

練習実験報告

肖宇笑

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Galvano Sepctrum



Fig. 1: Wavelen. correction

Galvano Sepctrum

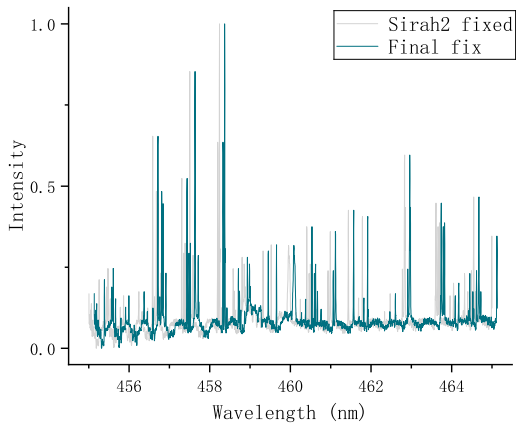


Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

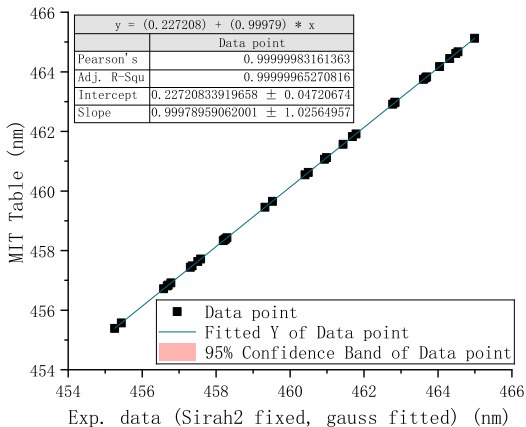


Fig. 2: Correction function

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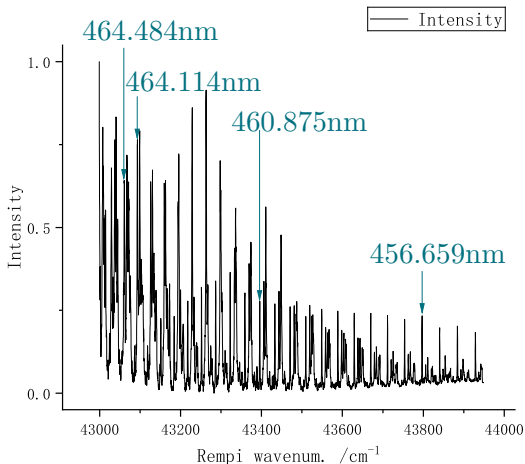
- Selected peaks

- Peak assignments

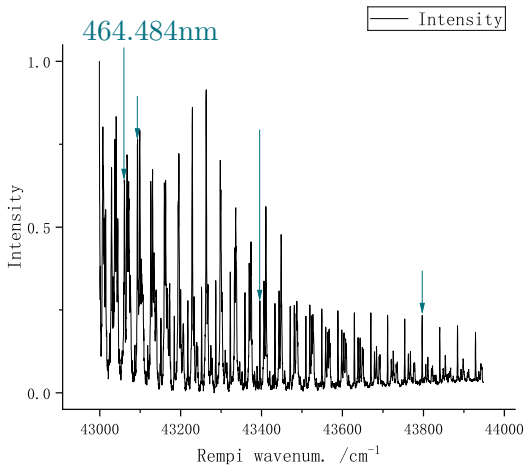
- Speed correction

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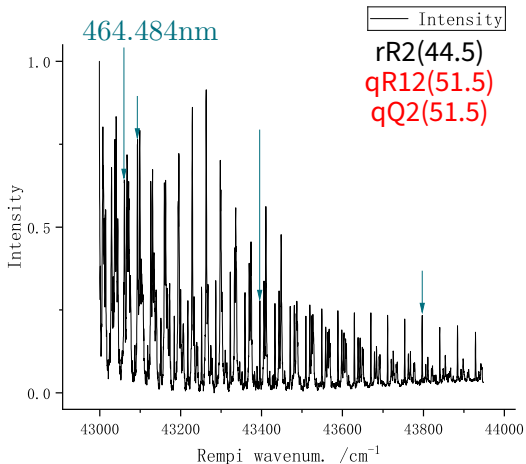
Selected peaks



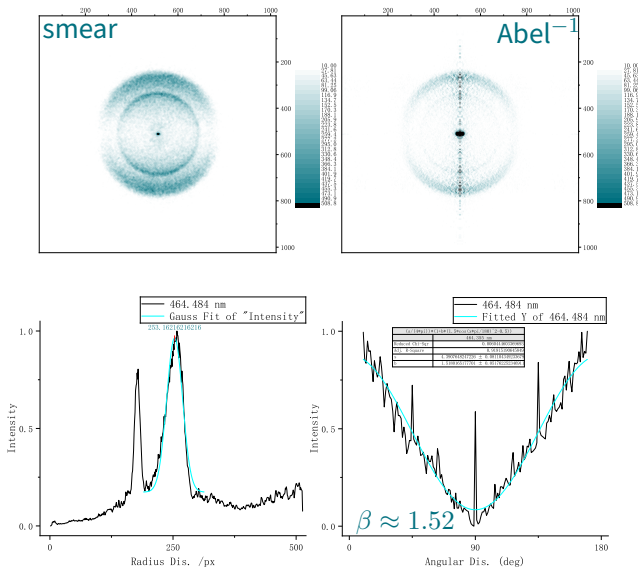
Peak 1



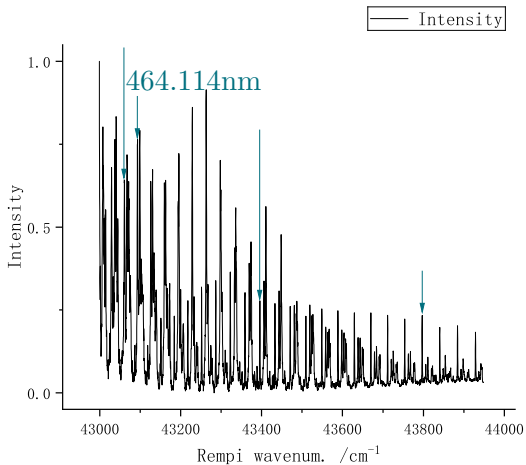
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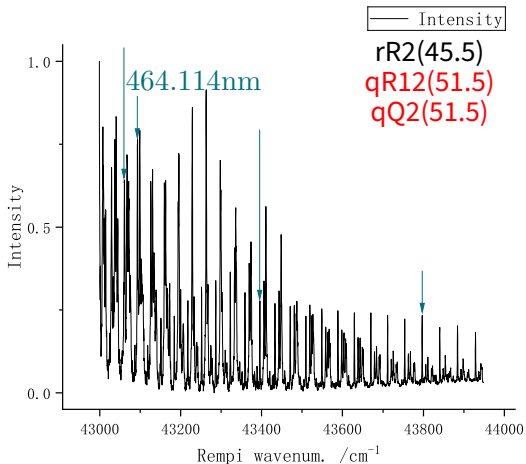
Peak 1



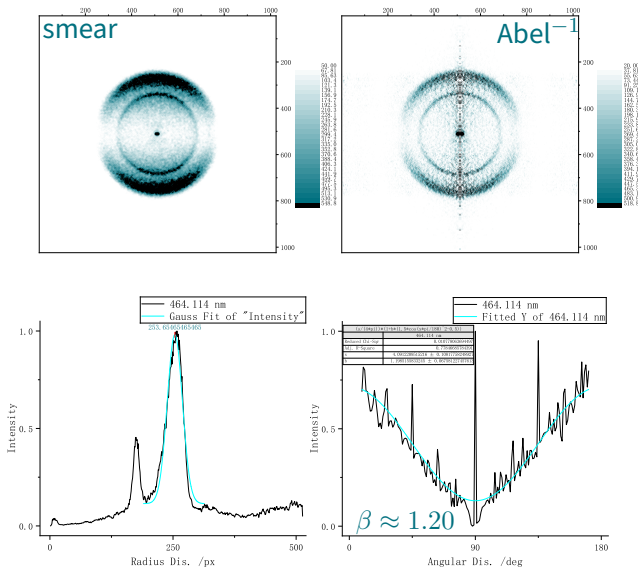
Peak 2



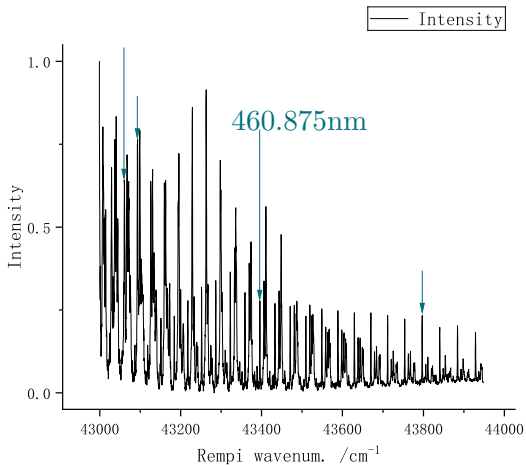
Peak 2



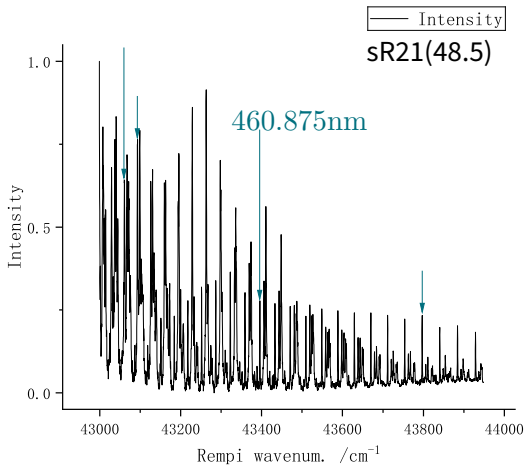
Peak 2



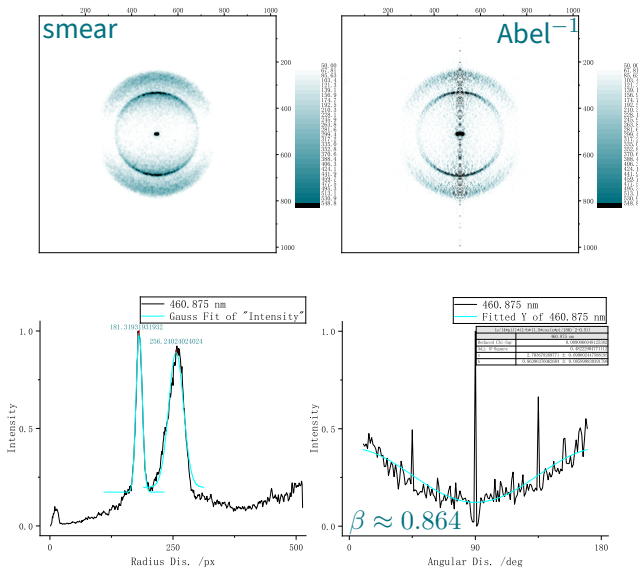
Peak 3



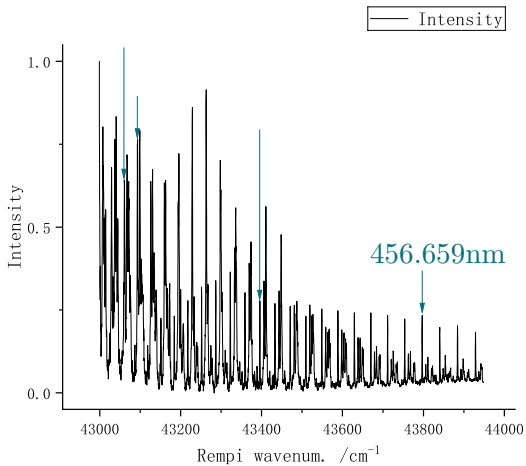
Peak 3



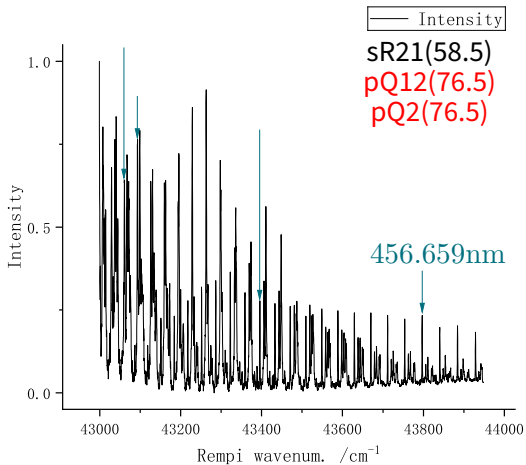
Peak 3



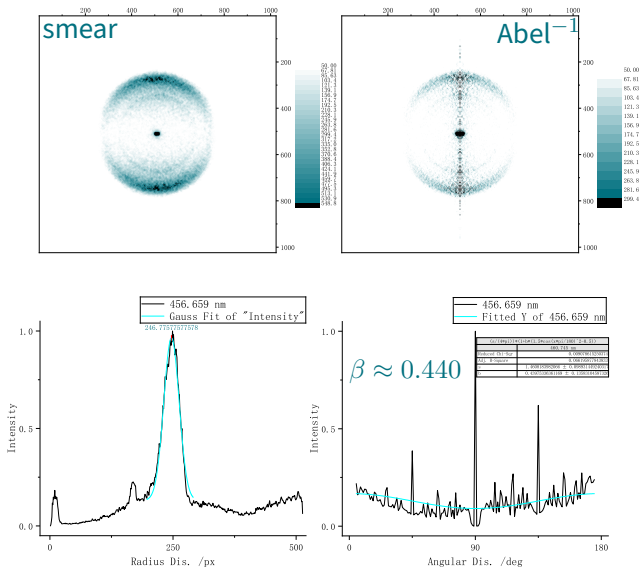
Peak 4



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 $\approx 43796.34\text{cm}^{-1}$
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<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_{total}	$E_{\text{bond}}(\text{O}-\text{NO})^1$	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	43 058.49cm ⁻¹	25 128.57cm ⁻¹	$\Delta E_v(1 \rightarrow 0) + E(J = 44)$
Peak 2 464.114nm	43 092.81cm ⁻¹		$\Delta E_v(1 \rightarrow 0) + E(J = 45)$
Peak 3 460.875nm	43 395.69cm ⁻¹		$\Delta E_v(1 \rightarrow 0) + E(J = 48)$
Peak 4 456.659nm	43 796.34cm ⁻¹		$\Delta E_v(1 \rightarrow 0) + E(J = 58)$

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

Speed correction

Trans. energy of NO

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

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

Speed correction

Trans. energy of NO

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

Vib. energy level

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

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

Speed correction

Trans. energy of NO

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

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

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

Speed correction

Trans. energy of NO

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

Rot. energy level

Simulated data generated by PGOPHER⁴.

³Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).

⁴Colin 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 ⁻¹	4375.588cm ⁻¹
	10964.609cm ⁻¹	4334.685cm ⁻¹
	10794.143cm ⁻¹	4344.824cm ⁻¹
(0cm ⁻¹)	9398.766cm ⁻¹	3870.489cm ⁻¹
3P_1	10922.731cm ⁻¹	4320.423cm ⁻¹
	10805.984cm ⁻¹	4279.520cm ⁻¹
	10635.518cm ⁻¹	4289.659cm ⁻¹
(158.625cm ⁻¹)	9240.141cm ⁻¹	3815.324cm ⁻¹
3P_0	10854.379cm ⁻¹	4296.653cm ⁻¹
	10737.632cm ⁻¹	4255.749cm ⁻¹
	10567.166cm ⁻¹	4265.888cm ⁻¹
(226.977cm ⁻¹)	9171.789cm ⁻¹	3791.553cm ⁻¹

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

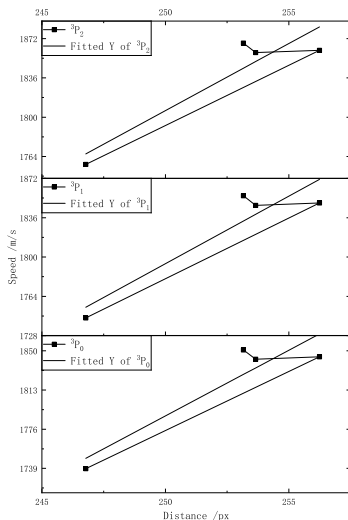
Speed correction

Trans. speed of NO

$E_{\text{int.}}(\text{O})$	$v(\text{NO}) = \sqrt{\frac{2E_{\text{trans}}(\text{NO})}{m(\text{NO})}}$	Δy
3P_2 (0cm^{-1})	1867.845m s ⁻¹	253.177
	1859.094m s ⁻¹	253.650
	1861.267m s ⁻¹	256.147
	1756.732m s ⁻¹	246.776
3P_1 (158.625cm^{-1})	1856.033m s ⁻¹	253.177
	1847.226m s ⁻¹	253.650
	1849.413m s ⁻¹	256.148
	1744.168m s ⁻¹	246.776
3P_0 (226.977cm^{-1})	1850.920m s ⁻¹	253.177
	1842.089m s ⁻¹	253.650
	1844.282m s ⁻¹	256.147
	1738.726m s ⁻¹	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 $\approx -1298 \text{ m s}^{-1}$

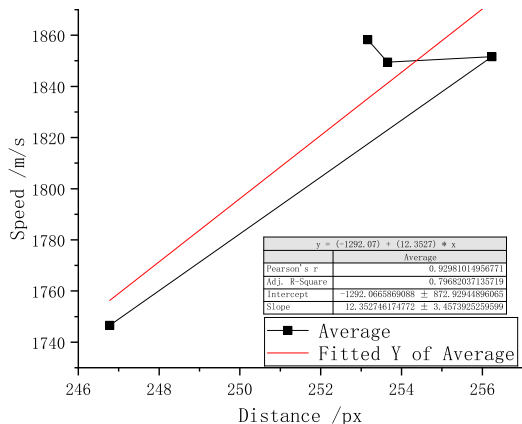
3P_0

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

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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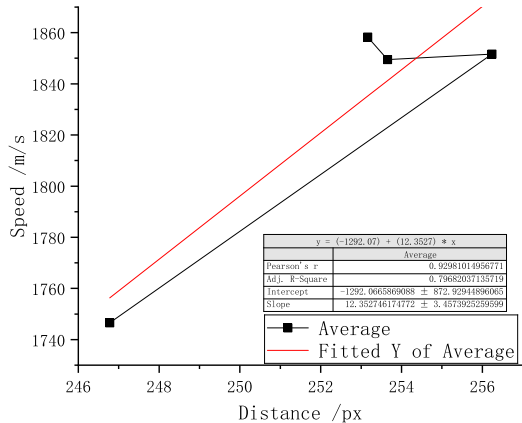
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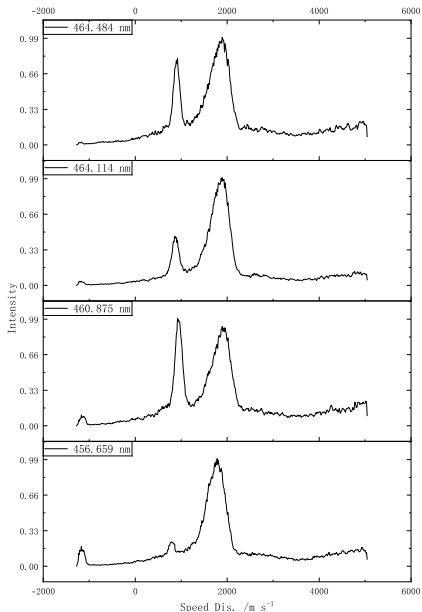


Average

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

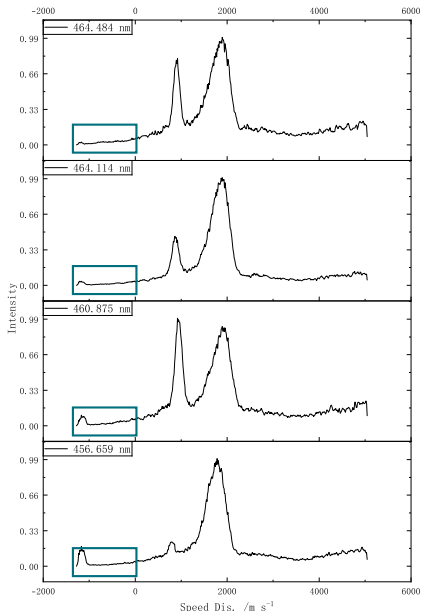
Intercept $\approx -1292 \text{ m s}^{-1}$

Error



^aMaybe $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.

Error



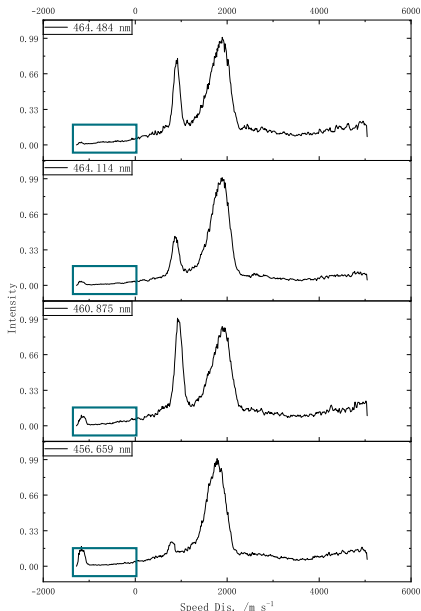
Average

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

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

^aMaybe $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.

Error



Average

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

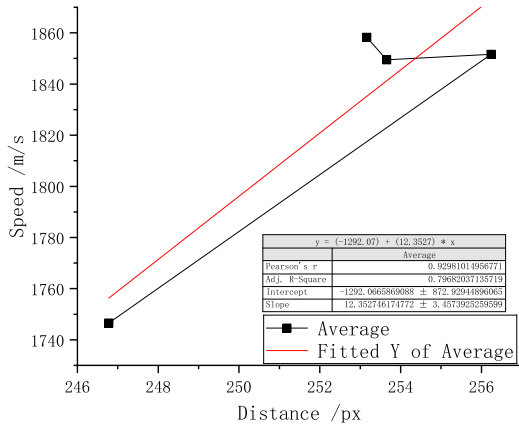
$$\text{Intercept} \approx -1292 \text{ m s}^{-1}$$

Notice

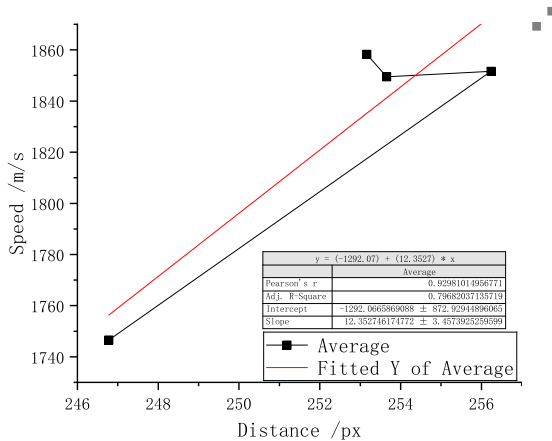
What we are calculating here are actually $|\mathbf{v}_{\text{NO}}|$, which are not supposed to be **minus**^a.

^aMaybe $\pm 5 \text{ m s}^{-1}$ -level intercept noise is permitted.

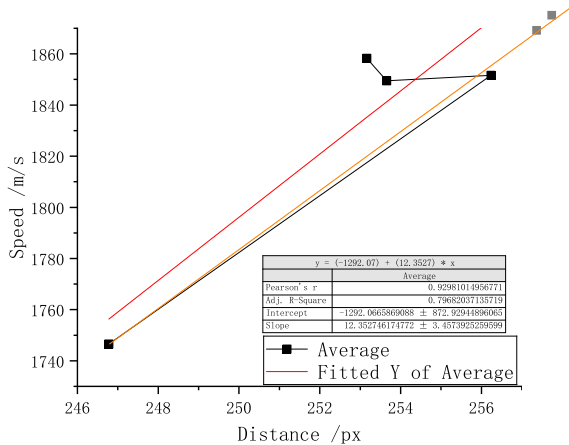
Error



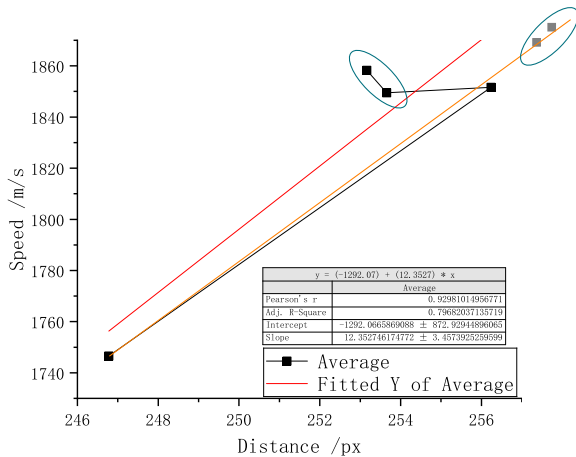
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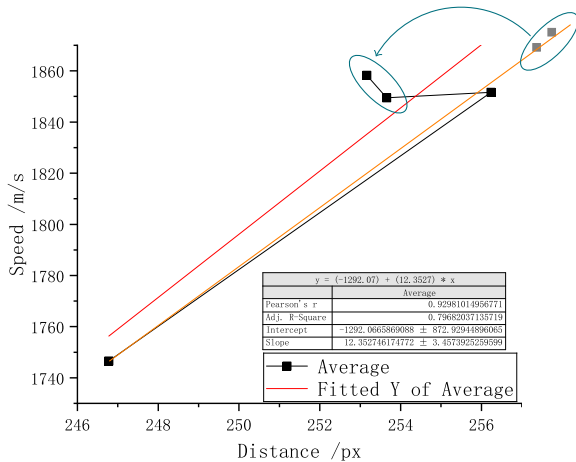
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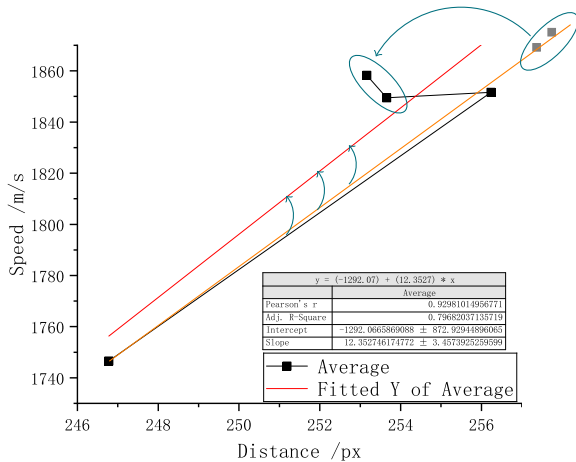
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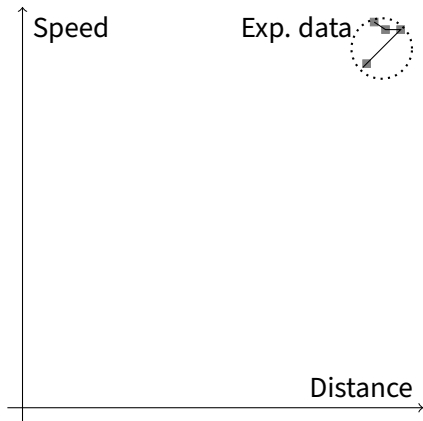
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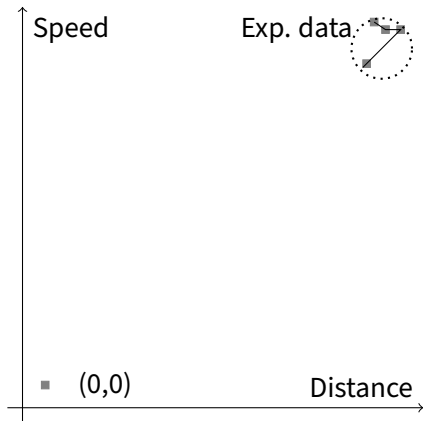
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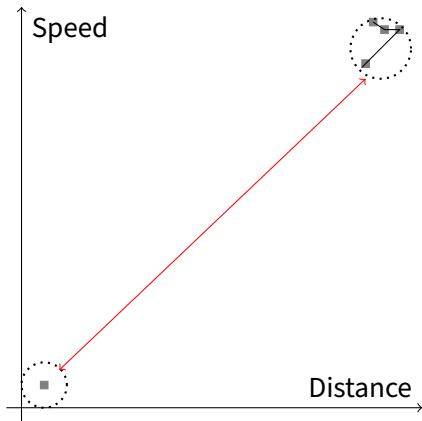
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Error

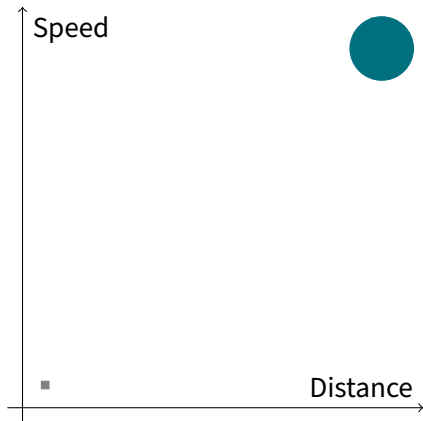


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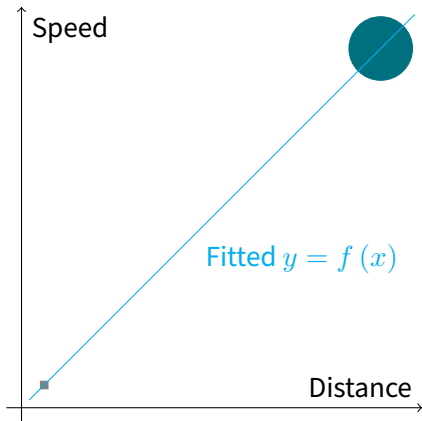
If we assume a virtual zero point:
The fake data obtains a huge **weight**!
Statistics tools always treat all data
as proper indications.

Error



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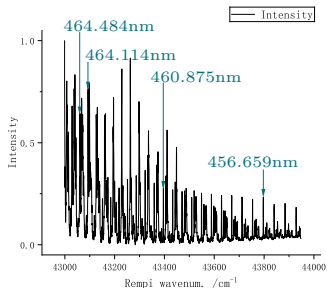
Error



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Statistics tools always treat all data
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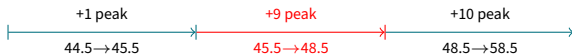
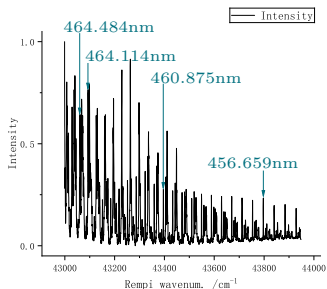
⇒ After assignments, which are the
points we should use?

Assignment for Assignment



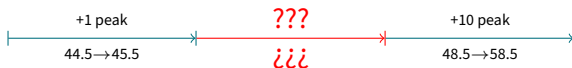
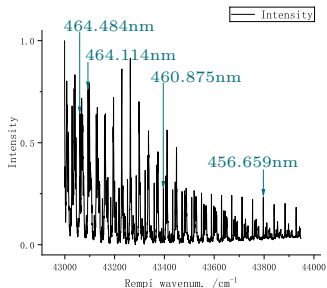
464.484nm $\approx 43058.49\text{cm}^{-1}$	464.114nm $\approx 43092.81\text{cm}^{-1}$	460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 253.162	px = 253.655	px = 256.240	px = 246.776
<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

Assignment for Assignment



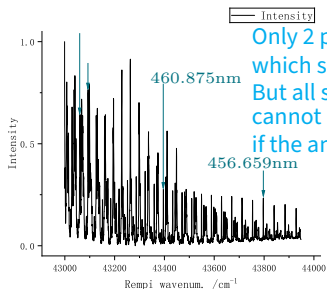
464.484nm ≈ 43058.49cm ⁻¹	464.114nm ≈ 43092.81cm ⁻¹	460.875nm ≈ 43395.69cm ⁻¹	456.659nm ≈ 43796.34cm ⁻¹
px = 253.162	px = 253.655	px = 256.240	px = 246.776
<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

Assignment for Assignment



464.484nm ≈ 43058.49cm ⁻¹	464.114nm ≈ 43092.81cm ⁻¹	460.875nm ≈ 43395.69cm ⁻¹	456.659nm ≈ 43796.34cm ⁻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



Only 2 peaks
which seem more valid.
But all statistics tools
cannot be properly applied
if the amount of data ≤ 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] J. Danielak et al. *Journal of Molecular Spectroscopy* **181.2** (1997), pp. 394–402.
- [2] Rémy Jost et al. *The Journal of Chemical Physics* **105.3** (July 1996).
- [3] Charlotte Emma Moore and Jean W. Gallagher. “Tables of spectra of hydrogen, carbon, nitrogen, and oxygen atoms and ions”. 1993.
- [4] Colin M. Western. *Journal of Quantitative Spectroscopy and Radiative Transfer* **186** (2017), pp. 221–242.