

練習実験報告

肖宇笑

May 30, 2024

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Galvano Sepctrum

Fig. 1: Wavelen. correction

Galvano Sepctrum

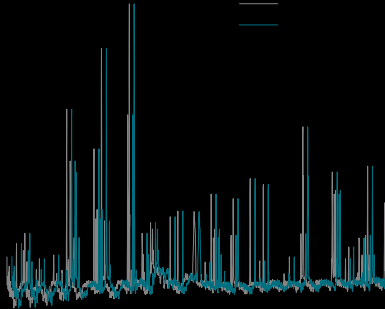


Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

$y = (0.227208) + (0.99979) * x$	
	Data point
Pearson's	0.99999983161363
Adj. R-Squ	0.99999965270816
Intercept	0.22720833919658 \pm 0.04720674
Slope	0.99978959062001 \pm 1.02564957

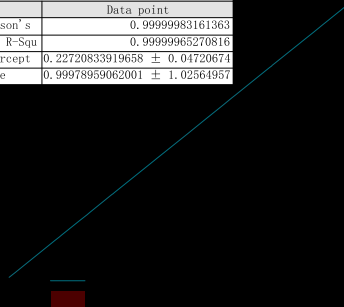


Fig. 2: Correction function

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Selected peaks

464.484nm

464.114nm

460.875nm

456.659nm

Peak 1

464.484nm

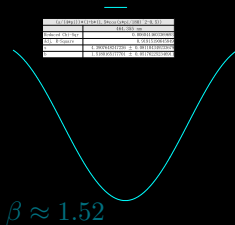
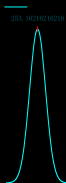
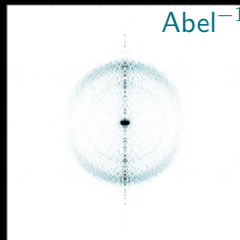
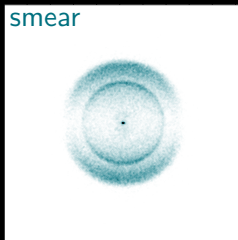


Peak 1

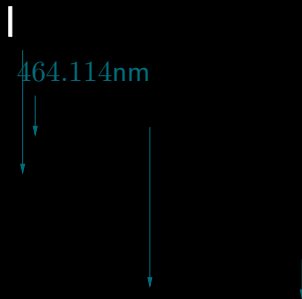
464.484nm

rR2(44.5)
qR12(51.5)
qQ2(51.5)

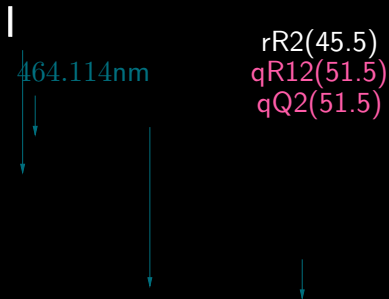
smear



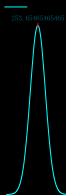
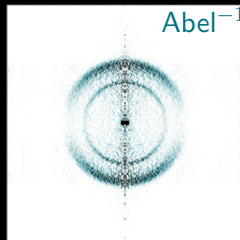
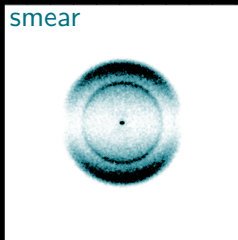
Peak 2



Peak 2

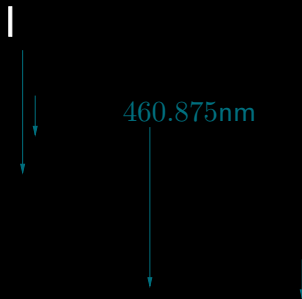


smear



$\text{Cu}(\text{I}4\text{py})\{\text{W}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}\} \cdot 10\text{H}_2\text{O} \cdot 2.8.21\}$	
	454, 454 nm
Induced Chl-5d	0.6189/0.5535/0.25
$\langle \chi^2 \rangle$, R-square	0.796/0.714/1.00
σ	4.185035/0.1195 \pm 8.185560/0.22
λ	1.20659/0.11896 \pm 0.306155/0.025

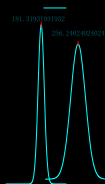
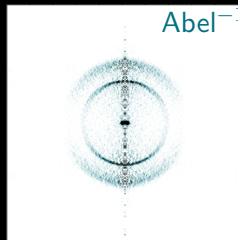
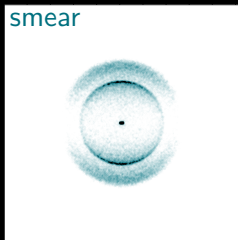
Peak 3



Peak 3



smear



Ca/(4Mg+3Fe+1)wt%, 5 wt% (atp/1.90-2.8.5)	
	498, 730 nm
Reduced Chi-Sqr	0.404034618252
Adj. R-Square	0.48222940711
n	2, 30818250711 ± 0.39602341548
σ	0.39602341548 ± 0.39602341548

$$\beta \approx 0.864$$

Peak 4

I

↓

↓

↓

456.659nm

↓

Peak 4

I

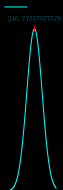
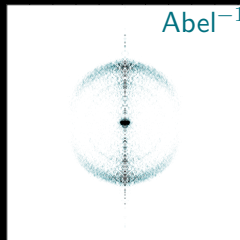
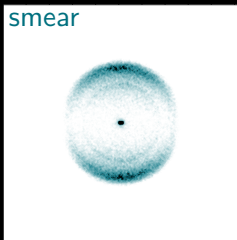


sR21(58.5)
pQ12(76.5)
pQ2(76.5)

456.659nm



Peak 4



$$\beta \approx 0.440$$

C:\Program Files\Foxit Software\Foxit Reader\Foxit Reader.exe	
100.000.000.000	
Product (S/N)	100.000.000.000
Model (S/N)	100.000.000.000
Serial (S/N)	100.000.000.000
Version (S/N)	100.000.000.000
Build (S/N)	100.000.000.000
Release (S/N)	100.000.000.000
Copyright (S/N)	100.000.000.000
License (S/N)	100.000.000.000
Support (S/N)	100.000.000.000
Help (S/N)	100.000.000.000
Exit (S/N)	100.000.000.000

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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 $\approx 43796.34\text{cm}^{-1}$
$\text{px} = 253.162$	$\text{px} = 253.655$	$\text{px} = 181.319 \& 256.240$	$\text{px} = 246.776$
<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_{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	$43\,058.49\text{cm}^{-1}$	$25\,128.57\text{cm}^{-1}$	$2341.932\,775\,0\text{cm}^{-1} + E(J = 44)$
Peak 2 464.114nm	$43\,092.81\text{cm}^{-1}$		$2341.932\,775\,0\text{cm}^{-1} + E(J = 45)$
Peak 3 460.875nm	$43\,395.69\text{cm}^{-1}$		$2341.932\,775\,0\text{cm}^{-1} + E(J = 48)$
Peak 4 456.659nm	$43\,796.34\text{cm}^{-1}$		$2341.932\,775\,0\text{cm}^{-1} + E(J = 58)$

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	43 058.49 cm^{-1}	25 128.57 cm^{-1}	5814.033 cm^{-1}
Peak 2 464.114nm	43 092.81 cm^{-1}		5965.969 cm^{-1}
Peak 3 460.875nm	43 395.69 cm^{-1}		6239.696 cm^{-1}
Peak 4 456.659nm	43 796.34 cm^{-1}		8004.278 cm^{-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

$E_{\text{int. (O)}}^5$	$E_{\text{trans}}(\text{total}) \approx 2.875464 E_{\text{trans}}(\text{NO})$ $= E_{\text{total}} - E_{\text{bond}}(\text{O}-\text{NO}) - E_{\text{int. (O)}} - E_{\text{int. (NO)}}$	$E_{\text{trans}}(\text{NO})$ $= \frac{1}{2} m(\text{NO}) v^2(\text{NO})$
3P_2 (0 cm ⁻¹)	11081.356 cm ⁻¹	4375.588 cm ⁻¹
	10964.609 cm ⁻¹	4334.685 cm ⁻¹
	10794.143 cm ⁻¹	4344.824 cm ⁻¹
	9398.766 cm ⁻¹	3870.489 cm ⁻¹
3P_1 (158.625 cm ⁻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
	9240.141 cm ⁻¹	3815.324 cm ⁻¹
3P_0 (226.977 cm ⁻¹)	10854.379 cm ⁻¹	4296.653 cm ⁻¹
	10737.632 cm ⁻¹	4255.749 cm ⁻¹
	10567.166 cm ⁻¹	4265.888 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

$3P_2$

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

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

$3P_1$

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

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

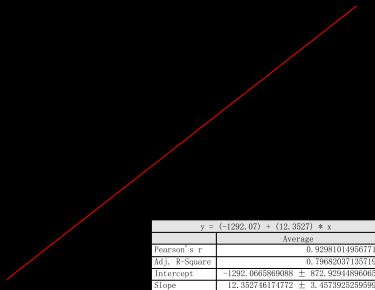
$3P_0$

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

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

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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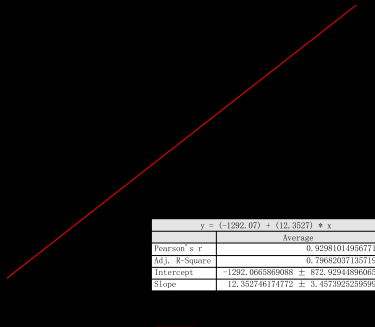
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Error



Average

 $12.35 \text{ m s}^{-1} \text{ px}^{-1}$ Intercept ≈ -1292

Error

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

Error



Average

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

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



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

Error

Average

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

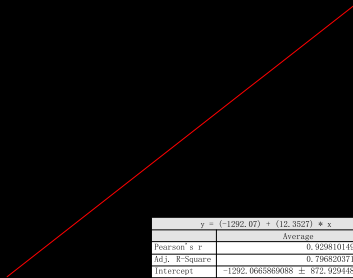
$$\text{Intercept} \approx -1292 \text{ m s}^{-1}$$

Notice

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

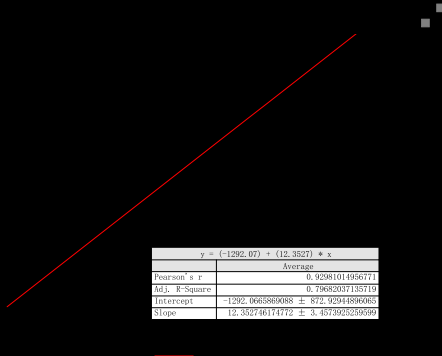
^aMaybe a $\pm 5 \text{ m s}^{-1}$ -level intercept noise are permitted.

Error

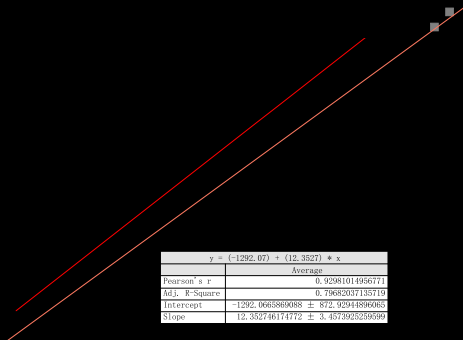


$y = (-1292.07) + (12.3527) \cdot x$	
Average	
Pearson's r	0.92981014956771
Adj. R-Square	0.79682037135719
Intercept	-1292.0665869088 ± 872.92944896065
Slope	12.352746174772 ± 3.4573925259599

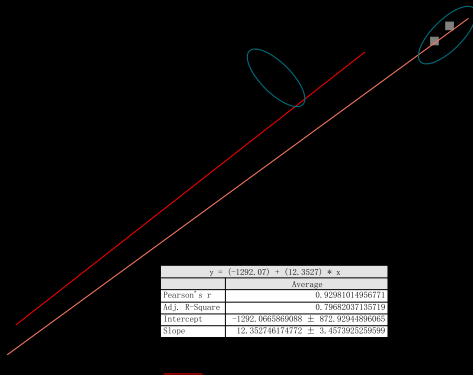
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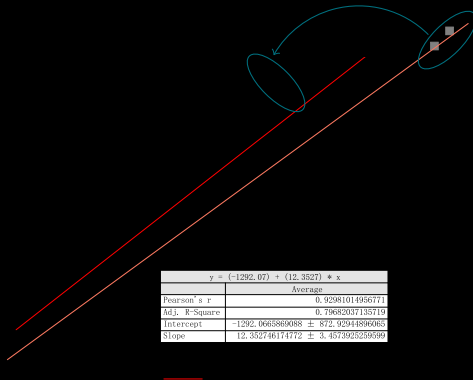
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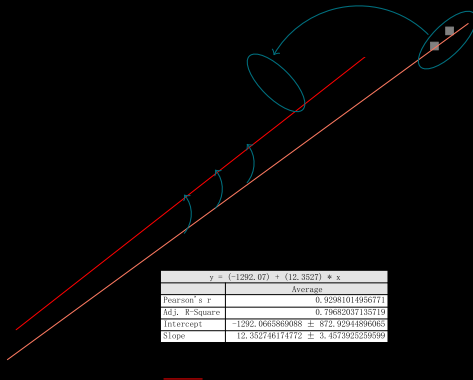
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Error



Error



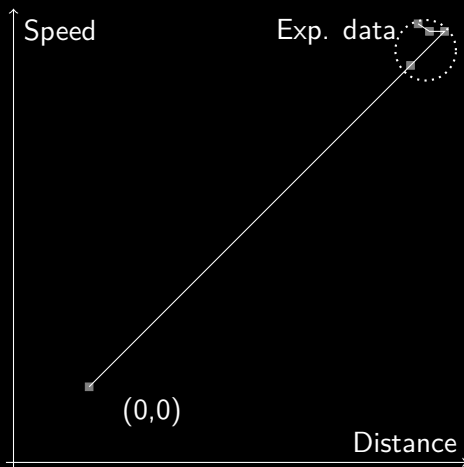
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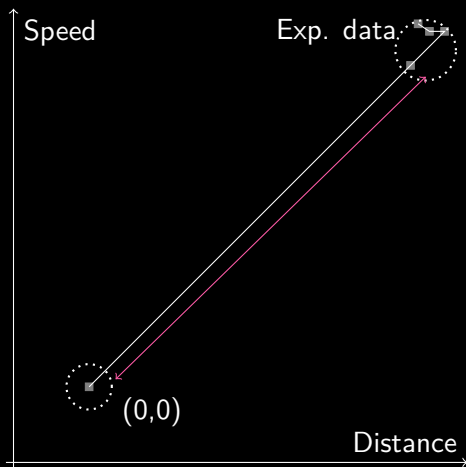
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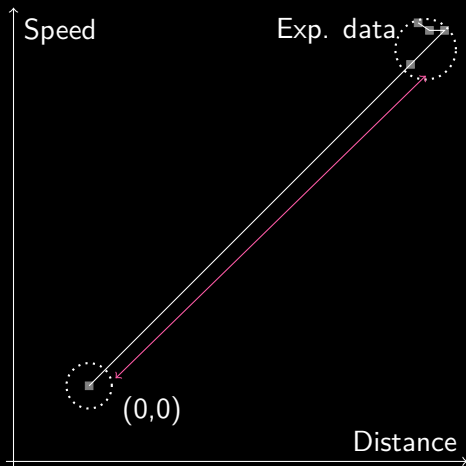
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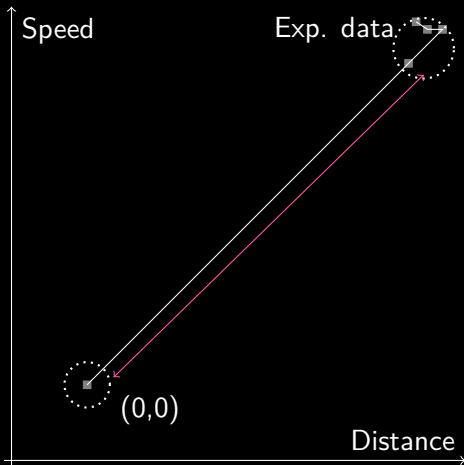


Error



If we assume a zero point:

Error



If we assume a zero point:
It obtains a huge **weight**!

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.