclear

structure of  $^{14}\text{N}$  is of special interest and well studied due to the anomalously long  $^{14}\text{C} \rightarrow ^{14}\text{N}$  half-life and their role in radio-carbon dating<sup>22</sup>.

Because  $iW$  is enhanced by  $\approx Z^2 A^{2/3}$  in heavy species<sup>41,42</sup>, RaOH appears especially promising<sup>29</sup>. However, the high mass is a hindrance to effective laser-slowing by the standard methods for molecules<sup>52,53</sup>. Moreover, the longest-lived Ra isotope possessing nuclear spin ( $^{225}\text{Ra}$ ) has a half-life of only 15 days. New techniques beyond those proposed here may be required to produce trapped RaOH in sufficient quantity for precision measurement. Nevertheless, MOTs of atomic  $^{225}\text{Ra}$  with typical  $N = 1000$  have been produced for atomic electric dipole measurements<sup>67</sup>; with our expected sensitivity, only  $N = 300$  total molecules would need to be detected for  $\delta W/W = 0.1$ .

We have shown that optically trapped polyatomic molecules offer a dramatically enhanced sensitivity to parity-violating effects and additional checks of systematic errors. Restriction to laser-coolable species still allows for measurement of NSD-PV in nuclei with a wide range of masses, necessary for the determination of key SM parameters and tests of beyond SM physics. The improved sensitivity should enable measurements of NSD-PV even in light nuclei where calculations are highly accurate.

Here, we have only considered linear asymmetric molecules. Symmetric top molecules possess  $k$ -doublets of opposite parity (similar to  $\ell$ -doublets) even in their vibrational ground state. For most  $^2A_1$  states (analogue of  $^2\Sigma$ ), the  $k$ -doublet splitting ( $\sim 10$  kHz) is smaller than SR/HF and thus not suitable for Zeeman tuning PV pairs to degeneracy for a NSD-PV measurement. However, the close spacing and miniscule differential Zeeman and ac Stark shifts of  $k$ -doublets may make symmetric top molecules in a magnetic or optical trap ideal for measuring NSI-PV.

### Data availability

The data that support the findings of this study are available from the corresponding author on request.

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### Author contributions

E.B.N. conceived the research proposal. E.B.N., D.S.B., S.E., J.A.F., N.N.K. and J.S. contributed to analysis and interpretation of the data, and in preparing the manuscript.

### Additional information

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