Journal of the Optical Society of America B
OPTICAL PHYSICS

Theoretical study of the measurement of electric field strength based on the pendular spectra of linear $(HCCCN)_n$ $(n = 1-3)$ molecules

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Received 23 April 2021; revised 13 August 2021; accepted 24 August 2021; posted 25 August 2021 (Doc. ID 428553); published 13 September 2021

The pendular spectra of linear $(HCCCN)_n$ $(n = 1-3)$ molecules at several rotational temperatures under a certain range of electric field strength E are calculated using the finite element matrix diagonalization method. In addition, the normalized "Q-branch" intensity (I_Q) and the gradient (K_E) of I_Q under corresponding conditions are investigated. Based on the results, the range and sensitivity of measuring the electric field strength with linear $(HCCCN)_n$ $(n = 1 - 3)$ molecules are analyzed. A scheme to measure electric field strength based on $(HCCCN)_n$ $(n = 1 - 3)$ with high sensitivity is proposed and the spatial resolution is also discussed. The feasibility of measuring the electric field strength of the electrostatic Stark decelerator based on a pendular spectrum is studied.

https://doi.org/10.1364/JOSAB.428553

1. INTRODUCTION

In research fields such as spectroscopic measurements [1], electrostatic Stark deceleration of molecules [2–5], and the measurement of the electron's electric dipole moment [6], the accurate value of the electrostatic field strength has a critical effect on the experimental results. There are two traditional electric field measurement methods. One is the electric potential difference method using the spherical electric field meter [7] and the field-mill electric field sensor [8]. The other is the electro-optical method, and corresponding applications include sensors using the electro-optical Kerr effect [9] and the electrostrictive effect [10]. These two measurement methods use detectors with large probes and complex internal structures, which means they are susceptible to interference and have a low spatial resolution (dozens of centimeters). Some other methods developed in the laboratory to measure electric fields that are based on microelectromechanical system sensors [11] and atomic and molecular Stark spectra [12,13], have limited measurement ranges (typically $1 - 10^4$ V/cm). Therefore, an electric field measurement method with a broader range and higher resolution is needed.

In the 1990s, Block *et al.* [14] and Rost *et al.* [15] reported experimental and theoretical studies on pendular spectra of $(HCN)_3$ in a strong electrostatic field, respectively. Under field-free conditions, the C-H vibrational spectra of the $(HCN)_3$ molecules have $P\,(\Delta J = -1)$ and $R\ (\Delta J = +1)$ branches. When $(HCN)_3$ are exposed in a strong external electric field, a so-called "Q-branch" spectrum appears. Then, Slenczka *et al.* studied the pendular spectrum driven by a magnetic field [16]. Yang *et al.* measured the pendular spectrum of the C-H vibration of $(HCCCN)_3$ [17]. Subsequently, pendular states and pendular spectra of molecules were studied in molecular dissociation processes [18], the manipulation of molecules [19], the orientation and alignment of polar molecules in laser fields [20–23], and quantum computing [24–26]. These studies have further broadened the application of pendular spectra. Our group proposed a method using the normalized "Q-branch" intensity of linear $(HCCCN)_3$ pendular spectra to measure the 3D vector and spatial distribution of electric fields [27].

In the present work, the pendular spectra and the corresponding normalized "Q-branch" intensity I_Q of $(HCCCN)_n$ $(n = 1 - 3)$ at various rotational temperatures (T = 1 K, 10 K, and 30 K) under different electric field strengths (E = 0 V/cm, 500 V/cm, 5000 V/cm, and 50,000 V/cm) are calculated. The gradient curves of I_Q with the variation of electrostatic field strength are also calculated. Finally, the feasibility of using $(HCCCN)_n$ $(n = 1 - 3)$ to measure the electric field strength in electrostatic Stark deceleration experiments is analyzed and discussed.

2. NUMERICAL CALCULATION METHOD

The detailed theory of pendular spectra has been introduced in our previous study [27]. Here, only a brief description is provided. The field-free linear $(\mathrm{HCCCN})_n$ $(\mathrm{n} = 1-3)$ molecules are free rotors, and the Schrödinger equation can be expressed as

$$\frac{\boldsymbol{J}^2}{2\boldsymbol{I}} |J, M\rangle = \boldsymbol{BJ}(\boldsymbol{J}+\mathbf{1})\, |J, M\rangle , \tag{1}$$

where, $\boldsymbol{J}^2$, I, J, M, and B are the square of the angular momentum operator, the momentum of inertia of the molecules, the rotational quantum number, the projection of J on the molecular axis, and the molecular rotational constant, respectively. In an external electric field E, the eigen equation of $(\mathrm{HCCCN})_n$ $(\mathrm{n} = 1-3)$ molecules is

$$\left(\boldsymbol{J}^2 - \boldsymbol{\omega} \cos \boldsymbol{\theta}\right) |J,\ M; \boldsymbol{\omega}\rangle = \boldsymbol{E}_{eigen}\, |J,\ M; \boldsymbol{\omega}\rangle , \tag{2}$$

where θ is the angle between the molecular axis and the direction of the external electric field, $\boldsymbol{E}_{eigen}$ is the eigen energy in units of the rotational constant, $\omega = \mu \cdot \mathrm{E}/B$ represents the strength of the interaction between molecules and the electric field; and μ is the permanent electric dipole moment of the molecule.

To calculate the transition between the upper and lower states, a Boltzmann distribution [28] is used to derive the population of molecules with a J rotational quantum number:

$$N_J = N_0(2J+1)e^{\frac{-hcBJ(J+1)}{k_B T}} , \tag{3}$$

where N_J is the population of molecules with a J quantum number, N_0 is the total population of molecules, k_B is the Boltzmann constant, and T is the rotational temperature.

In an electrostatic field, the eigenvalues of the energy levels of $(\mathrm{HCCCN})_n$ $(\mathrm{n} = 1-3)$ molecules are calculated using the finite element matrix diagonalization method [29]. By calculating the coupling strengths for each transition line, the pendular spectrum is obtained.

To describe the variation of "Q-branch" spectrum with the applied electric field, the ratio of "Q-branch" spectrum intensity to the whole spectrum intensity I_Q is calculated by

$$I_Q = \frac{\int_{\upsilon_{Q\min}}^{\upsilon_{Q\max}} S_Q(\upsilon)\mathrm{d}\upsilon}{\int_{\upsilon_{\min}}^{\upsilon_{\max}} S(\upsilon)\mathrm{d}\upsilon} , \tag{4}$$

where I_Q is the normalized "Q-branch" intensity, $S_Q(\upsilon)$ and $S(\upsilon)$ are the "Q-branch" spectrum function and the whole spectrum function of frequency υ, $\upsilon_{Q\max}$ and $\upsilon_{Q\min}$ are the maximum and minimum values in the frequency domain of the "Q-branch" spectrum, and $\upsilon_{\max}$ and $\upsilon_{\min}$ are the maximum and minimum values in the frequency domain of the whole spectrum.

3. RESULTS AND DISCUSSION

A. Pendular Spectra of HCCCN and $(\mathrm{HCCCN})_2$

The pendular spectra of $(\mathrm{HCCCN})_n$ $(\mathrm{n} = 1-3)$ were calculated at several different electric field strengths (range of $0-10^8$ V/cm) at three rotational temperatures: 1 K, 10 K, and 30 K. The pendular spectra of $(\mathrm{HCCCN})_3$ have been calculated (at 0.25 K, 1 K, and 5 K) in our previous paper [27]; here, the spectra of HCCCN and $(\mathrm{HCCCN})_2$ in four electric field strengths (0 V/cm, 500 V/cm, 5000 V/cm, and 50,000 V/cm) at different rotational temperatures are shown in Fig. 1 and Fig. 2, respectively. The molecular parameters used in the calculation are listed in Table 1. From [17] and Table 1, it can be derived that for the same electric field strength $\omega_{(\mathrm{HCCCN})_3} > \omega_{(\mathrm{HCCCN})_2} > \omega_{\mathrm{HCCCN}}$, which means that $(\mathrm{HCCCN})_3$ can be oriented in a weaker electric field than $(\mathrm{HCCCN})_2$, and HCCCN needs a stronger electric field to be oriented than $(\mathrm{HCCCN})_2$.

As shown in Figs. 1 and 2, the number of spectral peaks is relatively few at a low rotational temperature because the low J values of molecules [known from Eq. (3)] result in fewer transitions. With the rising rotational temperature, the population of molecules on high-J levels increases; thus, the number of spectral peaks increases. It is clearly shown in Figs. 1 and 2 that there is no "Q-branch" with $E = 0$ V/cm. With an increase in the electric field strength E, a so-called "Q-branch" appears and gets stronger. Under the condition that E is large enough, the molecules are almost fully oriented; thus the "Q-branch"

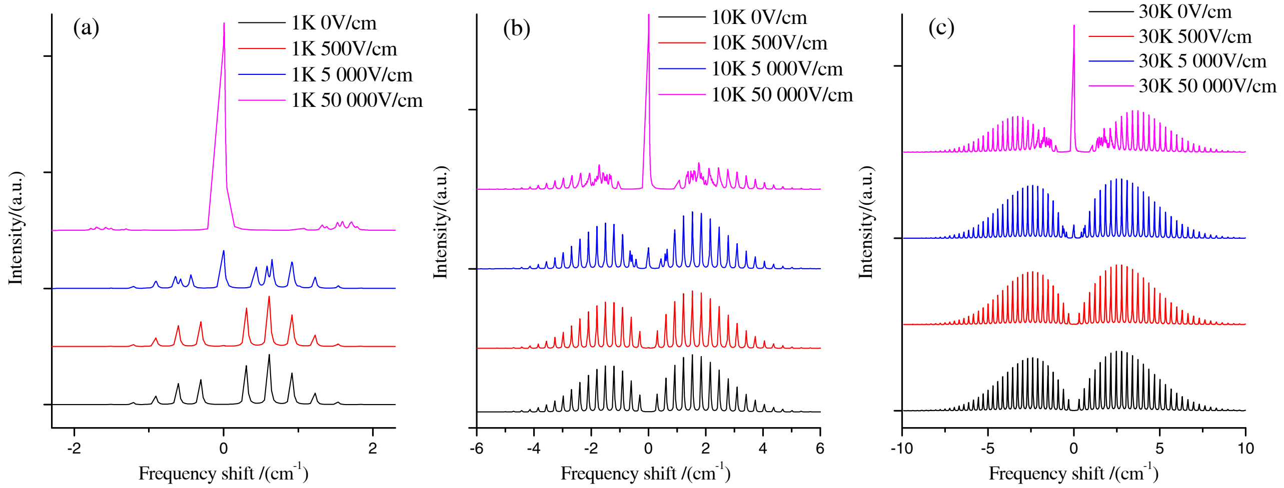

Fig. 1. Pendular spectra of HCCCN under 0 V/cm, 500 V/cm, 5000 V/cm, and 50,000 V/cm electric fields with rotational temperatures $T =$ (a) 1 K, (b) 10 K, and (c) 30 K, respectively.

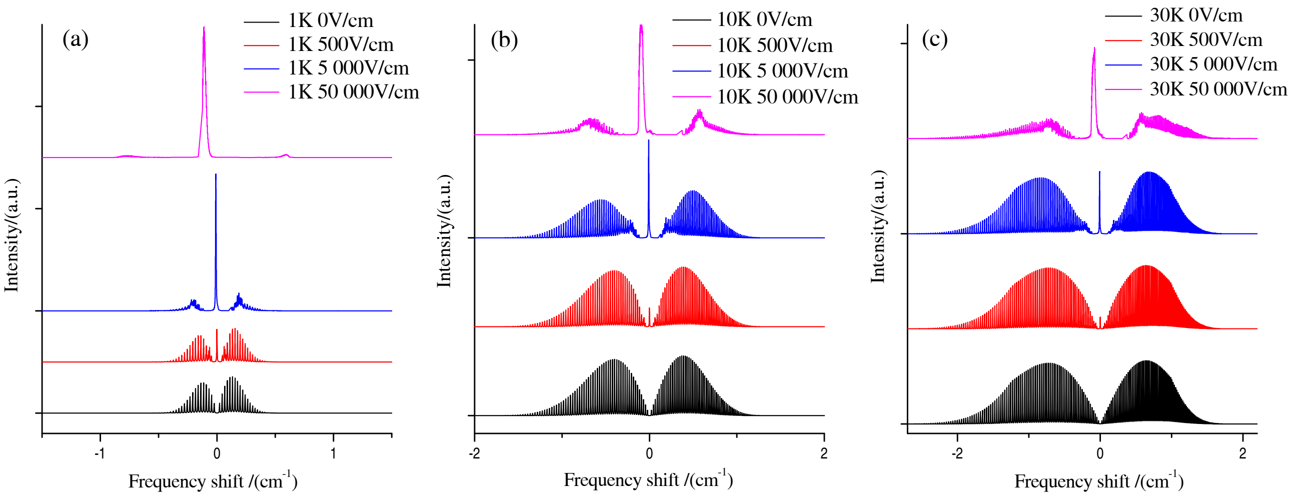

Fig. 2. Pendular spectra of $(HCCCN)_2$ under 0 V/cm, 500 V/cm, 5000 V/cm, and 50,000 V/cm electric fields with rotational temperatures $T =$ (a) 1 K, (b)10 K, and (c)30 K, respectively.

Table 1. Molecular Parameters of HCCCN and $(HCCCN)_2$ Molecules

	HCCCN		$(HCCCN)_2$	
	μ /Debye	B/cm^{-1}	μ /Debye	B/cm^{-1}
Lower state	3.73172[a]	0.15163530[b]	7.6228[c]	0.0113097[d]
Upper state	3.8063[e]	0.15149762[f]	7.7753[e]	0.01125979[d]

[a] From [30].

[b] From [31].

[c] Gaussian calculation result of electric dipole moment using the STO-3 G method.

[d] From [32].

[e] The difference in the electric dipole moment between the upper state and the ground state of $(HCCCN)_3$ in [17] is around 2%, so an estimated difference of 2% relative to the ground state is used for the upper state electric dipole moment of HCCCN and $(HCCCN)_2$.

[f] From [33].

dominates the spectrum. For the pendular spectra of HCCCN and $(HCCCN)_2$ at the same rotational temperature in the same electric field strength (e.g., Figs. 1(a) and 2(a), 1 K, 5000 V/cm), the relative intensity of the "Q-branch" of $(HCCCN)_2$ is stronger than that of HCCCN. This shows $(HCCCN)_2$ can be oriented more easily than HCCCN. This characteristic of the "Q-branch" intensity increasing with the electric field strength E suggests that HCCCN and $(HCCCN)_2$ have the potential to be used to measure the electric field.

B. Comparison of Electric Field Measurement with $(HCCCN)_n$ ($n = 1 - 3$)

To illustrate the relationship between the intensity of the "Q-branch" spectra of $(HCCCN)_n$ ($n = 1 - 3$) and the electric field strength E, the normalized "Q-branch" intensities I_Q of each molecule under different rotational temperatures were calculated and shown in Fig. 3. It can be seen for each molecule that when the electric field strength E increases gradually from 0 V/cm to 10^8 V/cm, the increment of I_Q first accelerates, then slows down, and ultimately reaches 1. This relationship between the I_Q of $(HCCCN)_n$ ($n = 1 - 3$) and E shows that the electric field strength measured can be up to 10^8 V/cm using this proposed method. From Fig. 3, two conclusions can be drawn. One is that, for the same molecule [Figs. 3(a)–3(c)] to get a certain normalized "Q-branch" intensity value I_Q, the molecule with a rotational temperature 30 K must be applied the strongest E, unlike those with rotational temperatures of 1 K and 10 K. This indicates that the molecule with higher rotational temperature must have a higher E applied to achieve the same I_Q. The other is at a certain rotational temperature, such as 30 K [Fig. 3(d)], to get the same normalized "Q-branch" intensity value I_Q, the highest E should be applied to HCCCN molecule compared to what is applied to the $(HCCCN)_2$ and $(HCCCN)_3$ molecules. This means the I_Q of HCCCN increases more slowly than that of $(HCCCN)_2$ and $(HCCCN)_3$ at the same rotational temperature. Based on the results of Fig. 3, it can be inferred that the HCCCN molecule with a rotational temperature higher than 30 K [34,35] can be used to measure an electric field with a strength of more than 10^8 V/cm.

In practical measurement, the gradient of I_Q dominates the sensitivity. Therefore, K_E, the gradient of I_Q, is defined to evaluate the sensitivity as

$$K_E = \frac{\mathrm{d}I_Q}{\mathrm{d}(\lg E)}. \tag{5}$$

The K_E of $(HCCCN)_n$ ($n = 1 - 3$) was calculated as a function of the electric field strength. The K_E curves of $(HCCCN)_n$ ($n = 1 - 3$) at 1 K, 10 K, and 30 K rotational temperatures are shown, respectively, in Fig. 4.

As shown in Fig. 4(a), if E is weaker than $10^{3.60}$ V/cm, the measurement sensitivity of $(HCCCN)_3$ is the highest when the rotational temperature is 1 K. When the electric field strength increases to the range of $10^{3.60} - 10^{3.81}$ V/cm, the measurement sensitivity of $(HCCCN)_2$ shows an advantage. When the electric field strength is higher than $10^{3.81}$ V/cm, the measurement sensitivity of HCCCN molecules is the highest. Similar conclusions can be drawn for 10 K and 30 K in Fig. 4. For the convenience of comparison, all the results are summarized in Table 2.

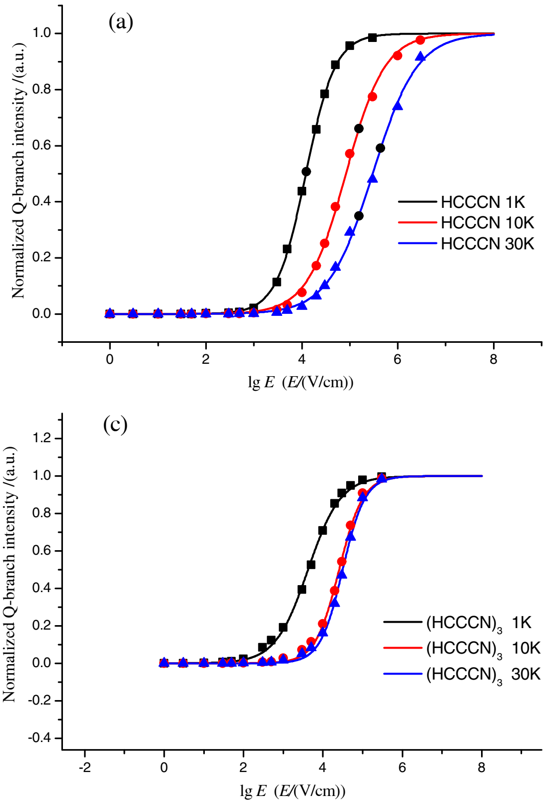

Fig. 3. Normalized "*Q*-branch" intensity of the pendular spectra of (a) HCCCN, (b) $(HCCCN)_2$, and (c) $(HCCCN)_3$ with 1 K, 10 K, and 30 K rotational temperatures, respectively. (d) Normalized "*Q*-branch" intensity of $(HCCCN)_n$ (n = 1 − 3) at 30 K (rotational temperature). The scatters are the calculated data, and the curves are the fitted lines.

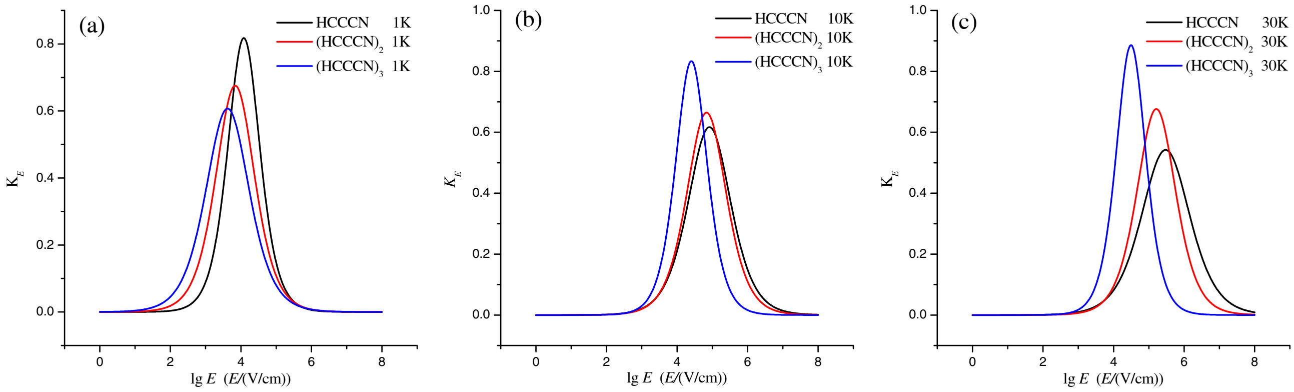

Fig. 4. Relationship between K_E and E of $(HCCCN)_n$ (n = 1 − 3) molecules at (a) 1 K, (b) 10 K, and (c) 30 K rotational temperatures, respectively.

Table 2. Sensitivity Range of Measuring Electric Field Strength with $(HCCCN)_n$ (n = 1 − 3) under 1 K, 10 K, and 30 K [Unit/(V/cm)]

	HCCCN	$(HCCCN)_2$	$(HCCCN)_3$
1 K	$>10^{3.81}$	$10^{3.60} - 10^{3.81}$	$<10^{3.60}$
10 K	$>10^{5.11}$	$10^{4.72} - 10^{5.11}$	$<10^{4.72}$
30 K	$>10^{5.58}$	$10^{4.89} - 10^{5.58}$	$<10^{4.89}$

As shown in Table 2, HCCCN, $(HCCCN)_2$, and $(HCCCN)_3$ molecules at the same rotational temperature are suitable to measure, respectively, relatively weak, medium strong, and relatively intense electric fields. It can be inferred that the suitable measurement range of electric field strength for each molecule increases with a rise in the rotational temperature. The range and varying trend of sensitivity shown in Fig. 4 gives clear instructions for the selection of the appropriate molecule and rotational temperature to measure the electric field strength.

Based on the results, a scheme to measure the electric field strength is proposed. In experimental measurement, the jetting of HCCCN sample forms the molecule beam with $(HCCCN)_n$ (n = 1 − 3) [17], and the corresponding rotational temperatures of the three molecules are the same. First, determine the range of the electric field to be measured under a certain condition (the applied voltage, the distance between electrodes). Then, choose the appropriate molecule by the range and rotational temperature according to Table 2, and collect the pendular spectrum. Finally, calculate the normalized "*Q*-branch" intensity I_Q, to obtain the electric field strength. In this way, a higher sensitivity can be achieved. The spatial resolution of this proposal depends directly on the focal diameter of the probe laser. For a Gaussian laser beam (quasi-parallel), the waist diameter d is expressed as

$$d = \frac{2\lambda f}{\pi \omega}, \tag{6}$$

where λ, f, and ω are the wavelength, focal length, and radius of the laser spot on the lens, respectively. For the C-H ν_1 vibration of (HCCCN)n ($n = 1 - 3$), the transition wavelength is around 3.3 μm. Considering f and ω to be 10 cm and 3 mm, respectively, which are common in the laboratory, the theoretical spatial resolution is 70 μm. Therefore, the spatial resolution of the pendular spectrum electric field measurement is far higher than those of the traditional methods [7–10].

One possible application of the measurement method mentioned above is the electrostatic Stark decelerators that have successfully decelerated polar molecules [2–5]. The exact value of the electric field strength has a significant influence on the deceleration result. The voltage applied on the Stark electrodes is 10–50 kV, and the electrode spacing is a few millimeters. As a result, the electric field strength of the Stark decelerator is on the magnitude of 10^5 V/cm. For such intense electric field in the narrow space, there is no suitable method to measure the electric field strength. However, the electric field distribution is generally calculated, so it can be quite different from the actual situation, which hinders further enhancement of the deceleration effect. The scheme proposed in this paper exactly covers this electric field strength. For the electrostatic field, assuming the rotational temperature of the prepared $(\mathrm{HCCCN})_n$ ($n = 1 - 3$) molecule beam is 30 K, it can be seen from Table 2 that the pendular spectrum of $(\mathrm{HCCCN})_2$ molecules can be used for the sensitive measurement of the electric field strength.

4. CONCLUSION

In this paper, the pendular spectra of linear $(\mathrm{HCCCN})_n$ ($n = 1 - 3$) molecules at certain rotational temperatures under different electric field strengths and the corresponding normalized "*Q*-branch" intensity I_Q are calculated. The measurement range and sensitivity with $(\mathrm{HCCCN})_n$ ($n = 1 - 3$) under the calculated conditions are analyzed. The results demonstrate that $(\mathrm{HCCCN})_n$ ($n = 1 - 3$) molecules can be used to measure an electric field, and the measured range can reach or even exceed 10^8 V/cm. A scheme is also proposed to achieve high sensitivity by choosing the appropriate molecule from $(\mathrm{HCCCN})_n$ ($n = 1 - 3$). In addition, the spatial resolution of this method can reach 70 μm, which, to the best of our knowledge, is far better than traditional methods. In conclusion, we believe the scheme based on pendular spectrum that has been proposed in this paper can significantly improve the range and sensitivity of the measurement of electric field strength and has great superiority.

Funding. National Natural Science Foundation of China (11674096, 11834003, 11874151); Natural Science Foundation of Shanghai (18ZR1412700).

Disclosures. The authors declare no conflicts of interest.

Data Availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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