

練習実験報告

肖宇笑

2024 年 6 月 18 日

Contents

Galvano Sepctrum

REMPI scan

- Selected peaks

- Peak assignments

- Speed correction

- Error

Contents

Galvano Sepctrum

REMPI scan

- Selected peaks

- Peak assignments

- Speed correction

- Error

Galvano Sepctrum



Fig. 1: Wavelen. correction

Galvano Sepctrum

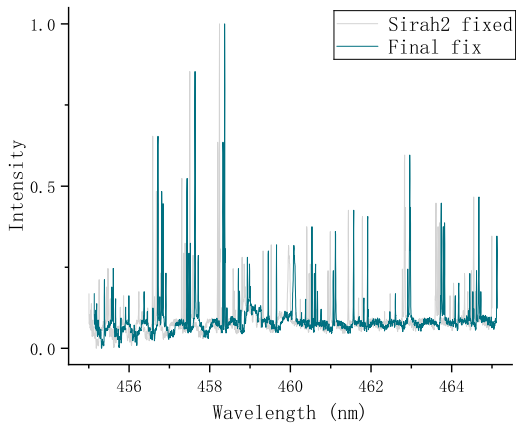


Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

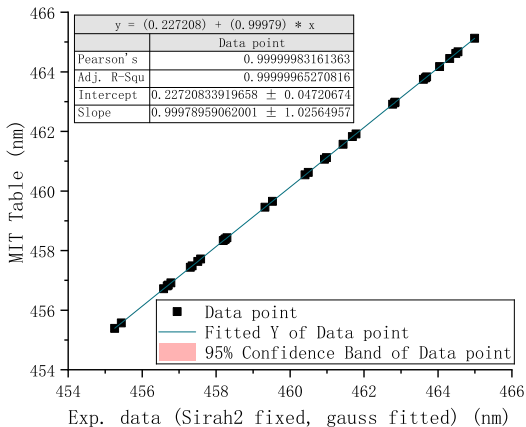


Fig. 2: Correction function

Contents

Galvano Sepctrum

REMPI scan

- Selected peaks

- Peak assignments

- Speed correction

- Error

Contents

Galvano Sepctrum

REMPI scan

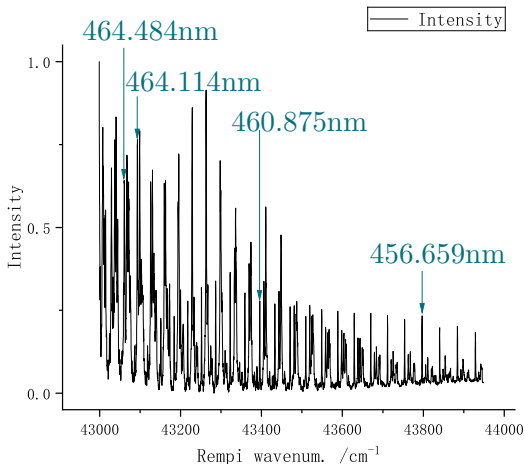
Selected peaks

Peak assignments

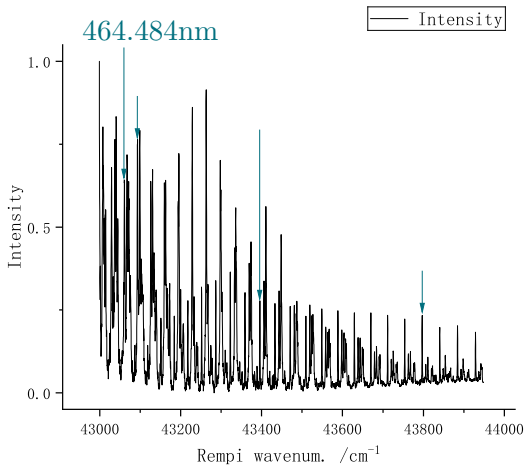
Speed correction

Error

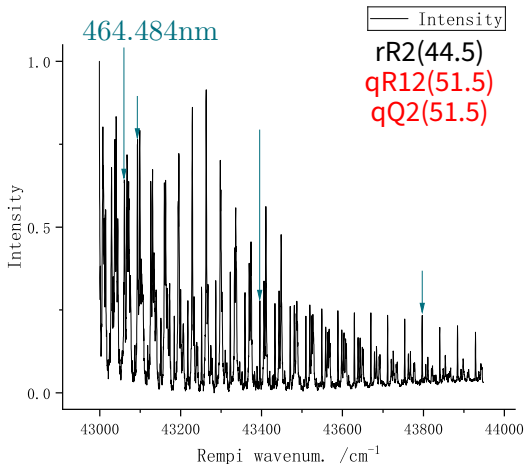
Selected peaks



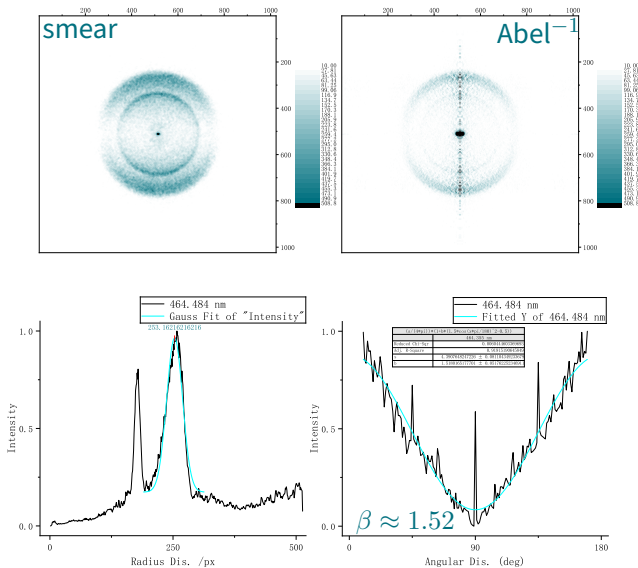
Peak 1



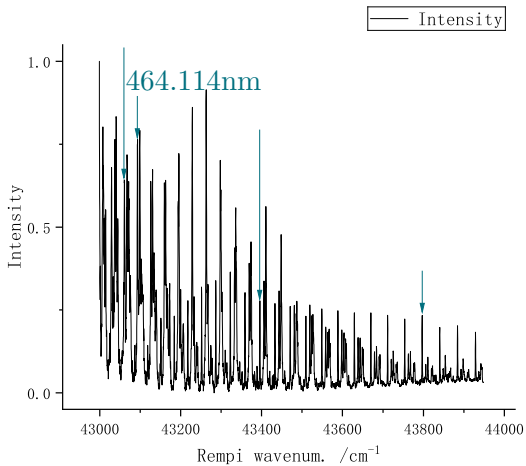
Peak 1



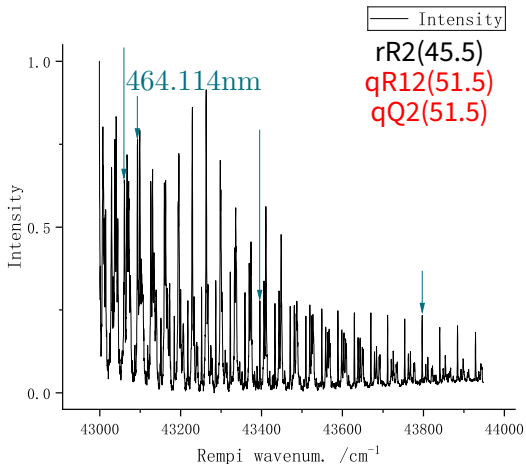
Peak 1



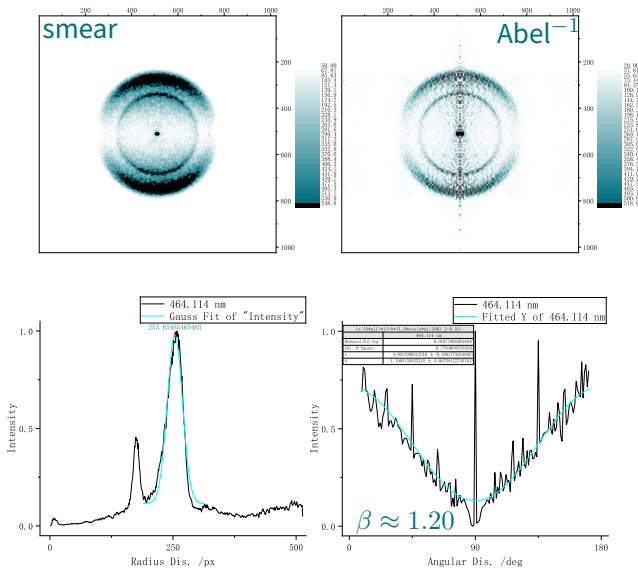
Peak 2



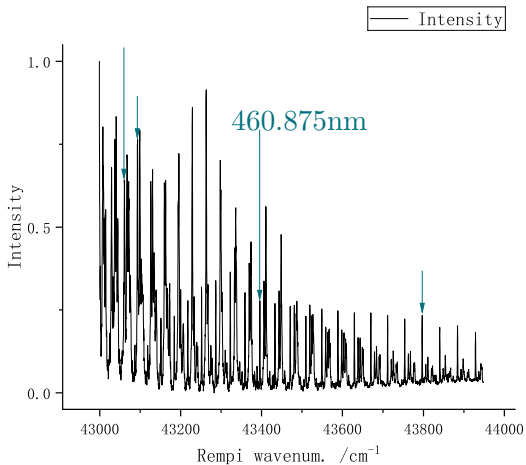
Peak 2



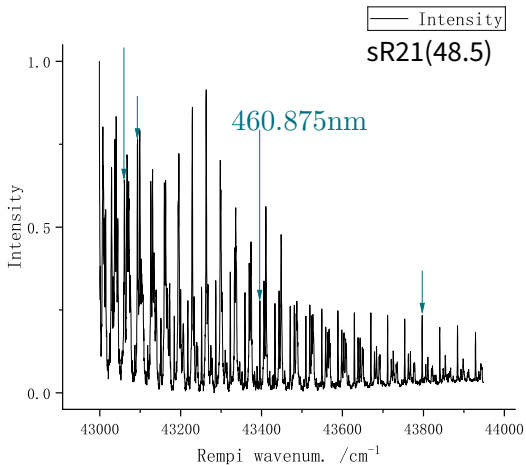
Peak 2



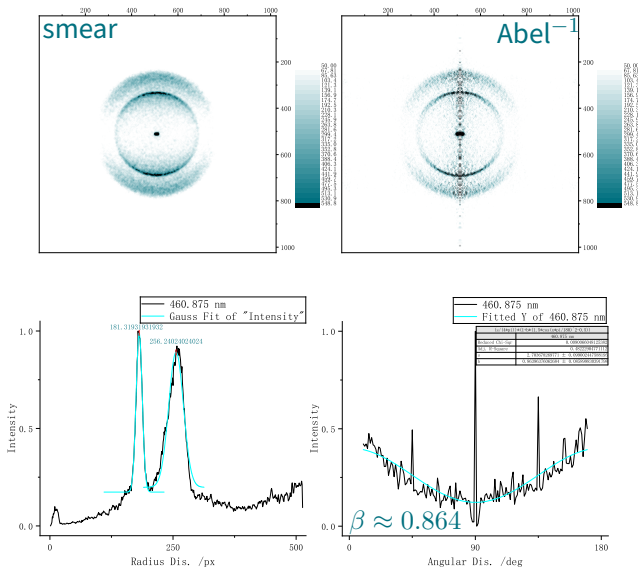
Peak 3



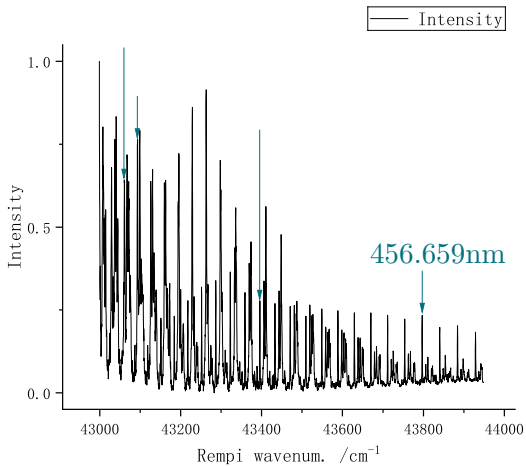
Peak 3



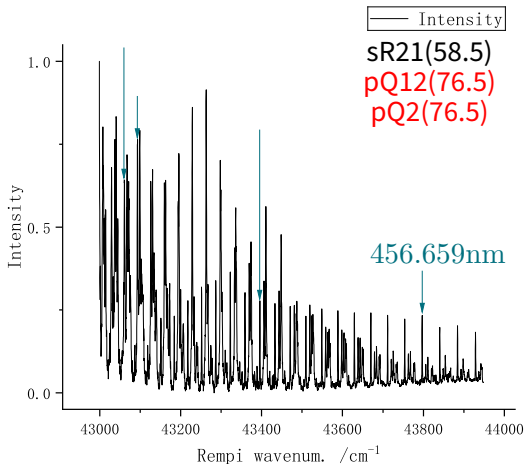
Peak 3



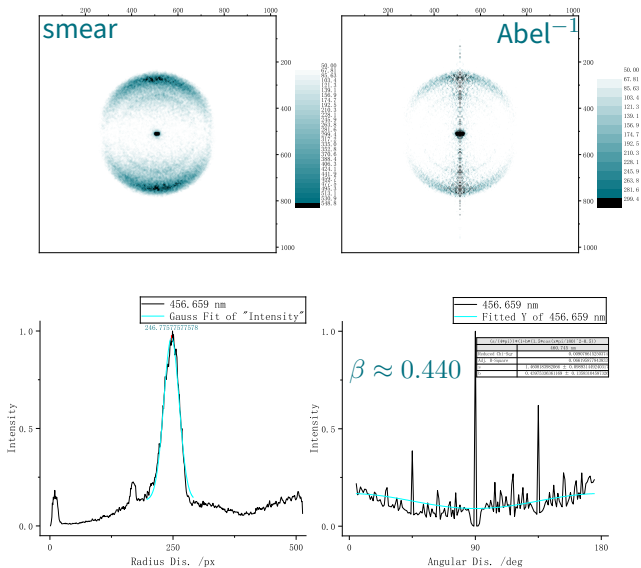
Peak 4



Peak 4



Peak 4



Contents

Galvano Sepctrum

REMPI scan

Selected peaks

Peak assignments

Speed correction

Error

Contents

Galvano Sepctrum

REMPI scan

Selected peaks

Peak assignments

Speed correction

Error

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
<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.

Contents

Galvano Sepctrum

REMPI scan

Selected peaks

Peak assignments

Speed correction

Error

Contents

Galvano Sepctrum

REMPI scan

Selected peaks

Peak assignments

Speed correction

Error

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

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

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

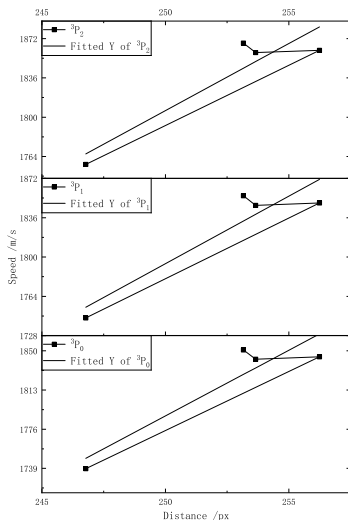
Speed correction

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



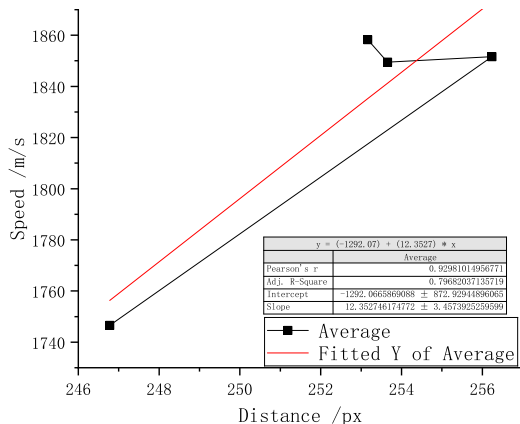
3P_2
 $12.28 \text{ m s}^{-1} \text{ px}^{-1}$
Intercept $\approx -1265 \text{ m s}^{-1}$

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

Contents

Galvano Sepctrum

REMPI scan

Selected peaks

Peak assignments

Speed correction

Error

Contents

Galvano Sepctrum

REMPI scan

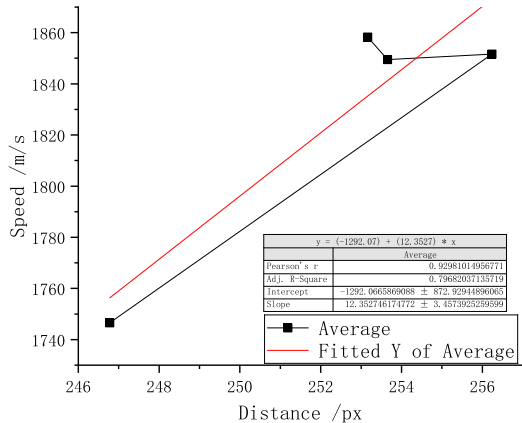
Selected peaks

Peak assignments

Speed correction

Error

Error

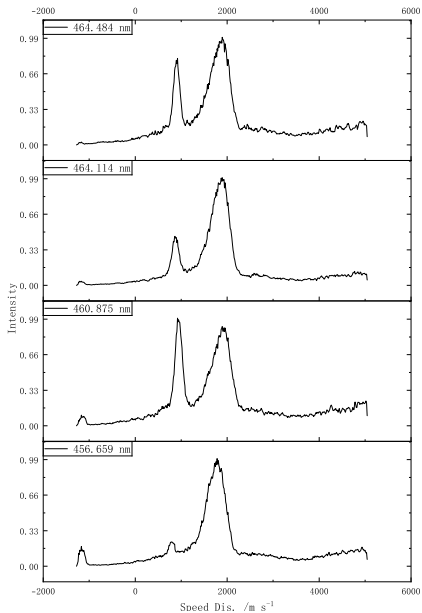


Average

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

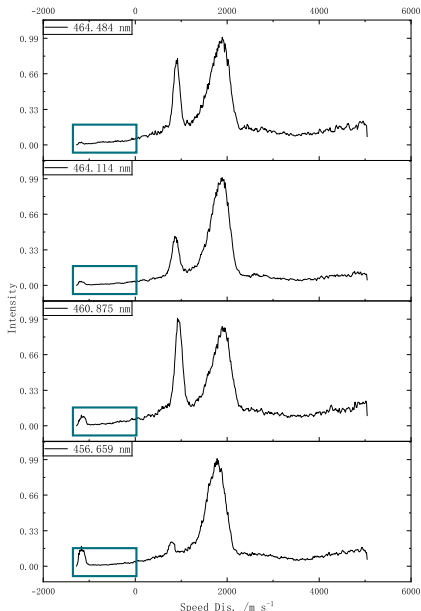
Intercept $\approx -1292 \text{ m s}^{-1}$

Error



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

Error



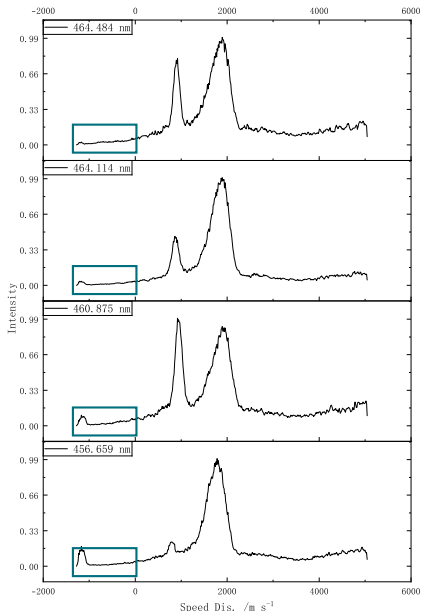
Average

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

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

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

Error



Average

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

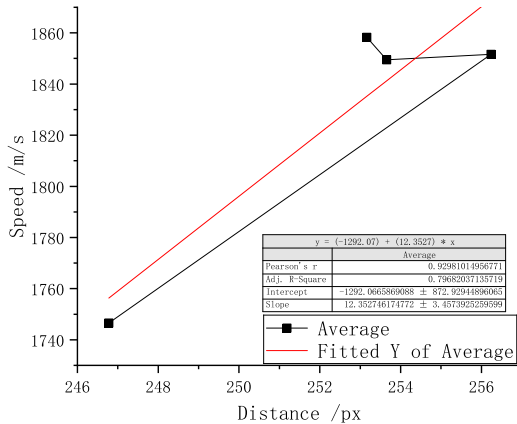
$$\text{Intercept} \approx -1292 \text{ m s}^{-1}$$

Notice

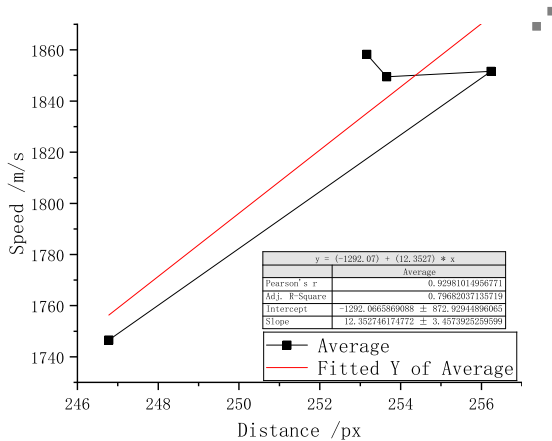
What we are calculating here are actually $|\mathbf{v}_{\text{NO}}|$, which are not supposed to be **minus**^a.

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

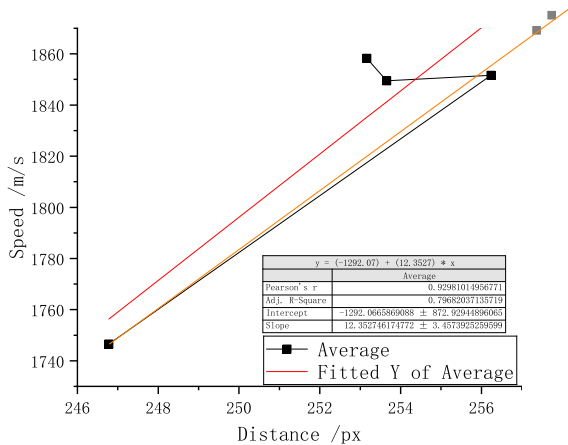
Error



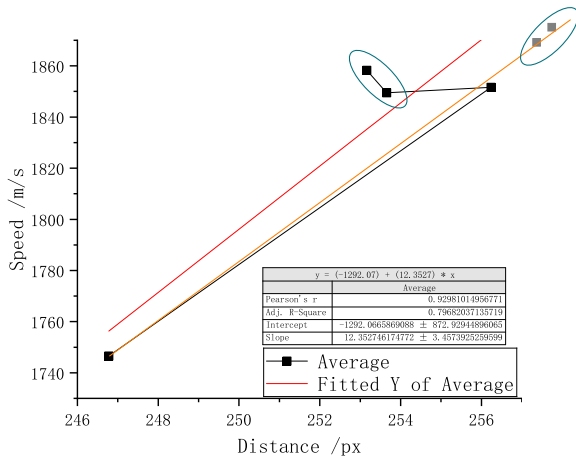
Error



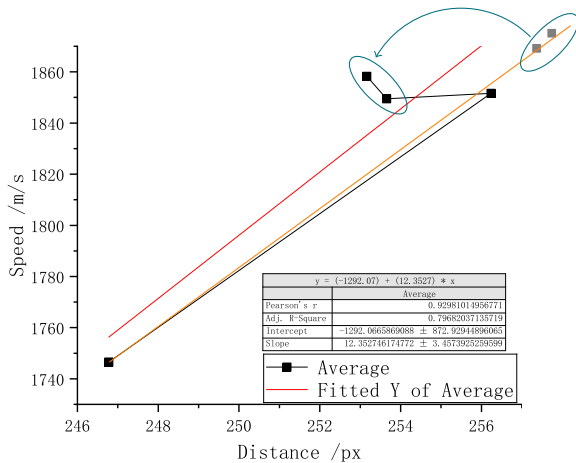
Error



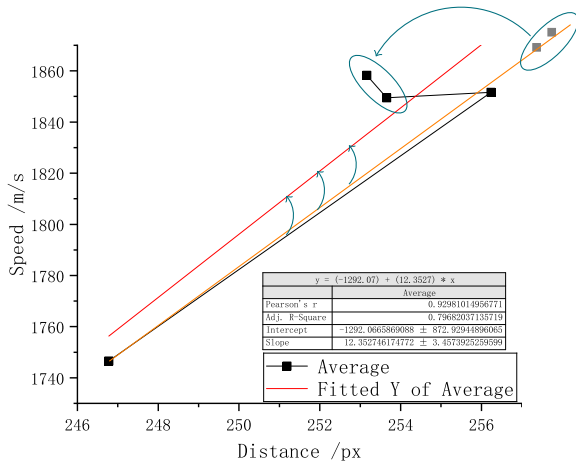
Error



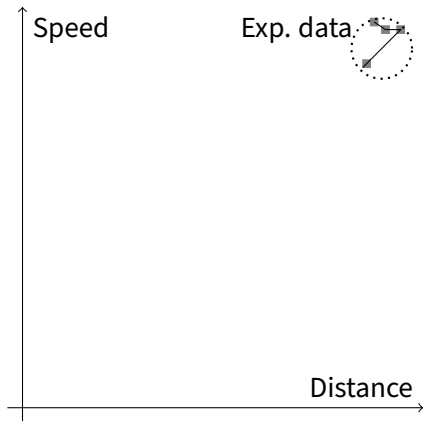
Error



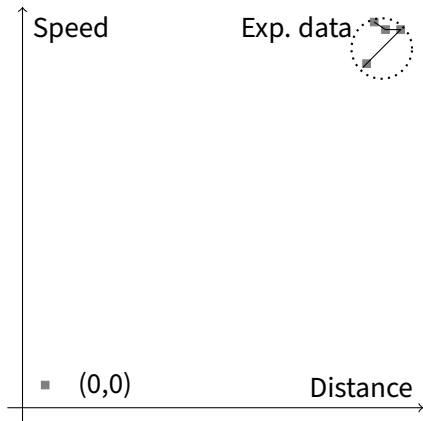
Error



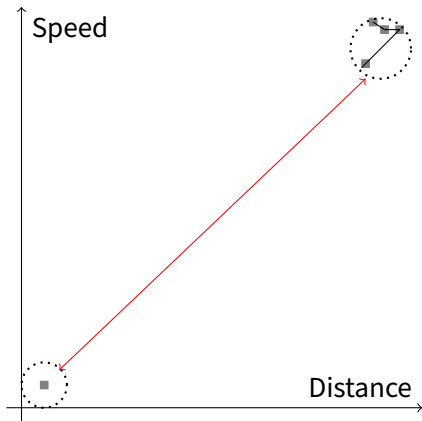
Error



Error

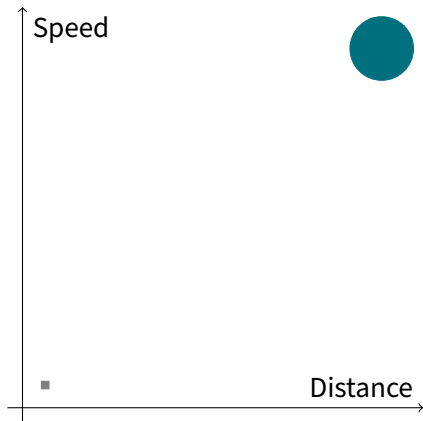


Error



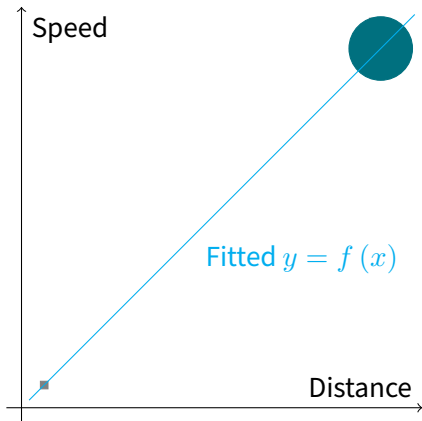
If we assume a virtual zero point:
The fake data obtains a huge **weight**!
Statistics tools always treat all data
as proper indications.

Error



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

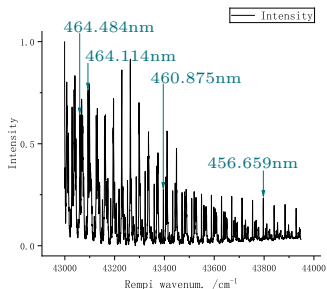
Error



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

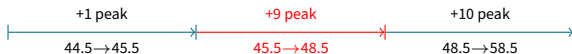
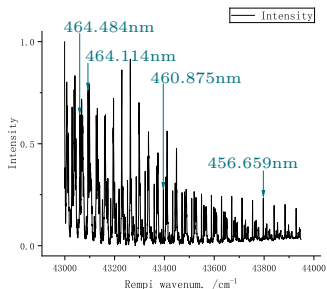
⇒ After assignments, which are the
points we should use?

Assignment for Assignment



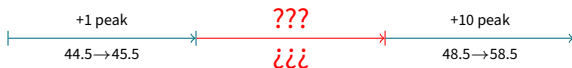
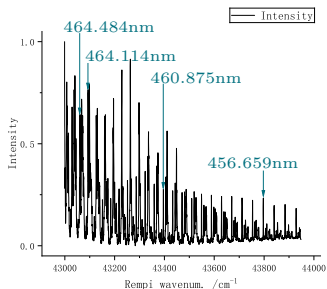
464.484nm $\approx 43058.49\text{cm}^{-1}$	464.114nm $\approx 43092.81\text{cm}^{-1}$	460.875nm $\approx 43395.69\text{cm}^{-1}$	456.659nm $\approx 43796.34\text{cm}^{-1}$
px = 253.162	px = 253.655	px = 256.240	px = 246.776
<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

Assignment for Assignment



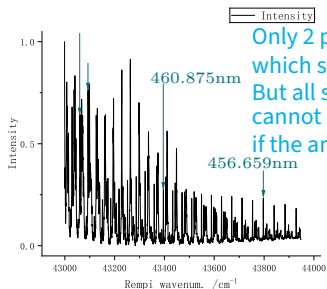
464.484nm ≈ 43058.49cm ⁻¹	464.114nm ≈ 43092.81cm ⁻¹	460.875nm ≈ 43395.69cm ⁻¹	456.659nm ≈ 43796.34cm ⁻¹
px = 253.162	px = 253.655	px = 256.240	px = 246.776
<i>rR2</i> (44.5)	<i>rR2</i> (45.5)	<i>sR21</i> (48.5)	<i>sR21</i> (58.5)

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 ≤ 2 .

+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.