

# 練習実験報告

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2024 年 6 月 2 日

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## Galvano Sepctrum

## REMPI scan

- Selected peaks

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## Galvano Sepctrum

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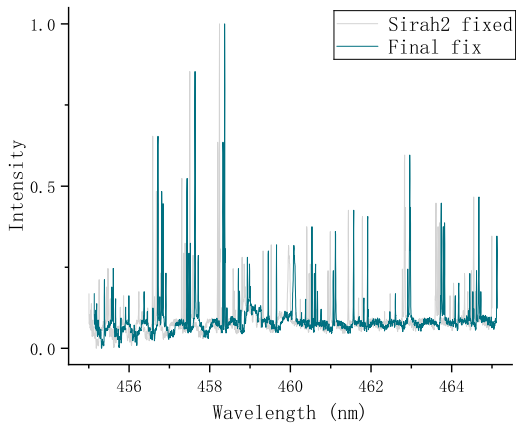
Error

# Galvano Sepctrum



**Fig. 1:** Wavelen. correction

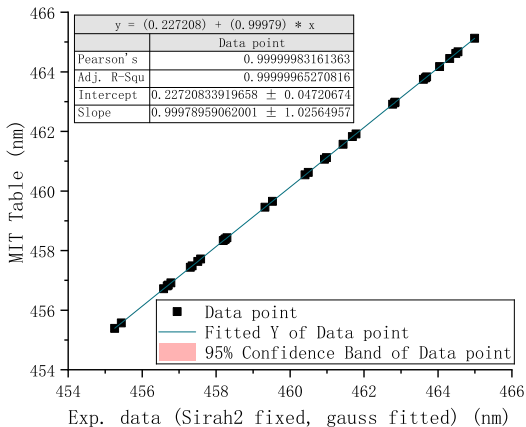
# Galvano Sepctrum



**Fig. 1:** Wavelen. correction

# Galvano Sepctrum

## Calibration



**Fig. 2:** Correction function

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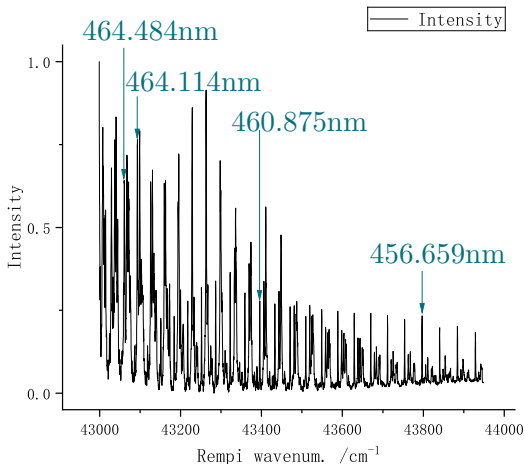
- Peak assignments

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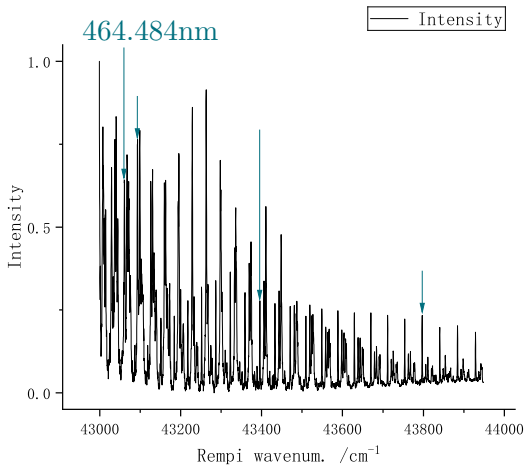
- Error



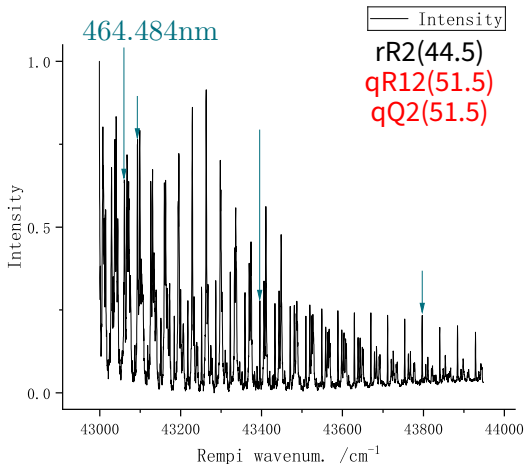
# Selected peaks



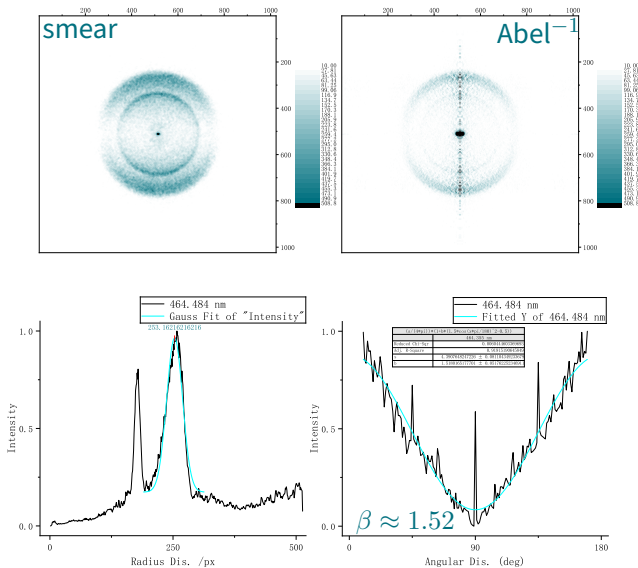
# Peak 1



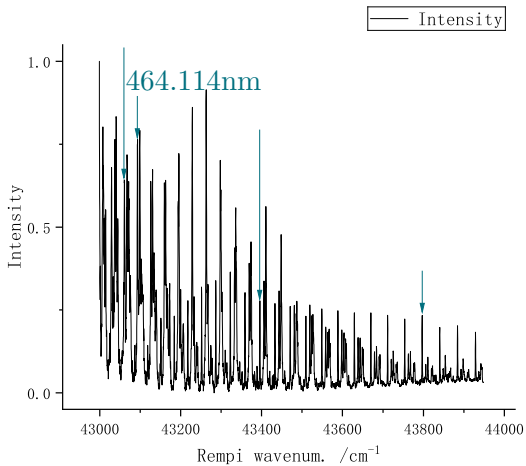
# Peak 1



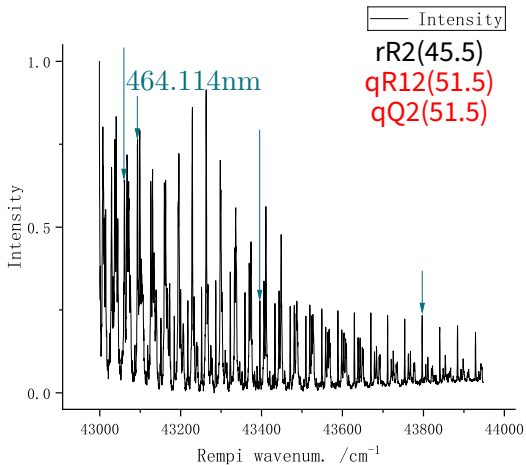
# Peak 1



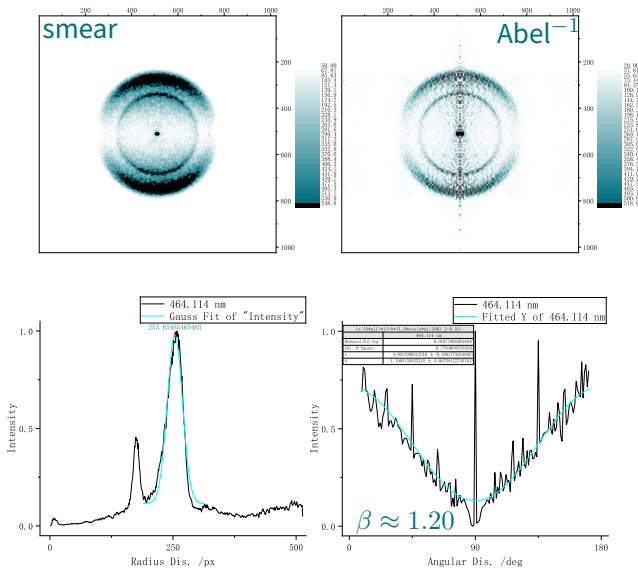
## Peak 2



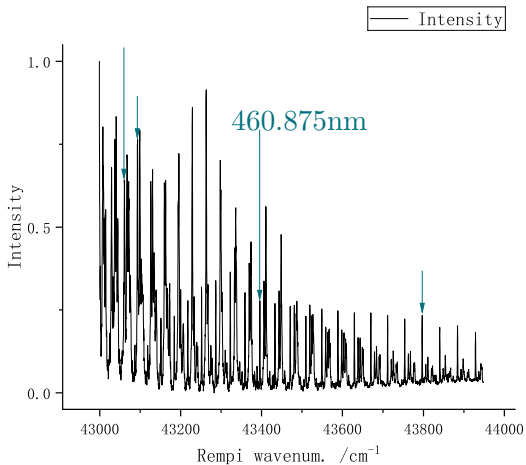
## Peak 2



# Peak 2

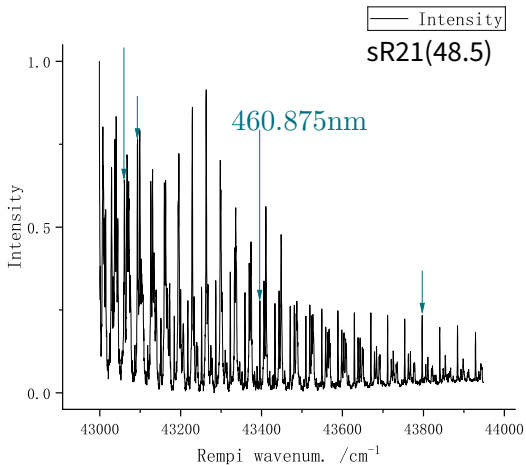


## Peak 3

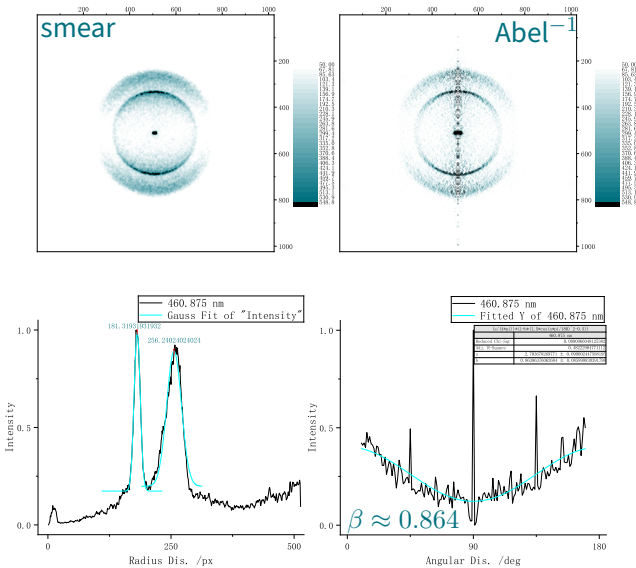




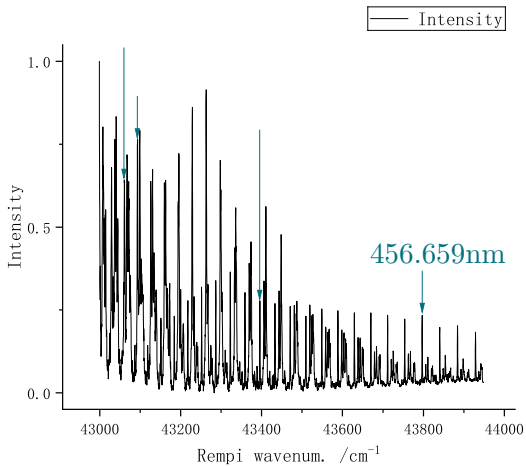
## Peak 3



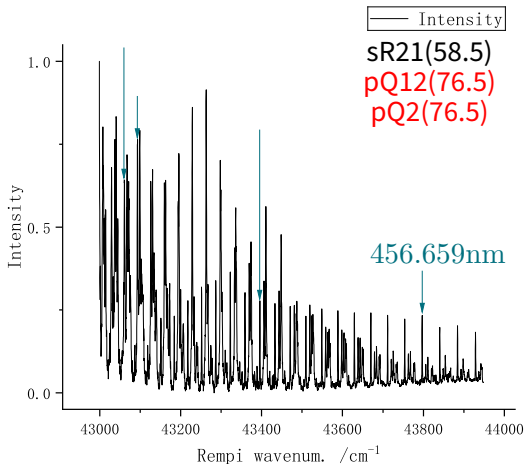
### Peak 3



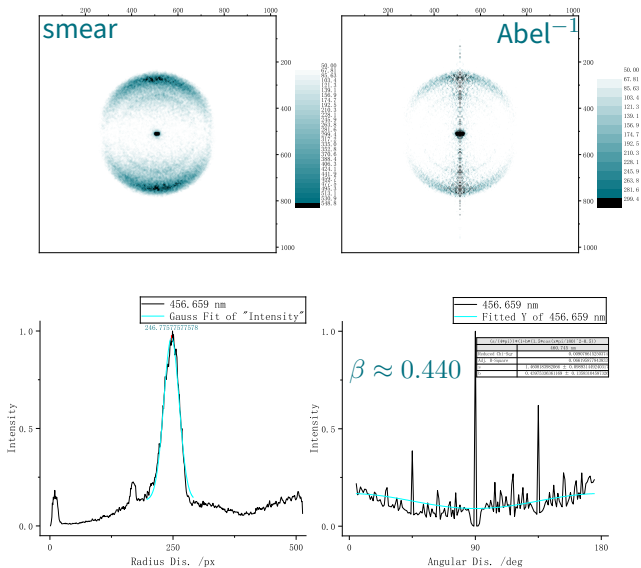
## Peak 4



## Peak 4



# Peak 4



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# Peak assignments

464.484nm $\approx 43058.49\text{cm}^{-1}$	464.114nm $\approx 43092.81\text{cm}^{-1}$	460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 253.162	px = 253.655	px = 181.319 & 256.240	px = 246.776
<i>rR2</i> (44.5) <i>qR12</i> (51.5) <i>qQ2</i> (51.5)	<i>rR2</i> (45.5) <i>qR12</i> (51.5) <i>qQ2</i> (51.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5) <i>pQ12</i> (76.5) <i>pP2</i> (76.5)



# Peak assignments

464.484nm $\approx 43058.49\text{cm}^{-1}$	464.114nm $\approx 43092.81\text{cm}^{-1}$	460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 253.162	px = 253.655	px = <b>181.319</b> & 256.240	px = 246.776
<i>rR2</i> (44.5) <i>qR12</i> (51.5) <i>qQ2</i> (51.5)	<i>rR2</i> (45.5) <i>qR12</i> (51.5) <i>qQ2</i> (51.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5) <i>pQ12</i> (76.5) <i>pP2</i> (76.5)

## Notice

Colored assignments are mismatched, and will not be used to calculate.

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# Speed correction

## Trans. energy of NO

	$E_{\text{total}}$	$E_{\text{bond}}(\text{O}-\text{NO})^1$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm <sup>-1</sup>	25 128.57cm <sup>-1</sup>	$\Delta E_v(1 \rightarrow 0) + E(J = 44)$
Peak 2 464.114nm	43 092.81cm <sup>-1</sup>		$\Delta E_v(1 \rightarrow 0) + E(J = 45)$
Peak 3 460.875nm	43 395.69cm <sup>-1</sup>		$\Delta E_v(1 \rightarrow 0) + E(J = 48)$
Peak 4 456.659nm	43 796.34cm <sup>-1</sup>		$\Delta E_v(1 \rightarrow 0) + E(J = 58)$

<sup>1</sup>Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).

# Speed correction

## Trans. energy of NO

	$E_{\text{total}}$	$E_{\text{bond}}(\text{O}-\text{NO})^2$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm <sup>-1</sup>	25 128.57cm <sup>-1</sup>	2341.932 775 0cm <sup>-1</sup> + $E(J = 44)$
Peak 2 464.114nm	43 092.81cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 45)$
Peak 3 460.875nm	43 395.69cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 48)$
Peak 4 456.659nm	43 796.34cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 58)$

<sup>2</sup>Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).

# Speed correction

## Trans. energy of NO

	$E_{\text{total}}$	$E_{\text{bond}}(\text{O}-\text{NO})^2$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm <sup>-1</sup>	25 128.57cm <sup>-1</sup>	2341.932 775 0cm <sup>-1</sup> + $E(J = 44)$
Peak 2 464.114nm	43 092.81cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 45)$
Peak 3 460.875nm	43 395.69cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 48)$
Peak 4 456.659nm	43 796.34cm <sup>-1</sup>		2341.932 775 0cm <sup>-1</sup> + $E(J = 58)$

## Vib. energy level

$$E_v = \omega_e \left( v + \frac{1}{2} \right) - \omega_e x_e \left( v + \frac{1}{2} \right)^2 + \omega_e y_e \left( v + \frac{1}{2} \right)^3.$$

<sup>2</sup>Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).

# Speed correction

## Trans. energy of NO

	$E_{\text{total}}$	$E_{\text{bond}}(\text{O}-\text{NO})^3$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm <sup>-1</sup>	25 128.57cm <sup>-1</sup>	5814.033cm <sup>-1</sup>
Peak 2 464.114nm	43 092.81cm <sup>-1</sup>		5965.969cm <sup>-1</sup>
Peak 3 460.875nm	43 395.69cm <sup>-1</sup>		6239.696cm <sup>-1</sup>
Peak 4 456.659nm	43 796.34cm <sup>-1</sup>		8004.278cm <sup>-1</sup>

<sup>3</sup>Rémy Jost et al. *The Journal of Chemical Physics* **105**.3 (July 1996).

<sup>4</sup>Colin M. Western. *Journal of Quantitative Spectroscopy and Radiative Transfer* **186** (2017), pp. 221–242.

# Speed correction

## Trans. energy of NO

	$E_{\text{total}}$	$E_{\text{bond}}(\text{O}-\text{NO})^3$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm <sup>-1</sup>	25 128.57cm <sup>-1</sup>	5814.033cm <sup>-1</sup>
Peak 2 464.114nm	43 092.81cm <sup>-1</sup>		5965.969cm <sup>-1</sup>
Peak 3 460.875nm	43 395.69cm <sup>-1</sup>		6239.696cm <sup>-1</sup>
Peak 4 456.659nm	43 796.34cm <sup>-1</sup>		8004.278cm <sup>-1</sup>

## Rot. energy level

Simulated data generated by PGOPHER<sup>4</sup>.

<sup>3</sup>Rémy Jost et al. *The Journal of Chemical Physics* **105**.3 (July 1996).

<sup>4</sup>Colin M. Western. *Journal of Quantitative Spectroscopy and Radiative Transfer* **186** (2017), pp. 221–242.



# Speed correction

## Trans. energy of NO

$E_{\text{int.}}^{(O)}$	$E_{\text{trans}}(\text{total}) \approx 2.875464 E_{\text{trans}}(\text{NO})$ $= E_{\text{total}} - E_{\text{bond}}(\text{O}-\text{NO}) - E_{\text{int.}}(\text{O}) - E_{\text{int.}}(\text{NO})$	$E_{\text{trans}}(\text{NO})$ $= \frac{1}{2} m(\text{NO}) v^2(\text{NO})$
$^3P_2$	11081.356cm <sup>-1</sup>	4375.588cm <sup>-1</sup>
	10964.609cm <sup>-1</sup>	4334.685cm <sup>-1</sup>
	10794.143cm <sup>-1</sup>	4344.824cm <sup>-1</sup>
(0cm <sup>-1</sup> )	9398.766cm <sup>-1</sup>	3870.489cm <sup>-1</sup>
$^3P_1$	10922.731cm <sup>-1</sup>	4320.423cm <sup>-1</sup>
	10805.984cm <sup>-1</sup>	4279.520cm <sup>-1</sup>
	10635.518cm <sup>-1</sup>	4289.659cm <sup>-1</sup>
(158.625cm <sup>-1</sup> )	9240.141cm <sup>-1</sup>	3815.324cm <sup>-1</sup>
$^3P_0$	10854.379cm <sup>-1</sup>	4296.653cm <sup>-1</sup>
	10737.632cm <sup>-1</sup>	4255.749cm <sup>-1</sup>
	10567.166cm <sup>-1</sup>	4265.888cm <sup>-1</sup>
(226.977cm <sup>-1</sup> )	9171.789cm <sup>-1</sup>	3791.553cm <sup>-1</sup>

<sup>5</sup>Charlotte Emma Moore and Jean W. Gallagher. "Tables of spectra of hydrogen, carbon, nitrogen, and oxygen atoms and ions". 1993.

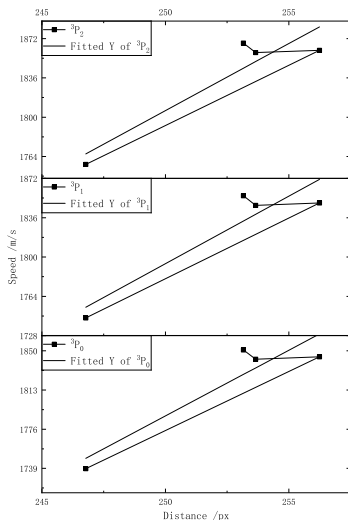
# Speed correction

## Trans. speed of NO

$E_{\text{int.}}(\text{O})$	$v(\text{NO}) = \sqrt{\frac{2E_{\text{trans}}(\text{NO})}{m(\text{NO})}}$	$\Delta y$
$^3P_2$ ( $0\text{cm}^{-1}$ )	1867.845m s <sup>-1</sup>	253.177
	1859.094m s <sup>-1</sup>	253.650
	1861.267m s <sup>-1</sup>	256.147
	1756.732m s <sup>-1</sup>	246.776
$^3P_1$ ( $158.625\text{cm}^{-1}$ )	1856.033m s <sup>-1</sup>	253.177
	1847.226m s <sup>-1</sup>	253.650
	1849.413m s <sup>-1</sup>	256.148
	1744.168m s <sup>-1</sup>	246.776
$^3P_0$ ( $226.977\text{cm}^{-1}$ )	1850.920m s <sup>-1</sup>	253.177
	1842.089m s <sup>-1</sup>	253.650
	1844.282m s <sup>-1</sup>	256.147
	1738.726m s <sup>-1</sup>	246.776

# Speed correction

## Trans. speed of NO



$^3P_2$

$12.28 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1265 \text{ m s}^{-1}$

$^3P_1$

$12.37 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1298 \text{ m s}^{-1}$

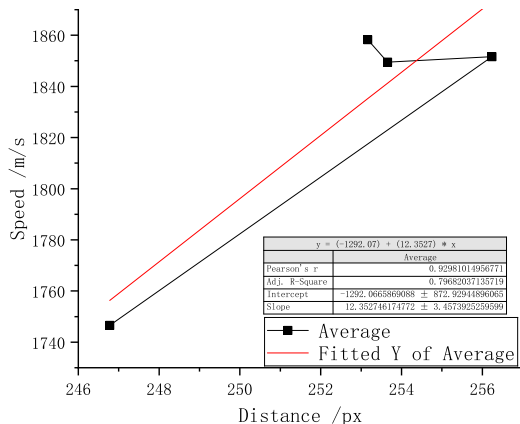
$^3P_0$

$12.40 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1313 \text{ m s}^{-1}$

# Speed correction

Trans. speed of NO



Average

$12.35 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1292 \text{ m s}^{-1}$

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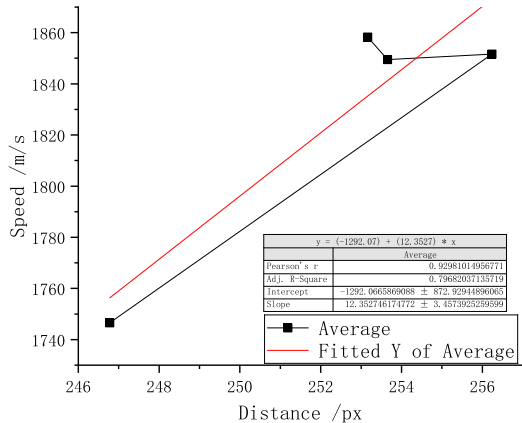
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# Error

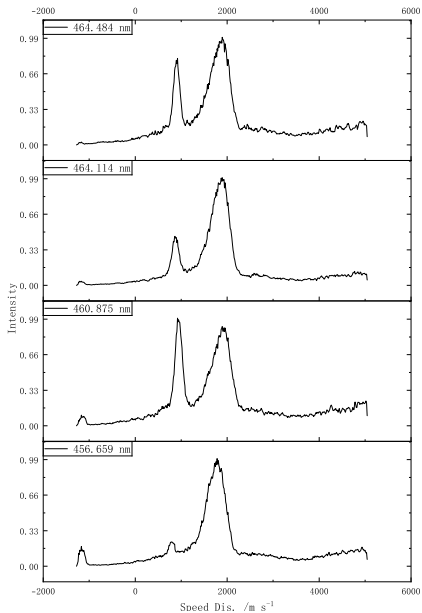


Average

$12.35 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1292 \text{ m s}^{-1}$

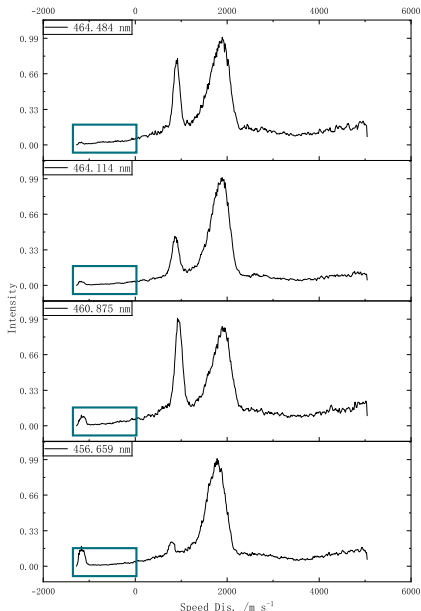
# Error



<sup>a</sup>Maybe  $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.



# Error



Average

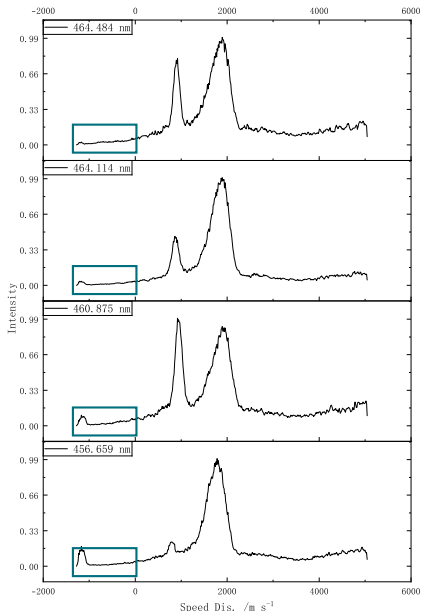
$12.35 \text{ m s}^{-1} \text{ px}^{-1}$

Intercept  $\approx -1292 \text{ m s}^{-1}$

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<sup>a</sup>Maybe  $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.

# Error



Average

$$12.35 \text{ m s}^{-1} \text{ px}^{-1}$$

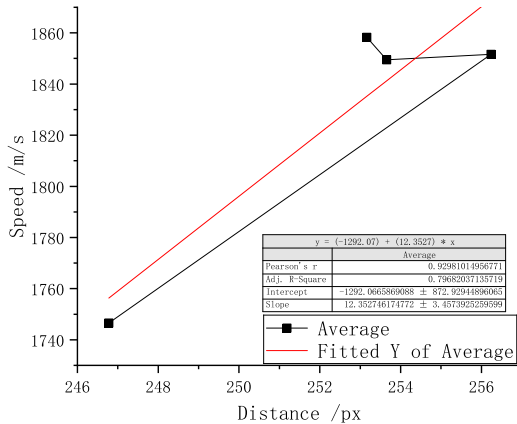
$$\text{Intercept} \approx -1292 \text{ m s}^{-1}$$

## Notice

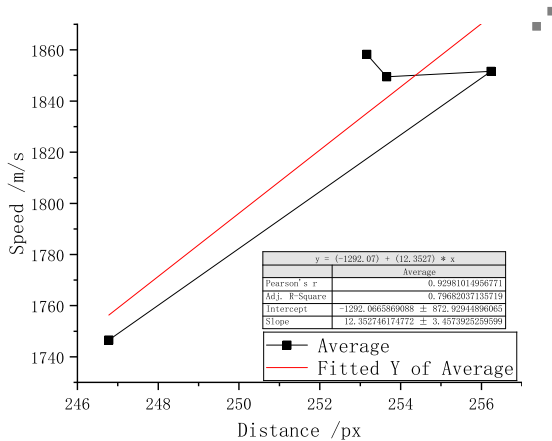
What we are calculating here are actually  $|\mathbf{v}_{\text{NO}}|$ , which are not supposed to be **minus**<sup>a</sup>.

<sup>a</sup>Maybe  $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.

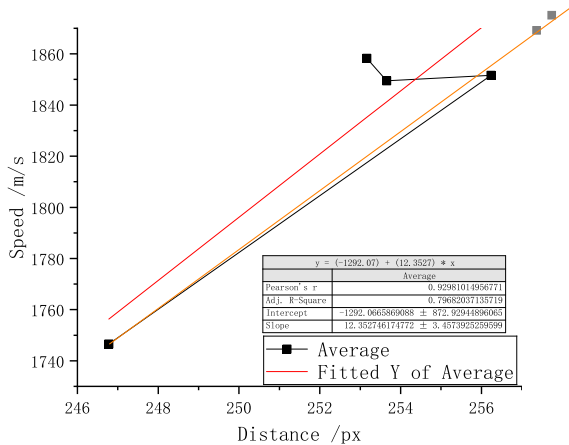
# Error



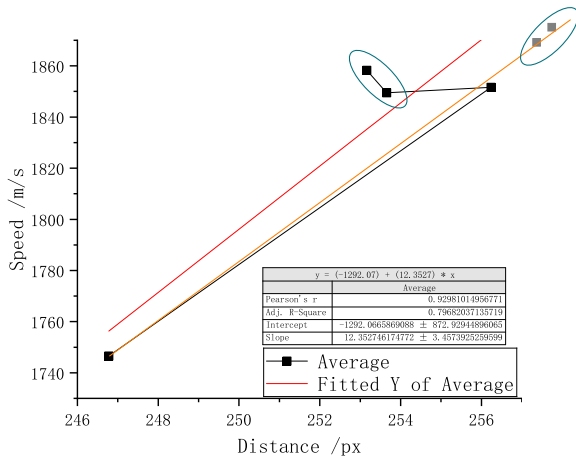
# Error



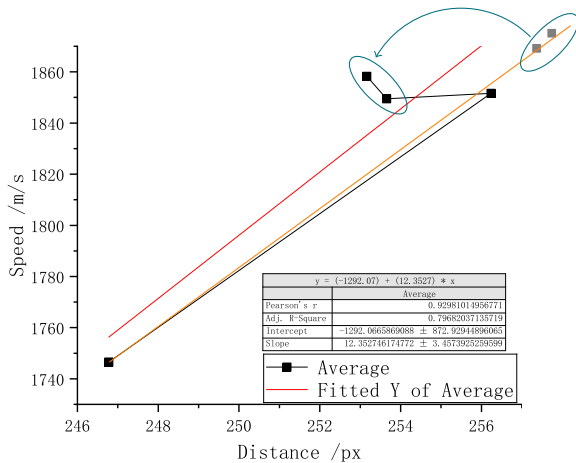
# Error



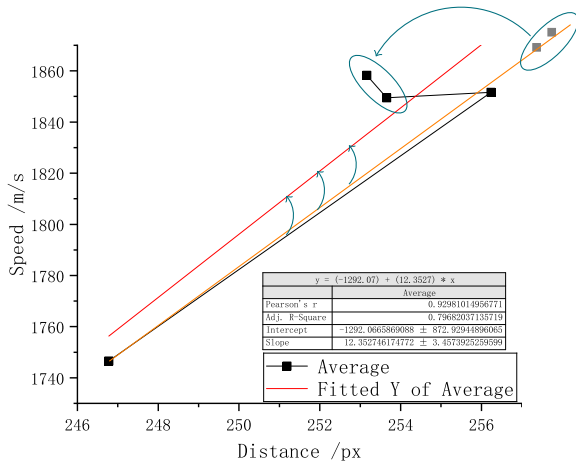
# Error



# Error

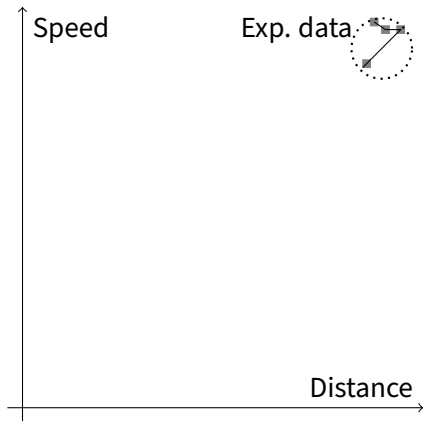


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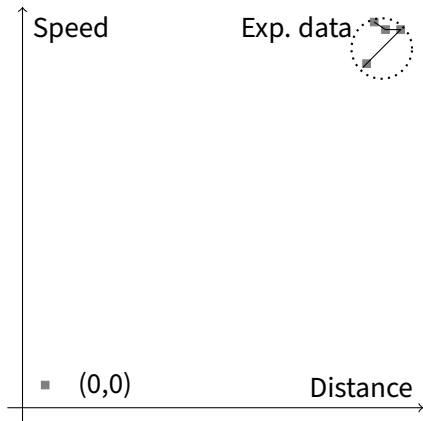




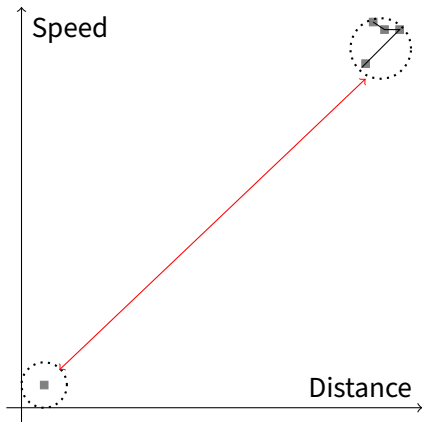
# Error



# Error

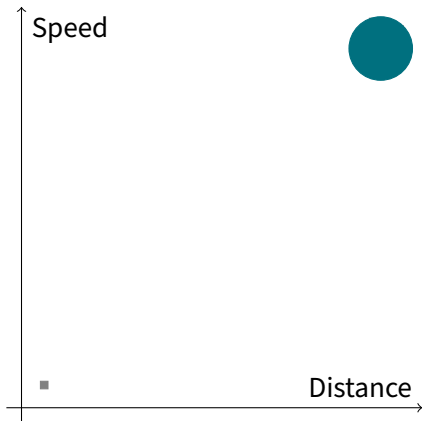


# Error



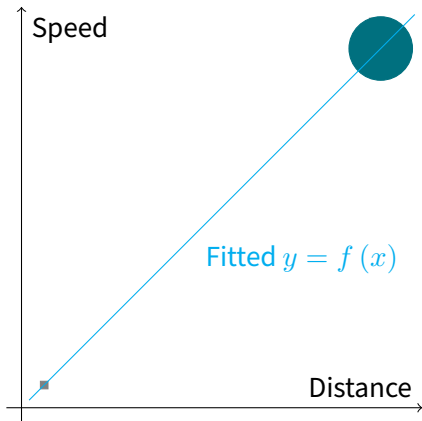
If we assume a virtual zero point:  
The fake data obtains a huge **weight**!  
Statistics tools always treat all data  
as proper indications.

# Error



If we assume a virtual zero point:  
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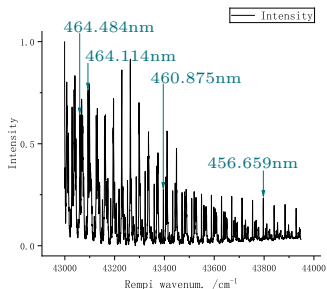
# Error



If we assume a virtual zero point:  
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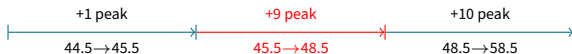
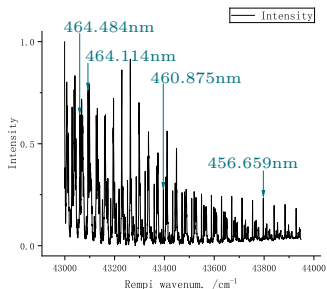
⇒ After assignments, which are the  
points we should use?

# Assignment for Assignment



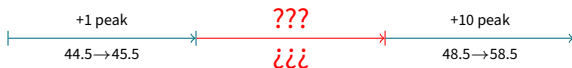
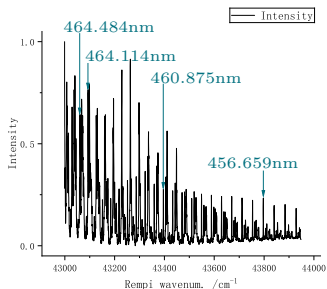
464.484nm $\approx 43058.49\text{cm}^{-1}$	464.114nm $\approx 43092.81\text{cm}^{-1}$	460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 253.162	px = 253.655	px = 256.240	px = 246.776
<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

# Assignment for Assignment



464.484nm ≈ 43058.49cm <sup>-1</sup>	464.114nm ≈ 43092.81cm <sup>-1</sup>	460.875nm ≈ 43395.69cm <sup>-1</sup>	456.659nm ≈ 43796.34cm <sup>-1</sup>
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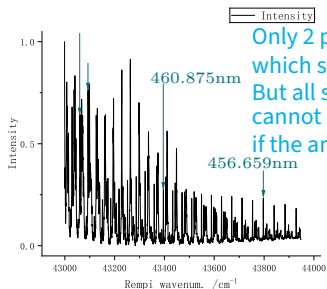
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<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)



# Assignment for Assignment



Only 2 peaks  
which seem more valid.  
But all statistics tools  
cannot be properly applied  
if the amount of data  $\leq 3$ .

+10 peak  
48.5 → 58.5

460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 256.240	px = 246.776
<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

# Reference

- [1] Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).
- [2] Charlotte Emma Moore and Jean W. Gallagher. “Tables of spectra of hydrogen, carbon, nitrogen, and oxygen atoms and ions”. 1993.
- [3] Colin M. Western. *Journal of Quantitative Spectroscopy and Radiative Transfer* **186** (2017), pp. 221–242.