練習実験報告

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2024 年 5 月 30 日

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Galvano Sepctrum

REMPI scan

    Selected peaks

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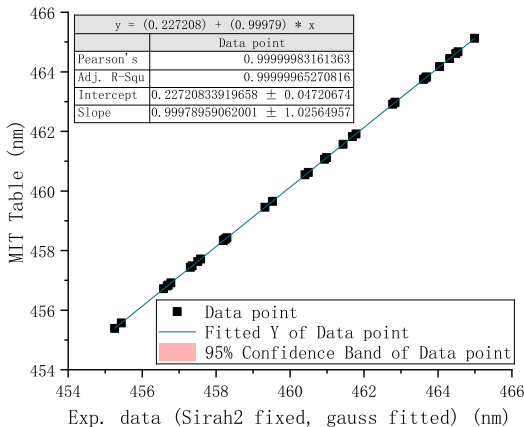
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Galvano Sepctrum
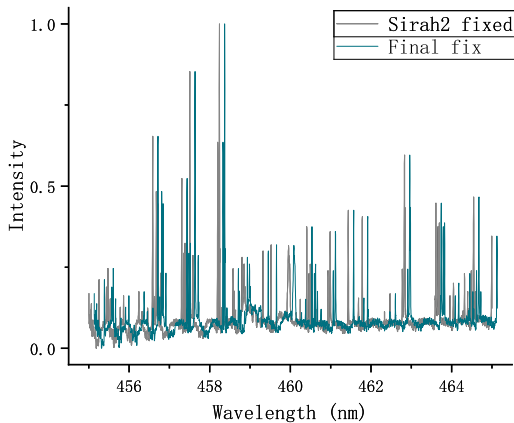
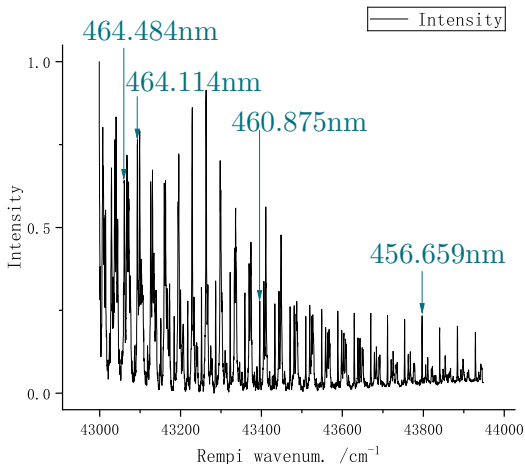# Galvano Sepctrum

Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

Fig. 2: Correction function

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Selected peaks

Peak 1
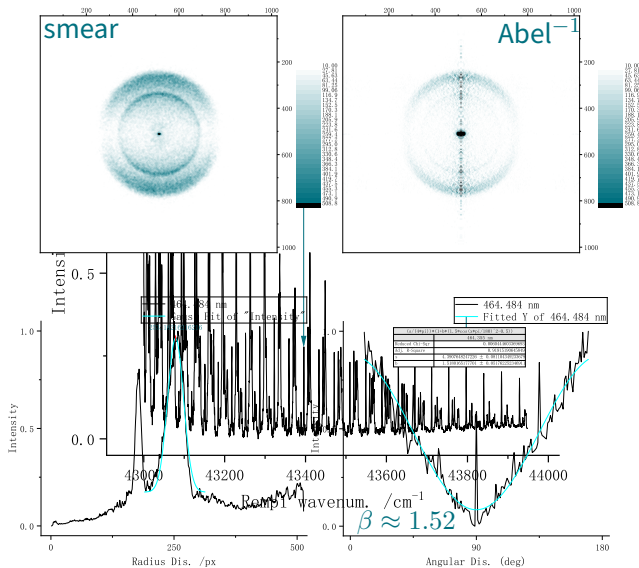
Peak 2

Peak 3

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

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

Speed correction
Trans. energy of NO

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

Vib. energy level

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

[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]	$E_{\text{trans}}(\text{total}) \approx 2.875464 E_{\text{trans}}(\text{NO})$ $= E_{\text{total}} - E_{\text{bond}}(\text{O-NO}) - E_{\text{int.}}(\text{O}) - E_{\text{int.}}(\text{NO})$	$E_{\text{trans}}(\text{NO})$ $= \frac{1}{2} m(\text{NO}) v^2(\text{NO})$
$^3P_2$	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}

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

Speed correction
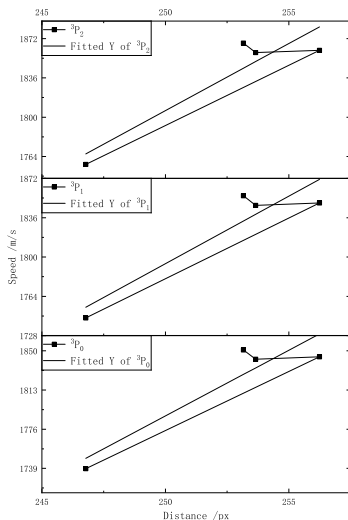
Trans. speed of NO

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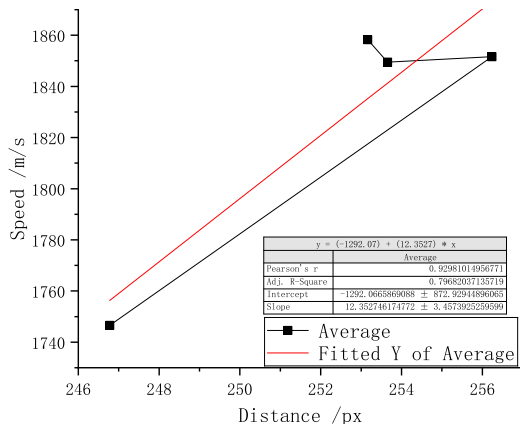
Average

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

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

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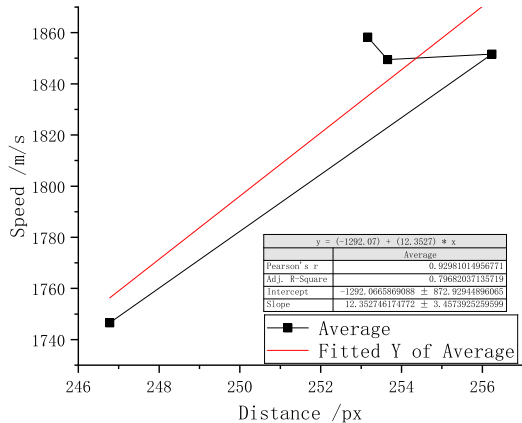
Error

Average

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

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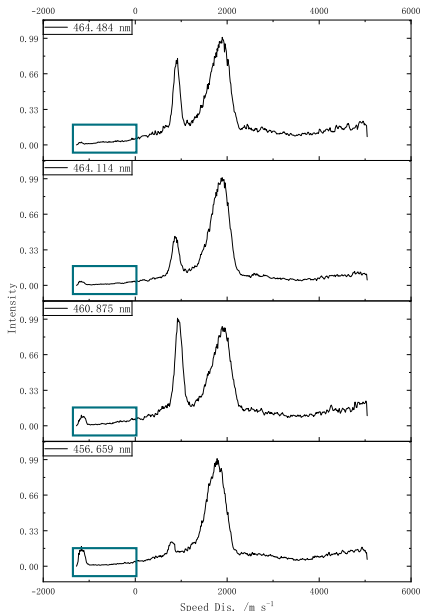
Error

Average
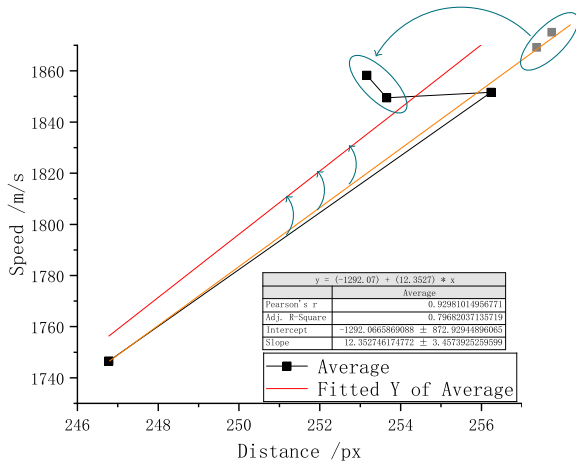$$12.35\,\mathrm{m\,s^{-1}\,px^{-1}}$$
Intercept $\approx -1292\,\mathrm{m\,s^{-1}}$

Notice

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

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

Error

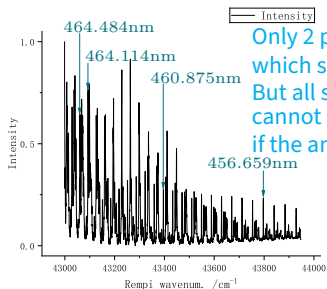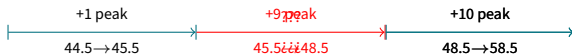# Error
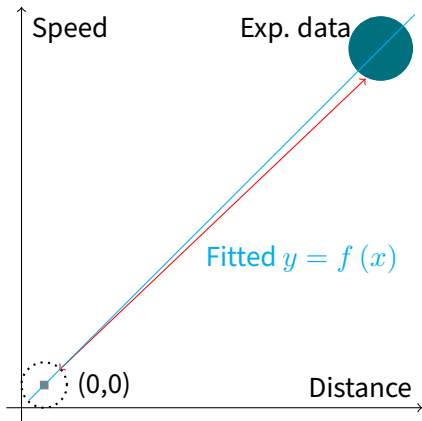
If we assume a virtual zero point:
The fake data obtains a huge weight!
Statistics tools always treat all data
as proper indications.

$\implies$ 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 $\leqslant 3$.

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.