練習実験報告

肖宇笑

2024 年 5 月 30 日

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Galvano Sepctrum

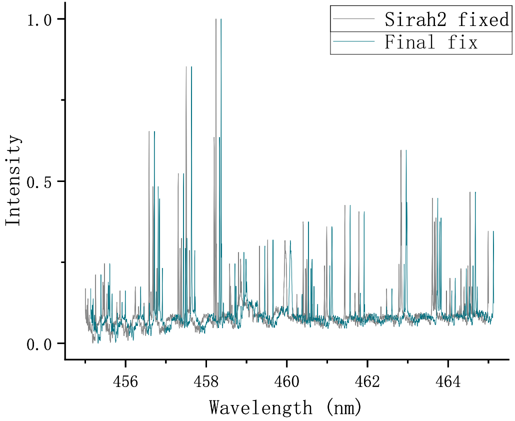

Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

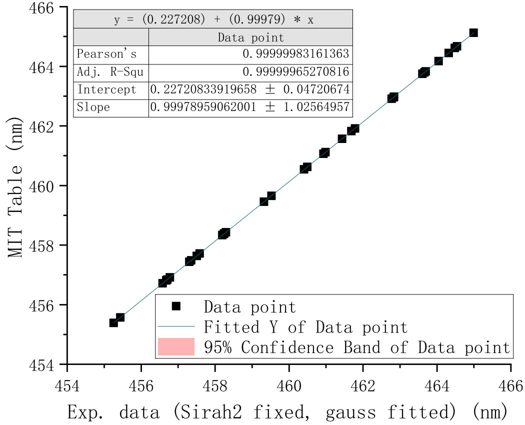

Fig. 2: Correction function

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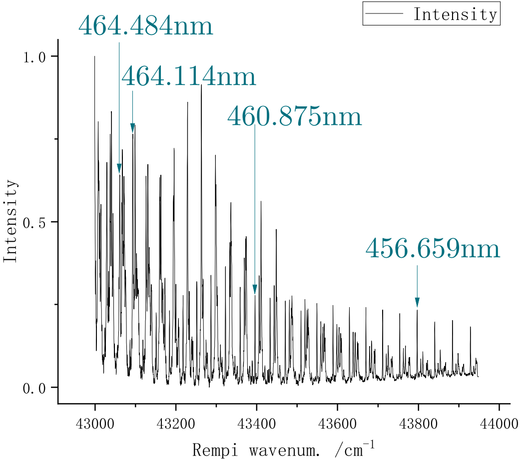
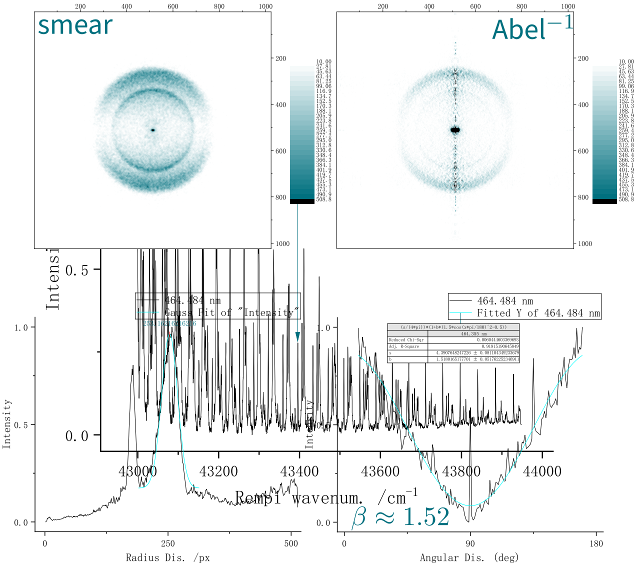
Selected peaks

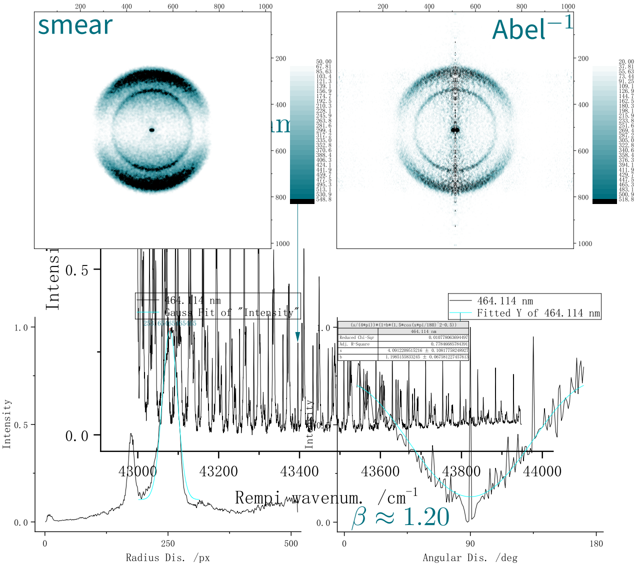


Peak 1



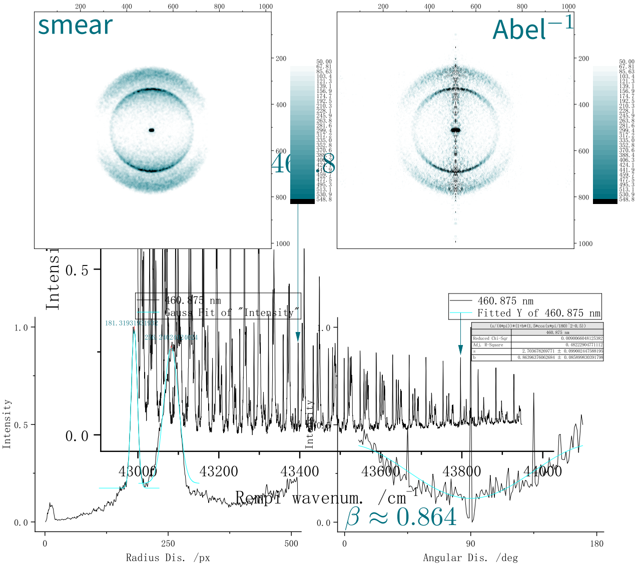
smear
Abel^{-1}
464.484 nm
Gauss Fit of "Intensity"
464.484 nm
Fitted Y of 464.484 nm
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
464.355 nm
Reduced Chi-Sqr 0.0060444603369693
Adj. R-Square 0.91915190645849
s 4.3907648247226 ± 0.081104349233679
b 1.5180165177701 ± 0.051762252346911
Intensity
Radius Dis. /px
Angular Dis. (deg)
Rempi wavenum. /cm^{-1}
$\beta \approx 1.52$

Peak 2



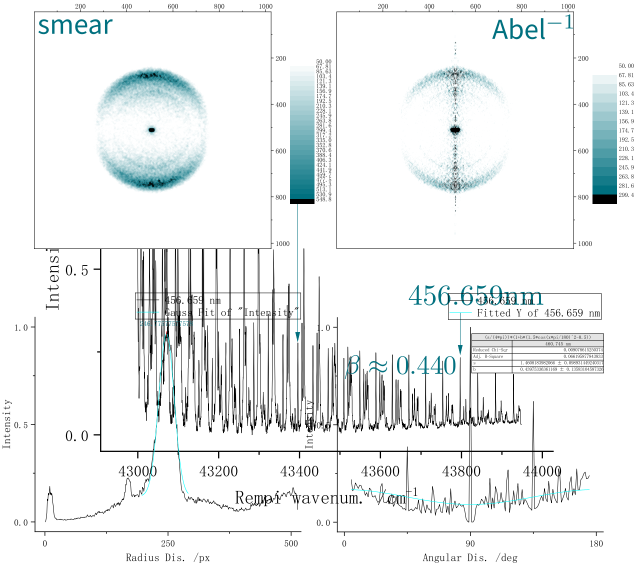
$\beta \approx 1.20$

Peak 3



$\beta \approx 0.864$

Peak 4


smear
Abel^{-1}
456.659nm
$\beta \approx 0.440$
Intensity
Rempi wavenum. /cm^{-1}
456.659 nm
Gauss Fit of "Intensity"
Fitted Y of 456.659 nm
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
Radius Dis. /px
Angular Dis. /deg

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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 $= 246.776$
$rR2\,(44.5)$ $qR12\,(51.5)$ $qQ2\,(51.5)$	$rR2\,(45.5)$ $qR12\,(51.5)$ $qQ2\,(51.5)$	$sR21\,(48.5)$	$sR21\,(58.5)$ $pQ12\,(76.5)$ $pP2\,(76.5)$

Notice

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

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Speed correction

Trans. energy of NO

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

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

Speed correction

Trans. energy of NO

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

Vib. energy level

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

[2] Rémy 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	$43\,058.49\text{cm}^{-1}$		5814.033cm^{-1}
Peak 2 464.114nm	$43\,092.81\text{cm}^{-1}$		5965.969cm^{-1}
Peak 3 460.875nm	$43\,395.69\text{cm}^{-1}$	$25\,128.57\text{cm}^{-1}$	6239.696cm^{-1}
Peak 4 456.659nm	$43\,796.34\text{cm}^{-1}$		8004.278cm^{-1}

Rot. energy level

Simulated data generated by PGOPHER[4].

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

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

Speed correction

Trans. energy of NO

$E_{\text{int.}}(\text{O})$ [5]	$E_{\text{trans}}(\text{total}) \approx 2.875464 E_{\text{trans}}(\text{NO})$ $= E_{\text{total}} - E_{\text{bond}}(\text{O}-\text{NO}) - E_{\text{int.}}(\text{O}) - E_{\text{int.}}(\text{NO})$	$E_{\text{trans}}(\text{NO})$ $= \frac{1}{2} m(\text{NO}) v^2(\text{NO})$
$^3P_2$ (0cm^{-1})	11081.356cm^{-1}	4375.588cm^{-1}
	10964.609cm^{-1}	4334.685cm^{-1}
	10794.143cm^{-1}	4344.824cm^{-1}
	9398.766cm^{-1}	3870.489cm^{-1}
$^3P_1$ (158.625cm^{-1})	10922.731cm^{-1}	4320.423cm^{-1}
	10805.984cm^{-1}	4279.520cm^{-1}
	10635.518cm^{-1}	4289.659cm^{-1}
	9240.141cm^{-1}	3815.324cm^{-1}
$^3P_0$ (226.977cm^{-1})	10854.379cm^{-1}	4296.653cm^{-1}
	10737.632cm^{-1}	4255.749cm^{-1}
	10567.166cm^{-1}	4265.888cm^{-1}
	9171.789cm^{-1}	3791.553cm^{-1}

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

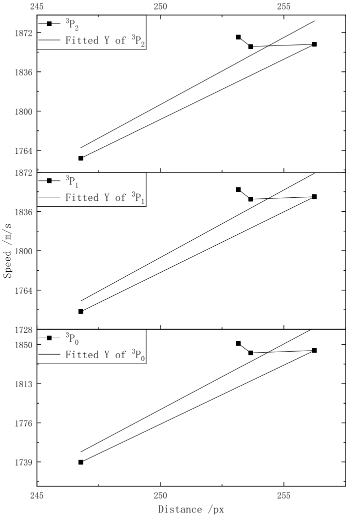
Speed correction

Trans. speed of NO

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

Speed correction

Trans. speed of NO



$^3P_2$

$12.28 \mathrm{m\,s^{-1}\,px^{-1}}$

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

$^3P_1$

$12.37 \mathrm{m\,s^{-1}\,px^{-1}}$

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

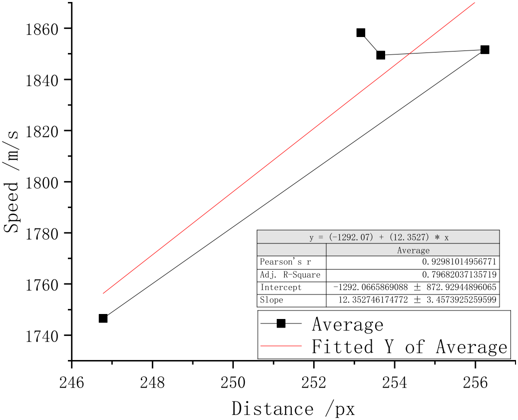
$^3P_0$

$12.40 \mathrm{m\,s^{-1}\,px^{-1}}$

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

Speed correction

Trans. speed of NO



Average

$12.35\,\mathrm{m\,s^{-1}\,px^{-1}}$

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

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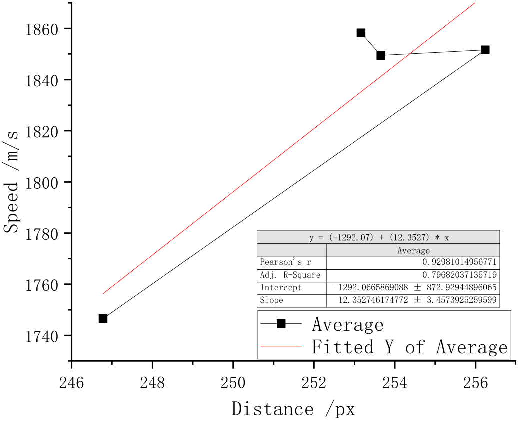
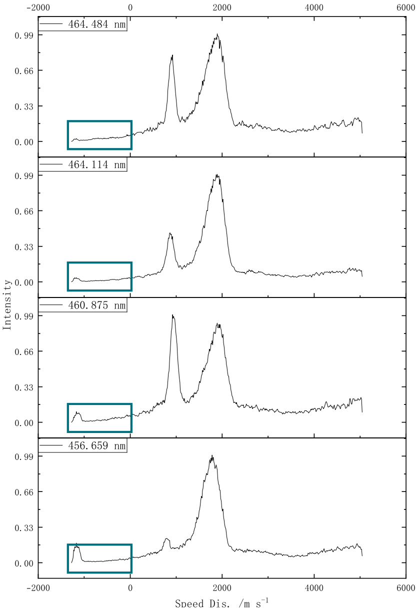


Average

$12.35\,\mathrm{m\,s^{-1}\,px^{-1}}$

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

Error



Average

$12.35 \mathrm{m\,s^{-1}\,px^{-1}}$

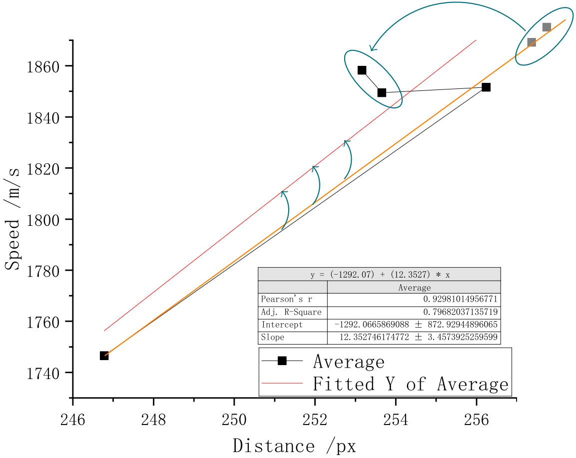
Intercept $\approx -1292 \mathrm{m\,s^{-1}}$

Notice

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

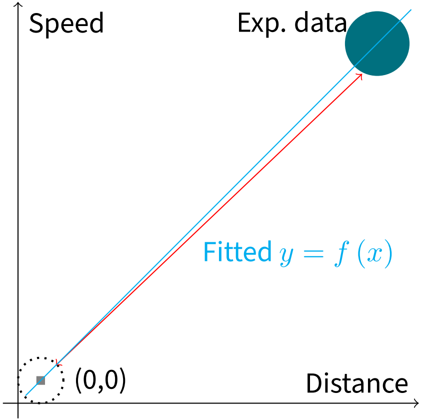
[a] Maybe a $\pm 5 \mathrm{m\,s^{-1}}$-level intercept noise are permitted.

Error



y = (-1292.07) + (12.3527) * x
Average
Pearson's r 0.92981014956771
Adj. R-Square 0.79682037135719
Intercept -1292.0665869088 ± 872.92944896065
Slope 12.352746174772 ± 3.4573925259599
Average
Fitted Y of Average
Speed /m/s
Distance /px
1740
1760
1780
1800
1820
1840
1860
246
248
250
252
254
256

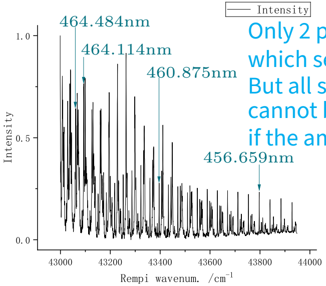
Error



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

$\Longrightarrow$ After assignments, which are the points we should use?

Assignment for Assignment



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

+1 peak	+9 peak	+10 peak
44.5⟶45.5	45.5⟶48.5	48.5⟶58.5

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 $= 246.776$
$rR2\,(44.5)$	$rR2\,(45.5)$	$sR21\,(48.5)$	$sR21\,(58.5)$

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.