

練習実験報告

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2024 年 6 月 11 日

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Galvano Sepctrum

REMPI scan

- Selected peaks

- Peak assignments

- Speed correction

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Galvano Sepctrum



Fig. 1: Wavelen. correction

Galvano Sepctrum

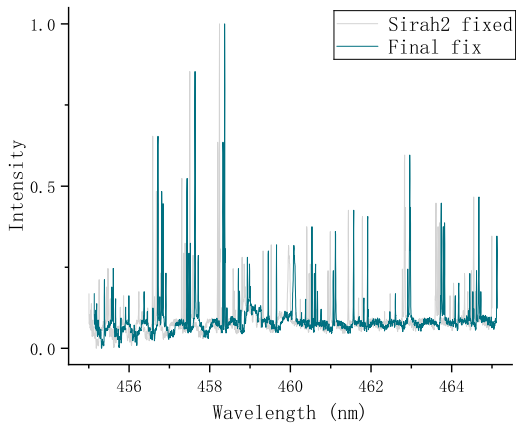


Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

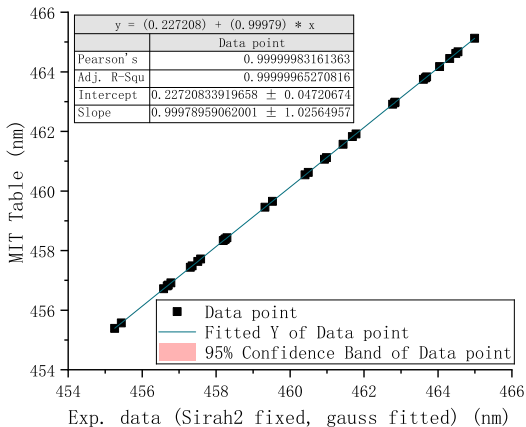


Fig. 2: Correction function

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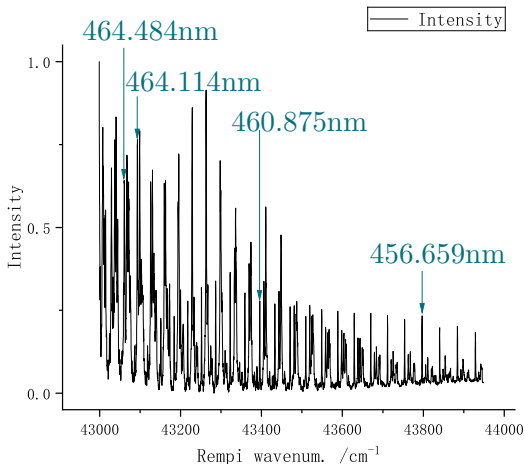
Selected peaks

Peak assignments

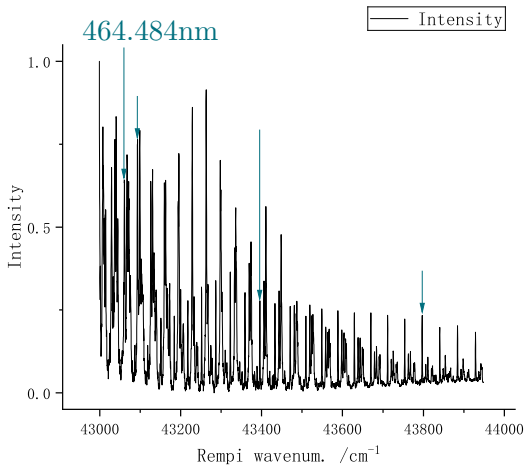
Speed correction

Error

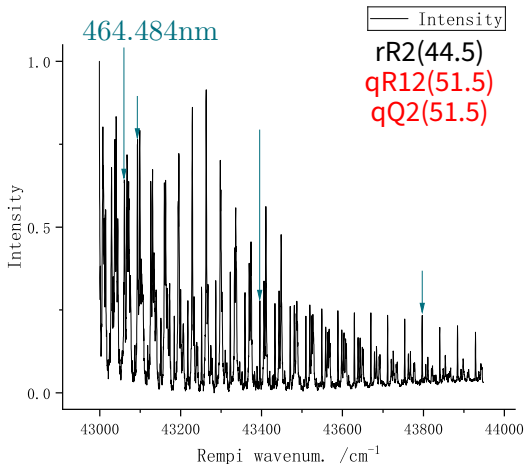
Selected peaks



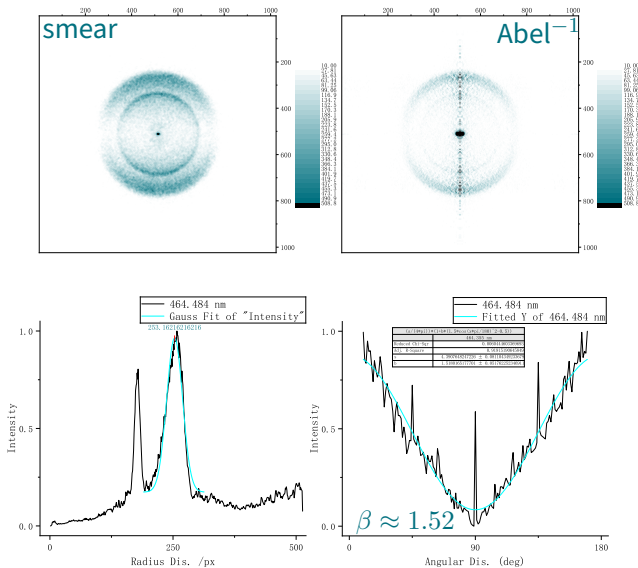
Peak 1



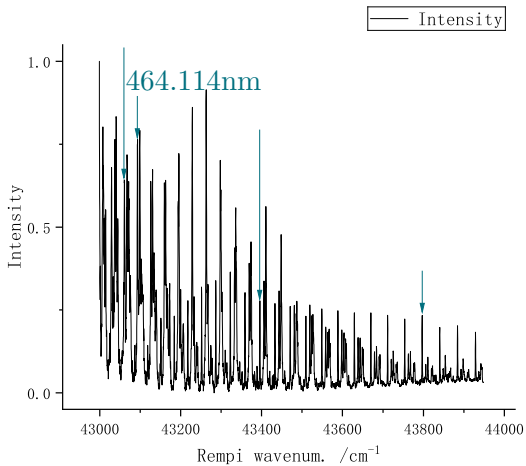
Peak 1



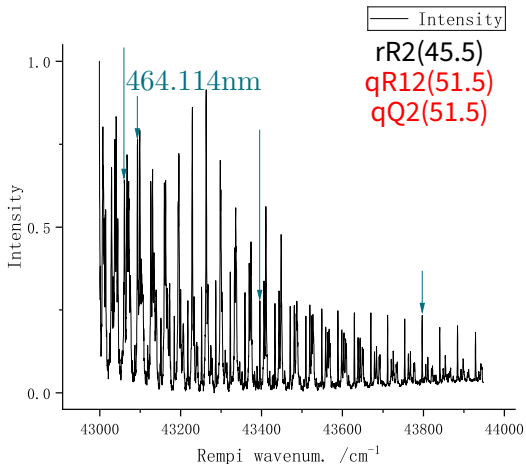
Peak 1



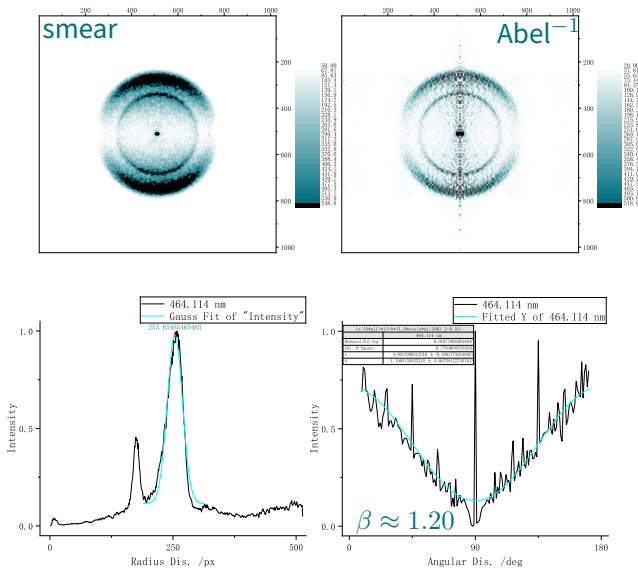
Peak 2



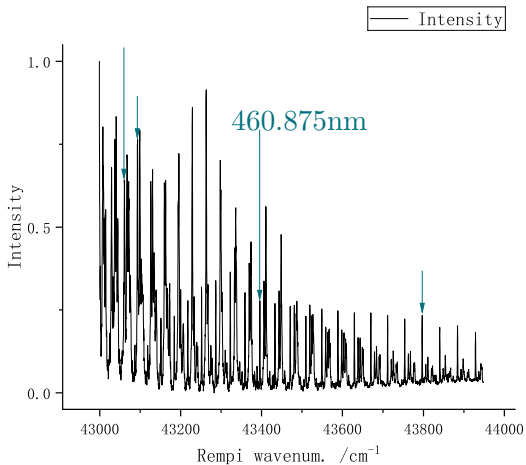
Peak 2



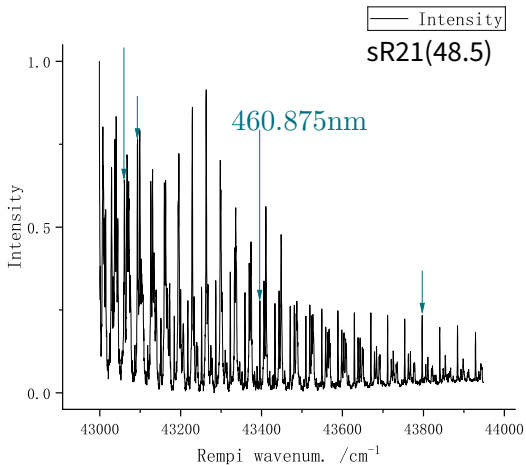
Peak 2



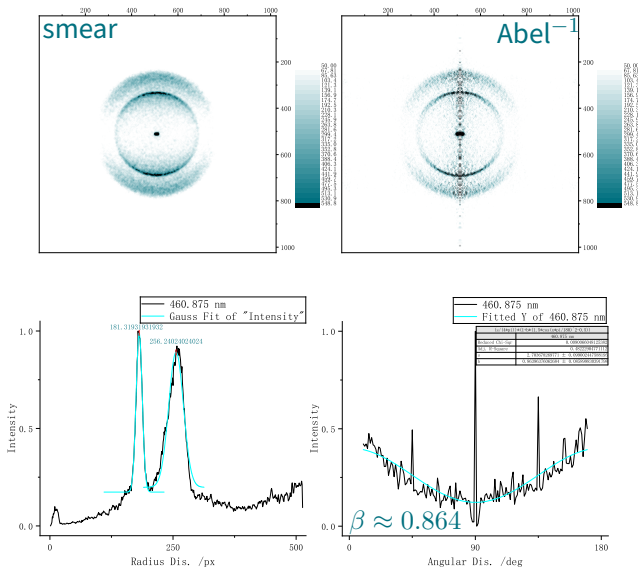
Peak 3



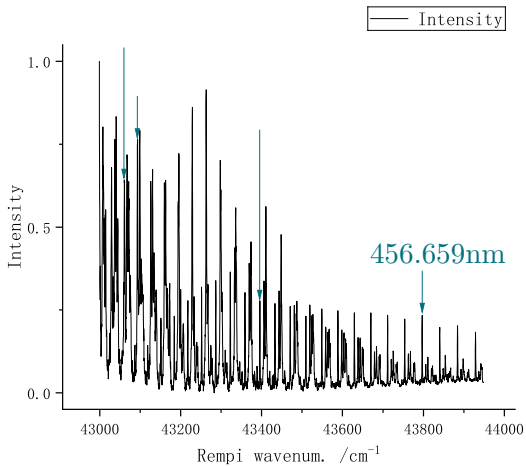
Peak 3



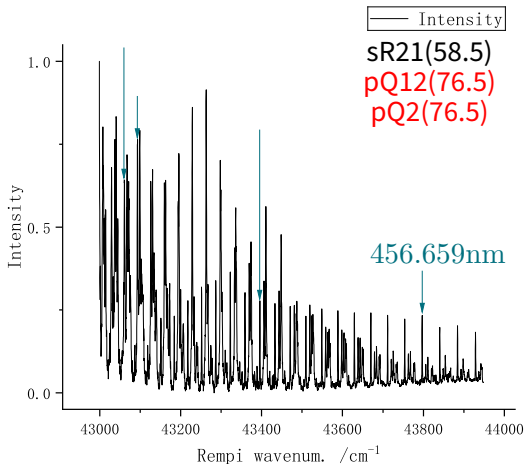
Peak 3



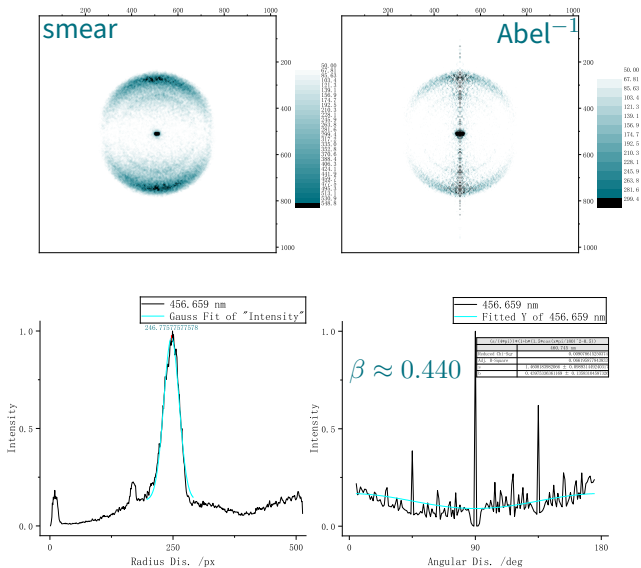
Peak 4



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 = 181.319 & 256.240 | px = 246.776 |
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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.

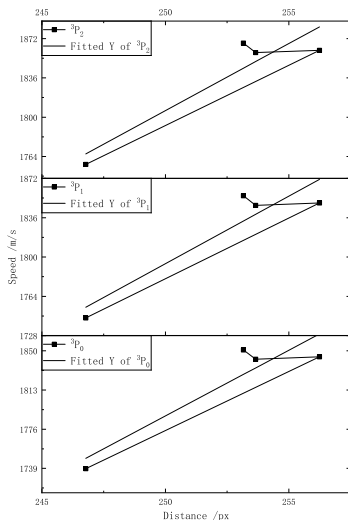
Speed correction

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

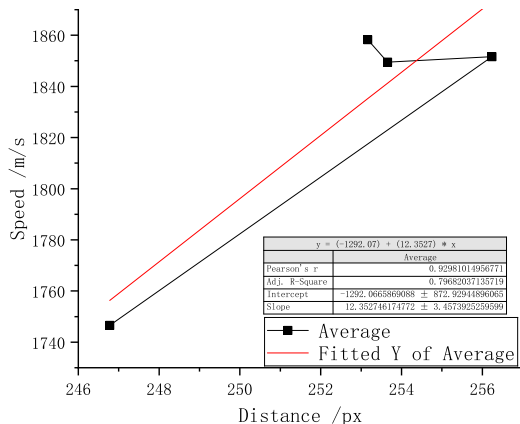
3P_0

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

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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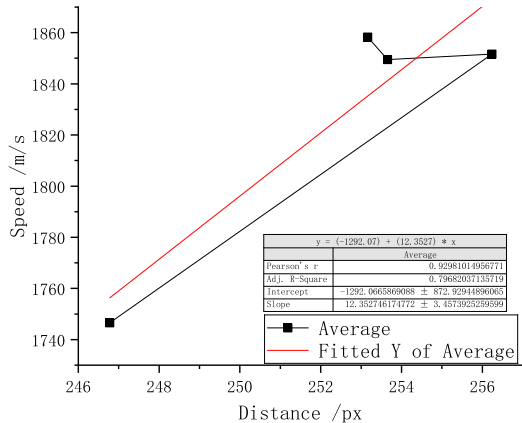
Selected peaks

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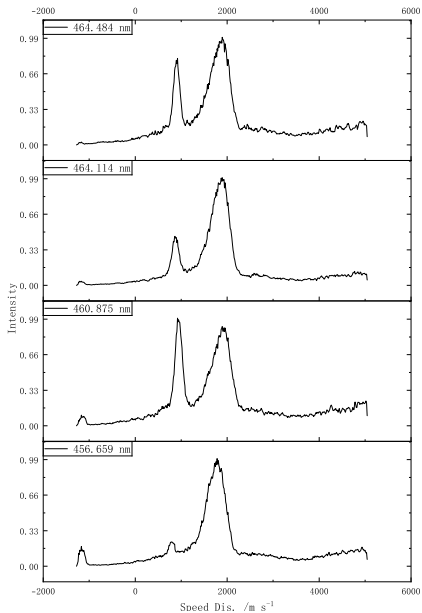


Average

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

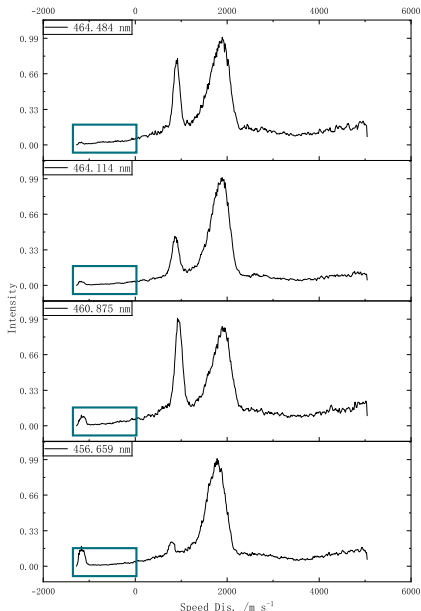
Intercept $\approx -1292 \text{ m s}^{-1}$

Error



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

Error



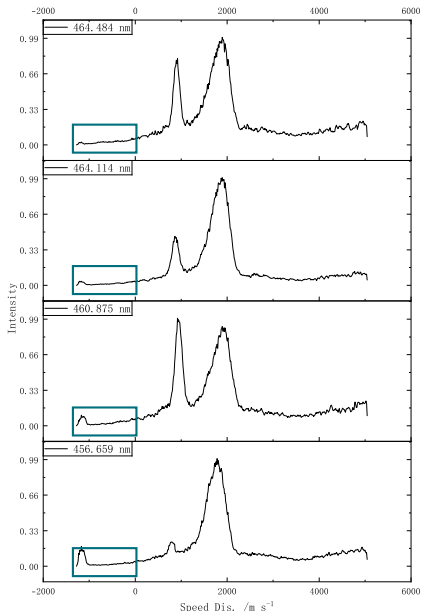
Average

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

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

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Error



Average

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

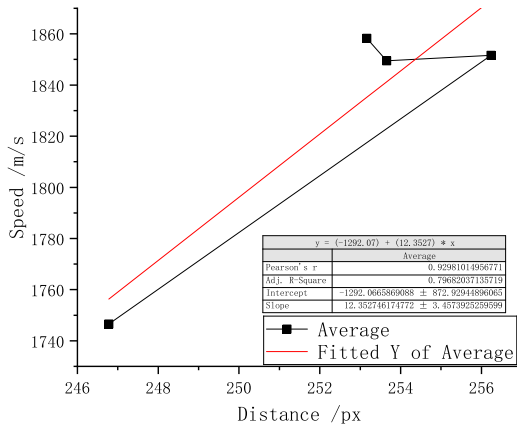
$$\text{Intercept} \approx -1292 \text{ m s}^{-1}$$

Notice

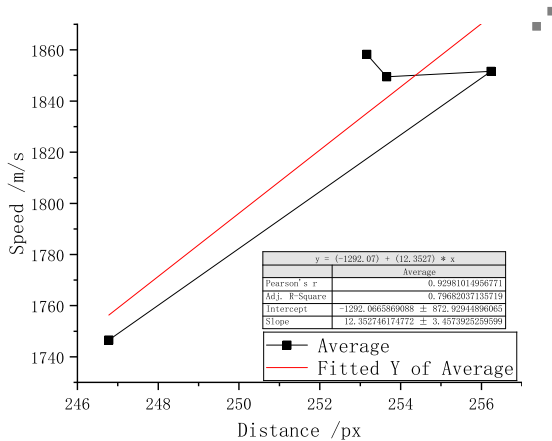
What we are calculating here are actually $|\mathbf{v}_{\text{NO}}|$, which are not supposed to be **minus**^a.

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

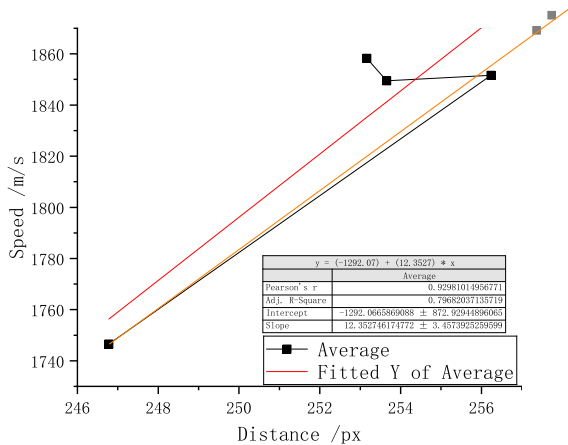
Error



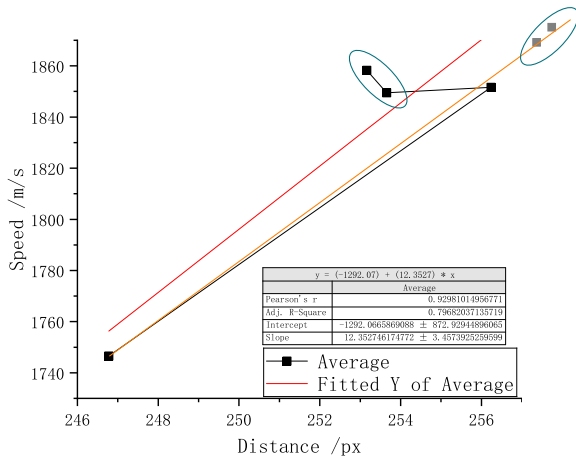
Error



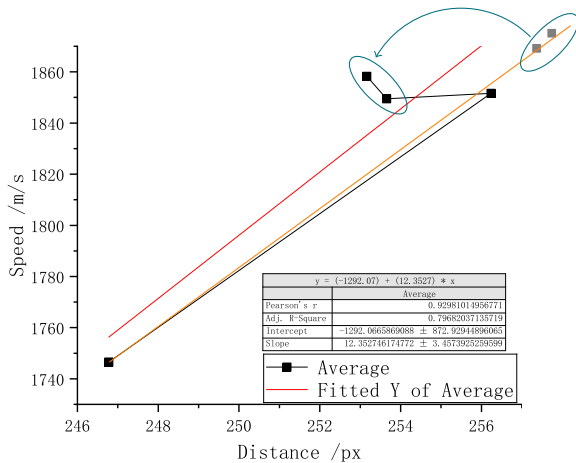
Error



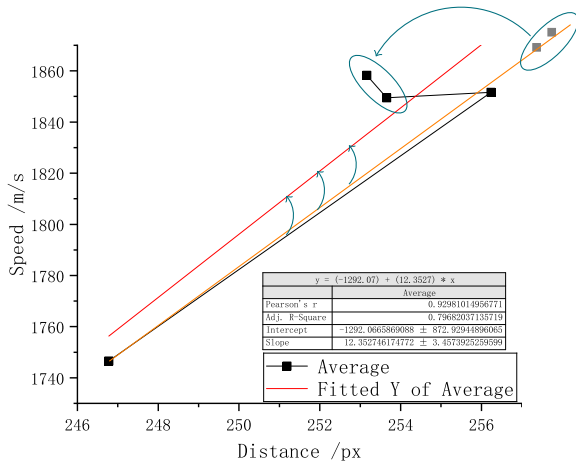
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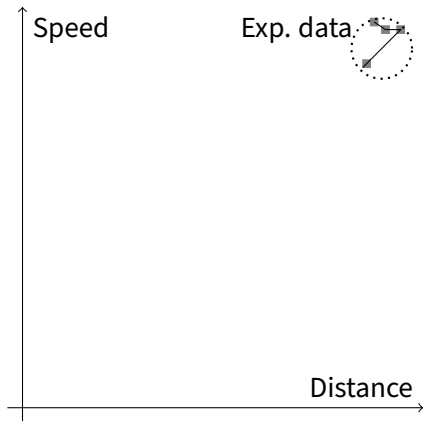
Error



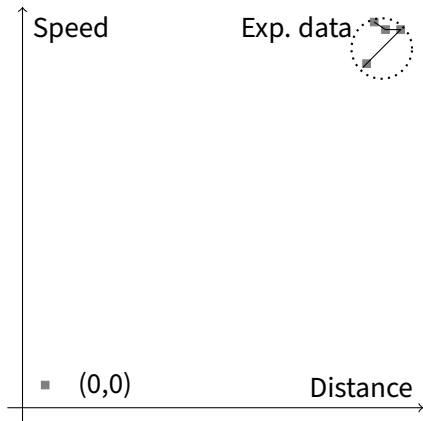
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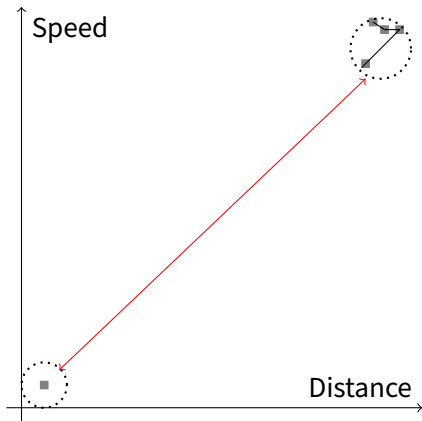
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Error

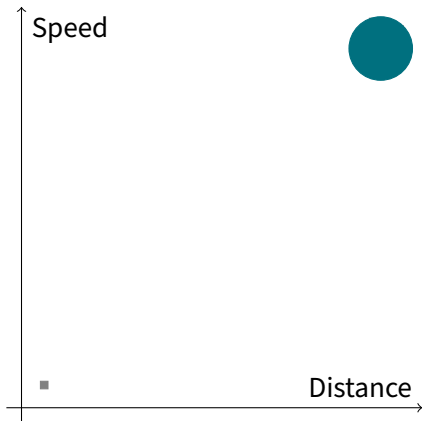


Error



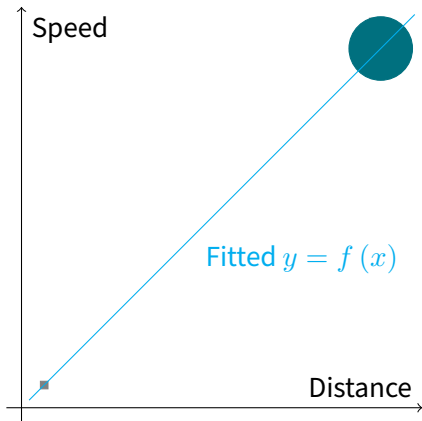
If we assume a virtual zero point:
The fake data obtains a huge **weight**!
Statistics tools always treat all data
as proper indications.

Error



If we assume a virtual zero point:
The fake data obtains a huge **weight**!
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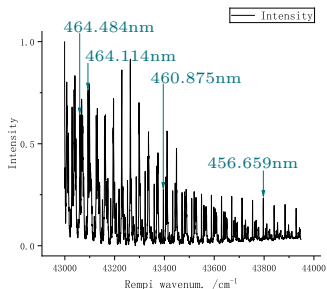
Error



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The fake data obtains a huge **weight**!
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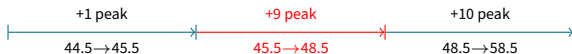
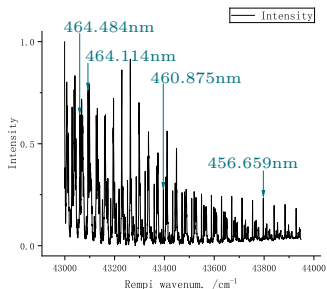
⇒ After assignments, which are the
points we should use?

Assignment for Assignment



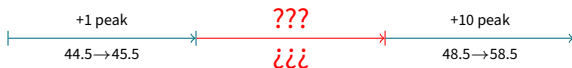
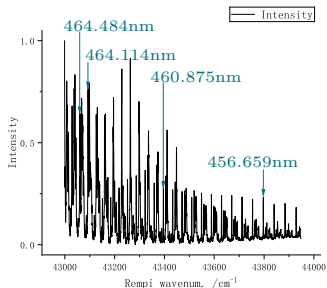
| | | | |
|---|---|---|---|
| 464.484nm $\approx 43058.49\text{cm}^{-1}$ | 464.114nm $\approx 43092.81\text{cm}^{-1}$ | 460.875nm $\approx 43395.69\text{cm}^{-1}$ | 456.659nm $\approx 43796.34\text{cm}^{-1}$ |
| px = 253.162 | px = 253.655 | px = 256.240 | px = 246.776 |
| <i>rR2</i> (44.5) | <i>rR2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

Assignment for Assignment



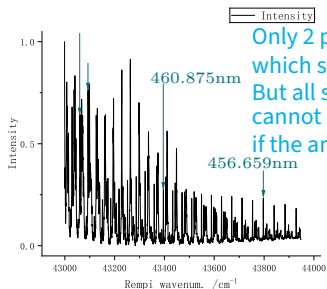
| | | | |
|---|---|---|---|
| 464.484nm ≈ 43058.49cm ⁻¹ | 464.114nm ≈ 43092.81cm ⁻¹ | 460.875nm ≈ 43395.69cm ⁻¹ | 456.659nm ≈ 43796.34cm ⁻¹ |
| px = 253.162 | px = 253.655 | px = 256.240 | px = 246.776 |
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Assignment for Assignment



| | | | |
|---|---|---|---|
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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] 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.