練習実験報告

肖宇笑

2024 年 6 月 2 日

Contents

Contents

Galvano Sepctrum

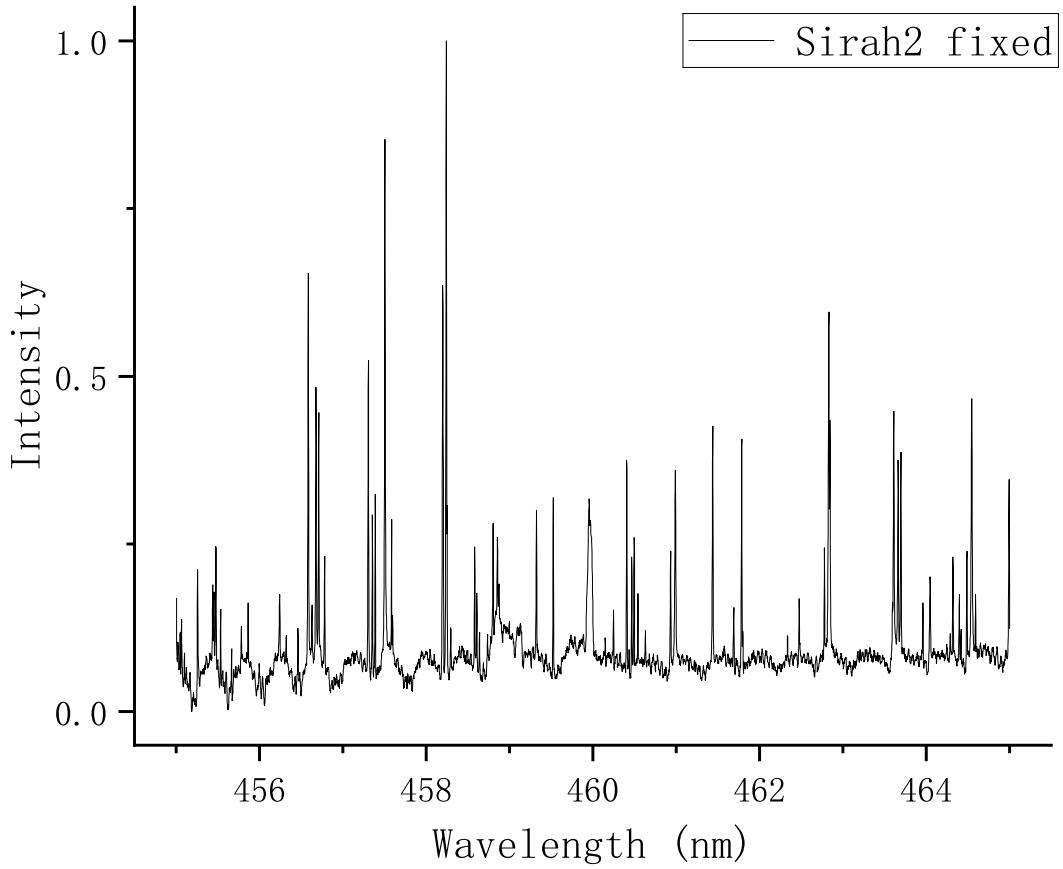

Fig. 1: Wavelen. correction

Galvano Sepctrum

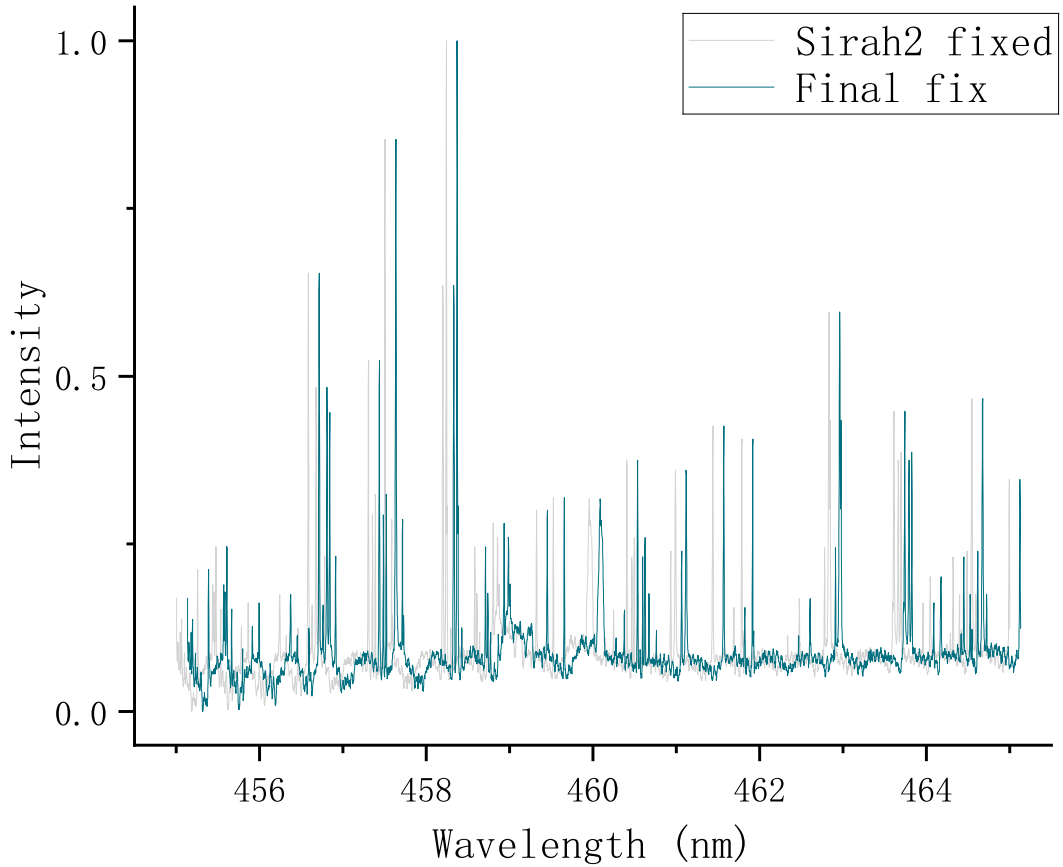

Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

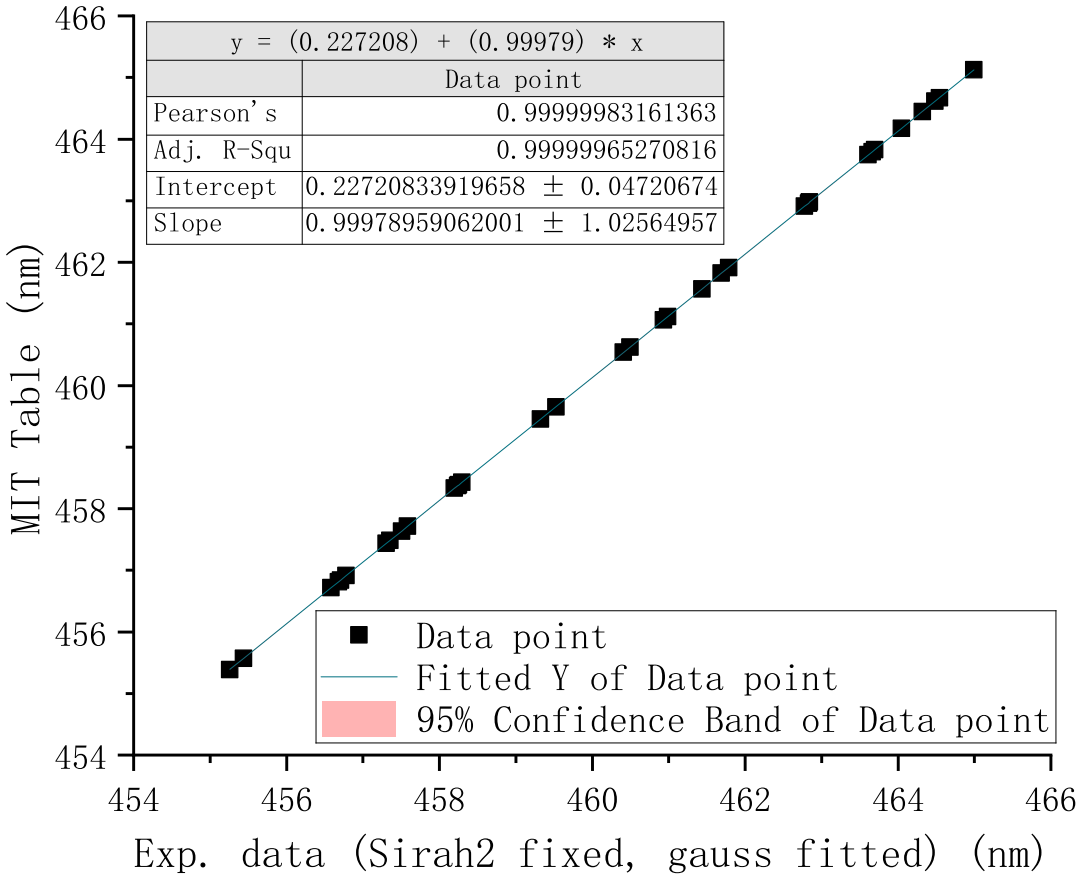

Fig. 2: Correction function

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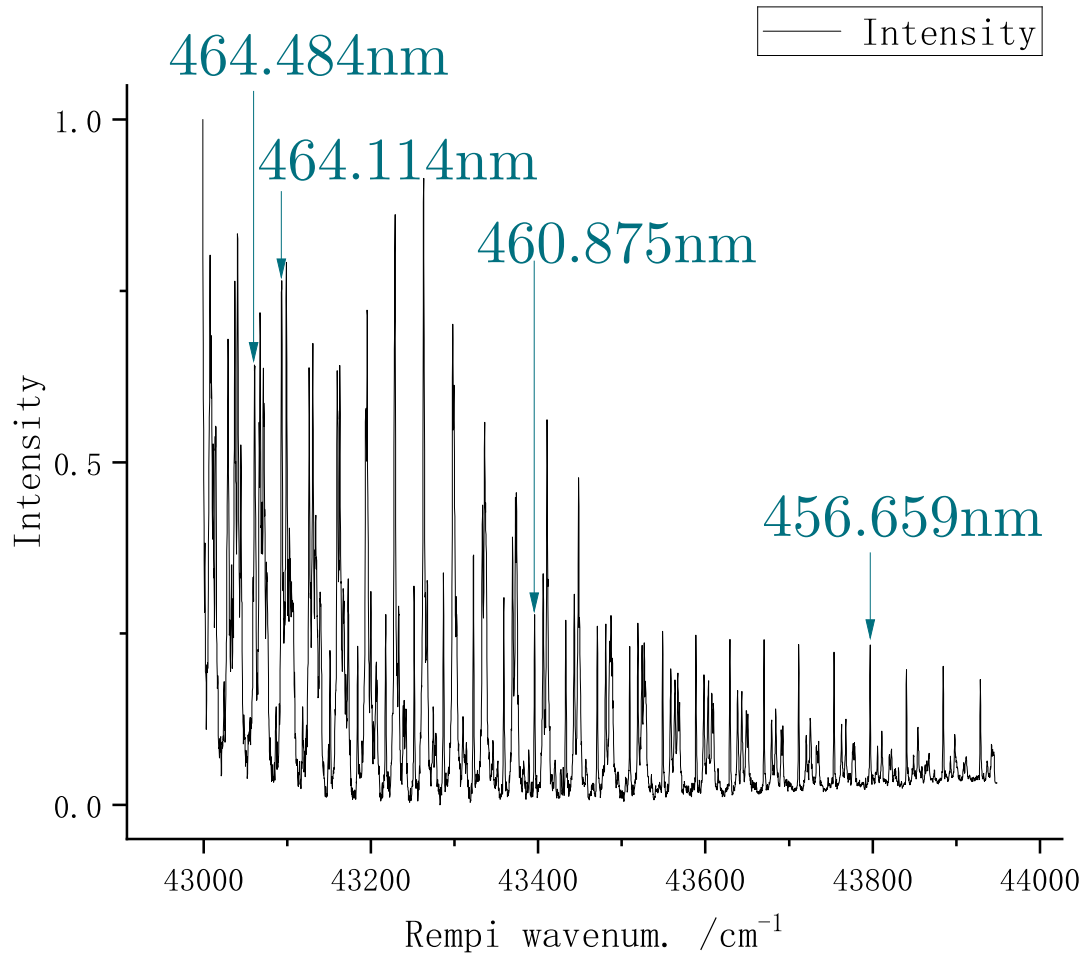
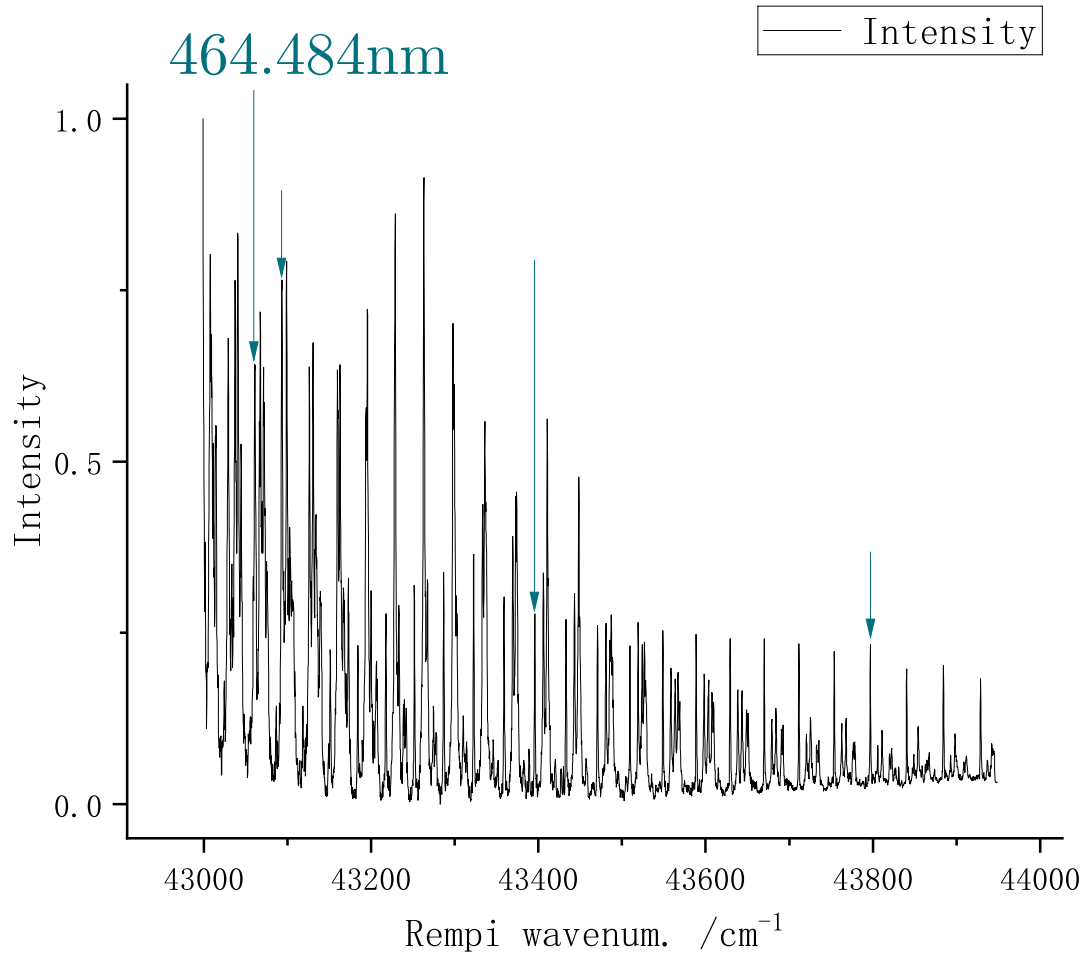
Contents

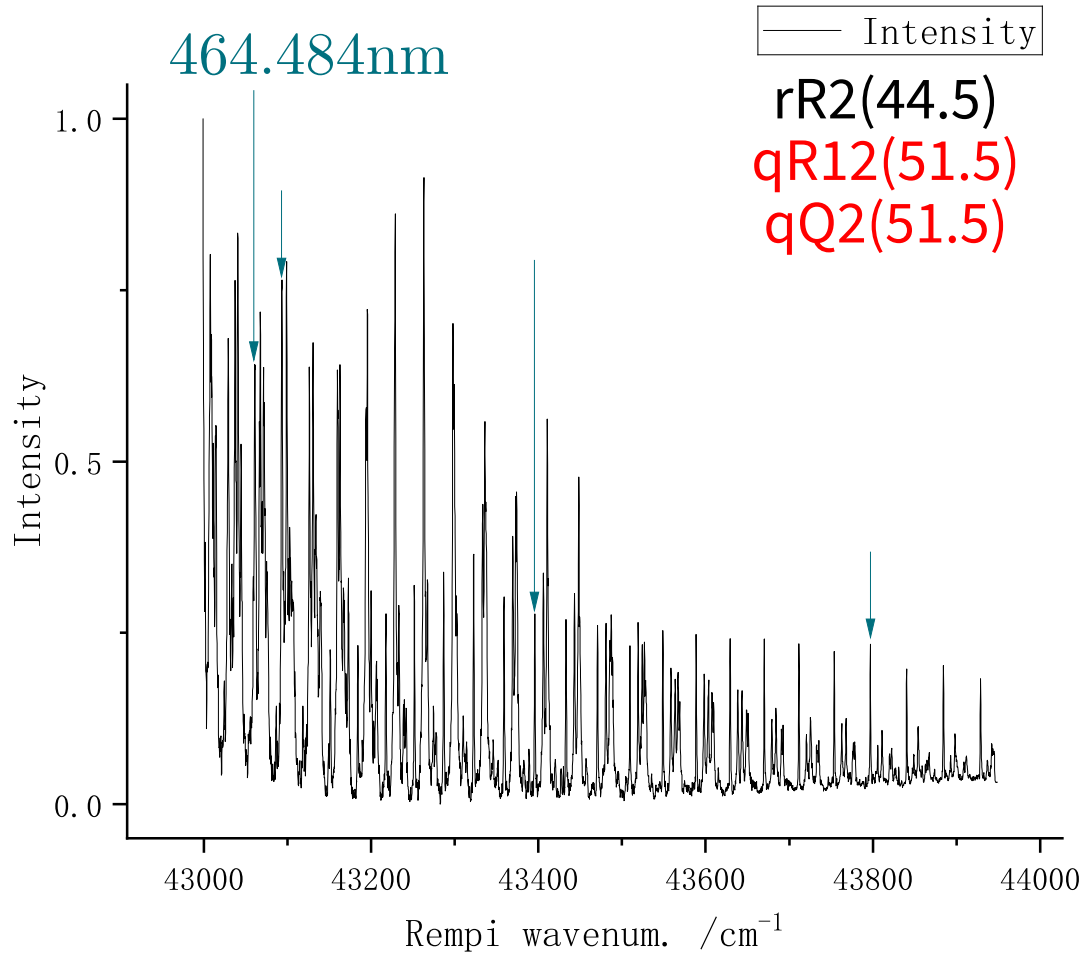
Selected peaks



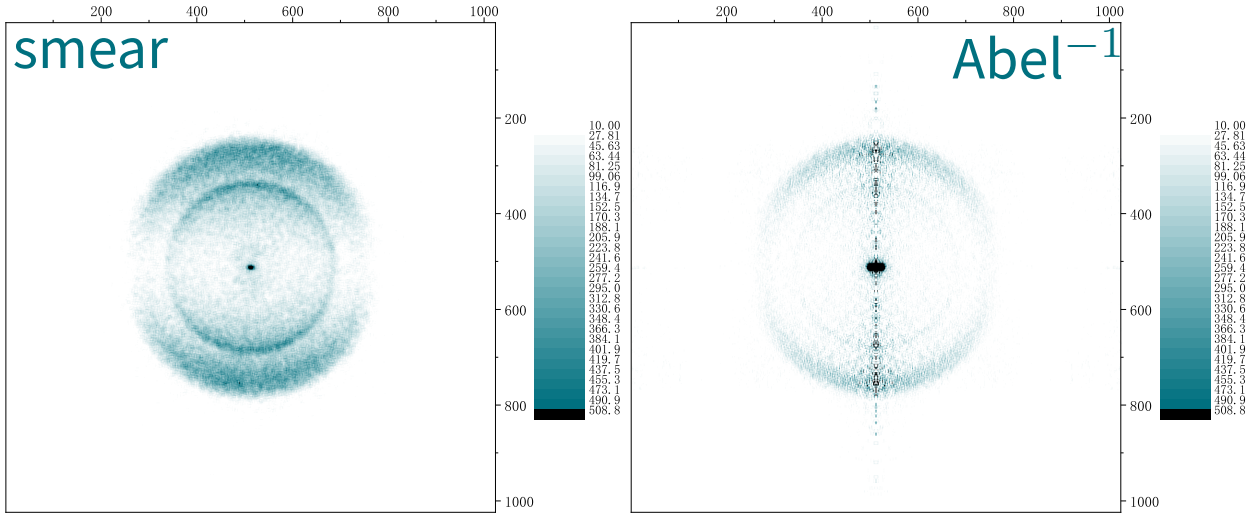
Peak 1


464.484nm
Intensity
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

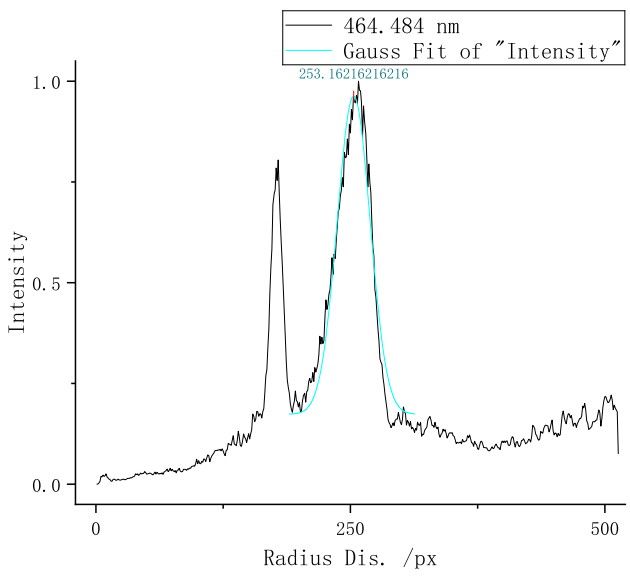
Peak 1

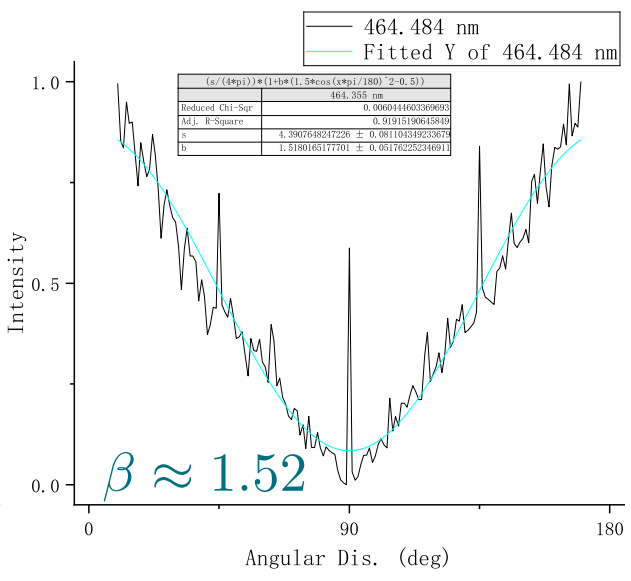

464.484nm
Intensity
rR2(44.5)
qR12(51.5)
qQ2(51.5)
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 1

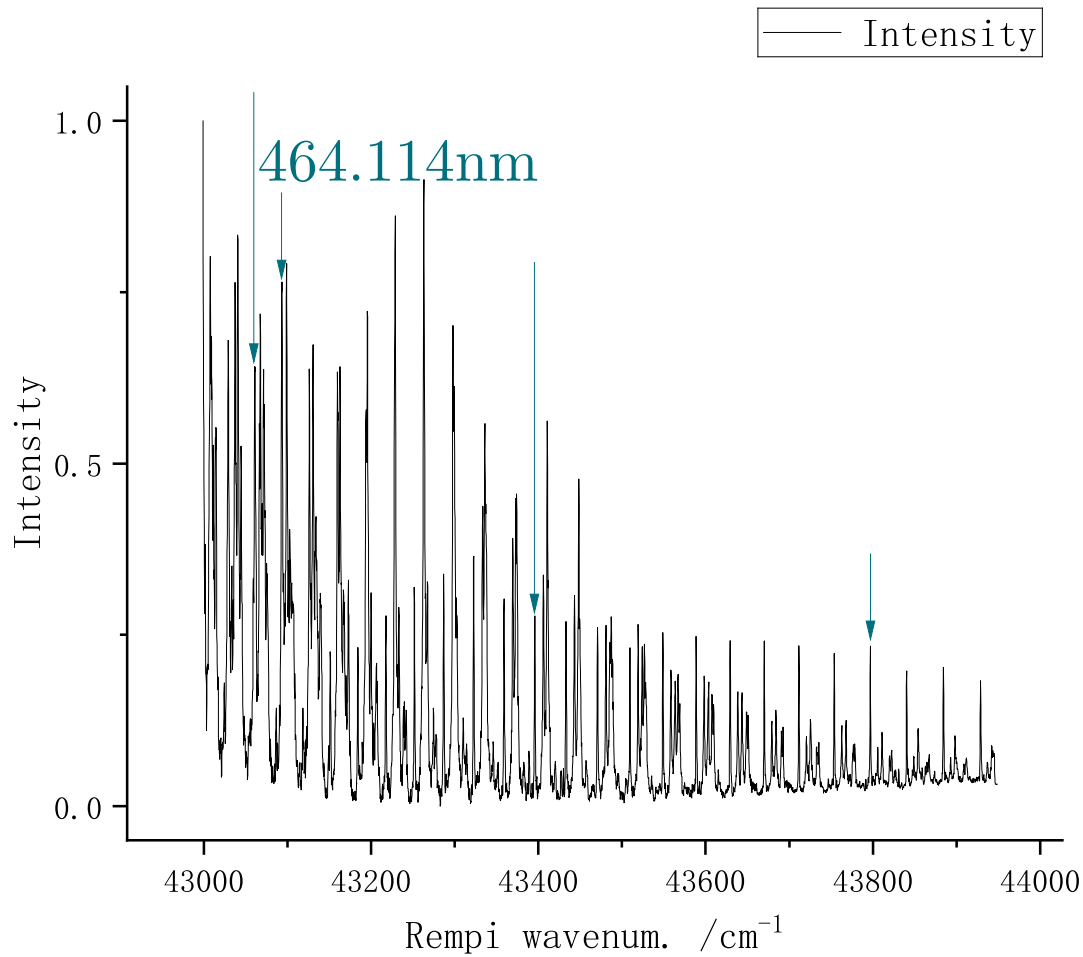

smear
200
400
600
800
1000
10.00
27.81
45.63
63.44
81.25
99.06
116.9
134.7
152.5
170.3
188.1
205.9
223.8
241.6
259.4
277.2
295.0
312.8
330.6
348.4
366.3
384.1
401.9
419.7
437.5
455.3
473.1
490.9
508.8

Abel^{-1}
200
400
600
800
1000
10.00
27.81
45.63
63.44
81.25
99.06
116.9
134.7
152.5
170.3
188.1
205.9
223.8
241.6
259.4
277.2
295.0
312.8
330.6
348.4
366.3
384.1
401.9
419.7
437.5
455.3
473.1
490.9
508.8

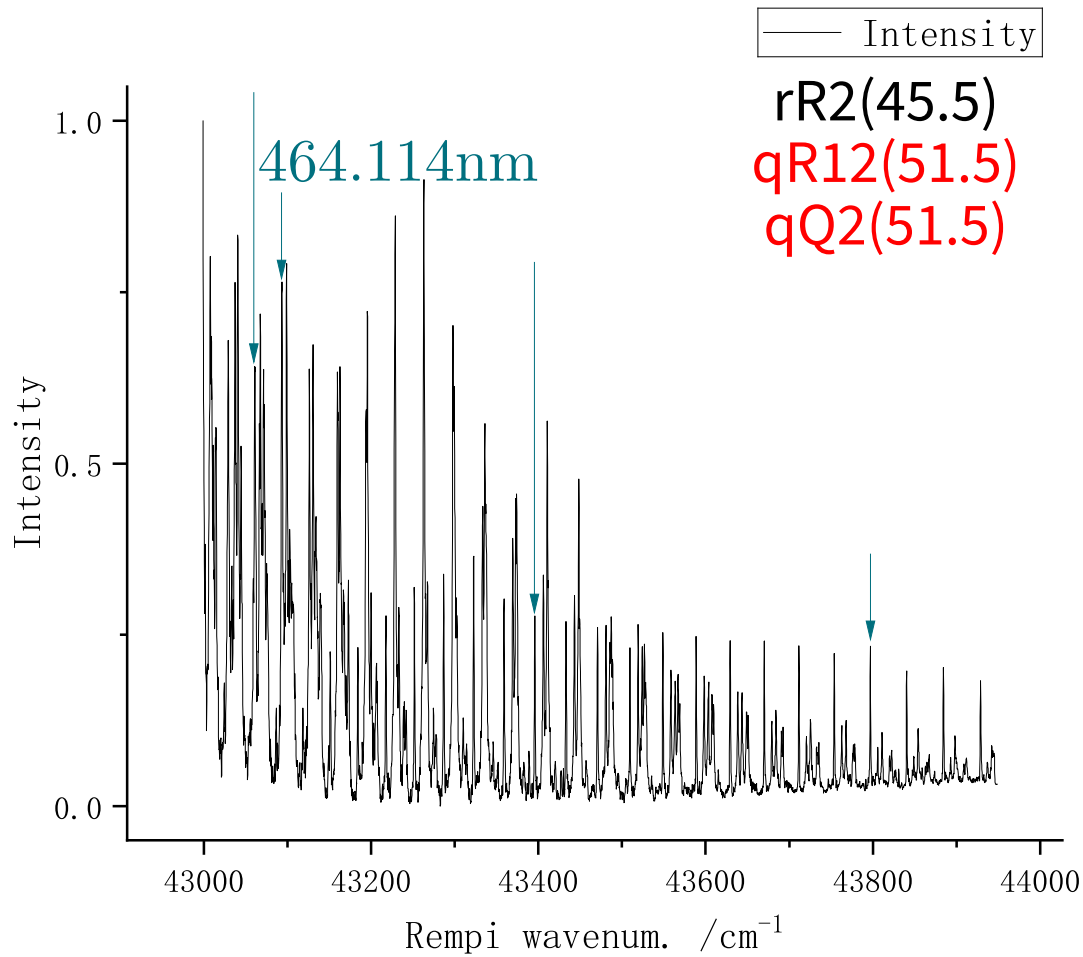

464.484 nm
Gauss Fit of "Intensity"
253.16216216216
Intensity
1.0
0.5
0.0
0
250
500
Radius Dis. /px


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
1.0
0.5
0.0
0
90
180
Angular Dis. (deg)
$\beta \approx 1.52$

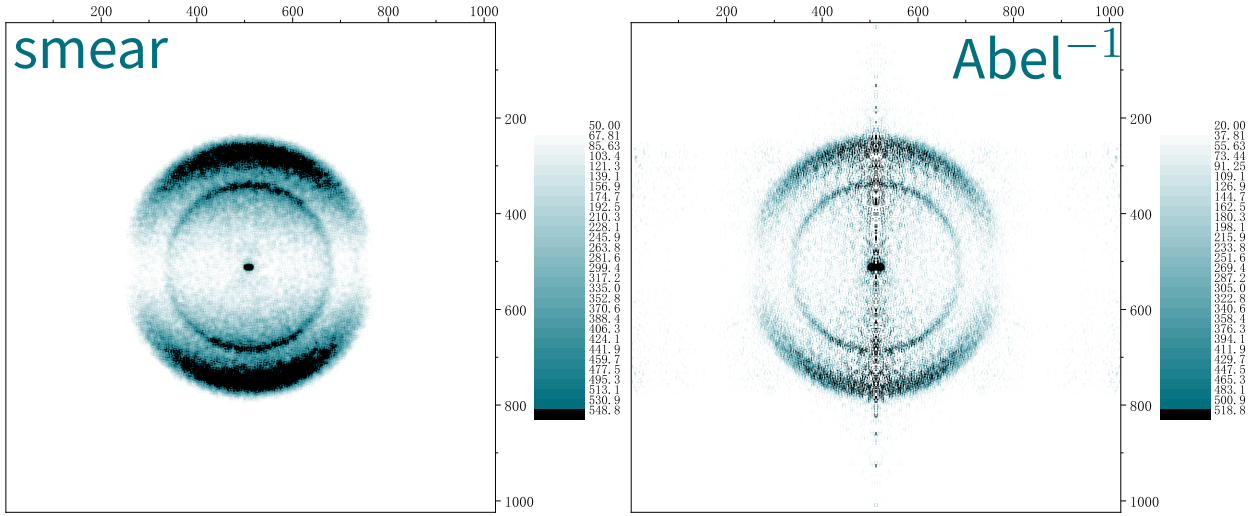
Peak 2

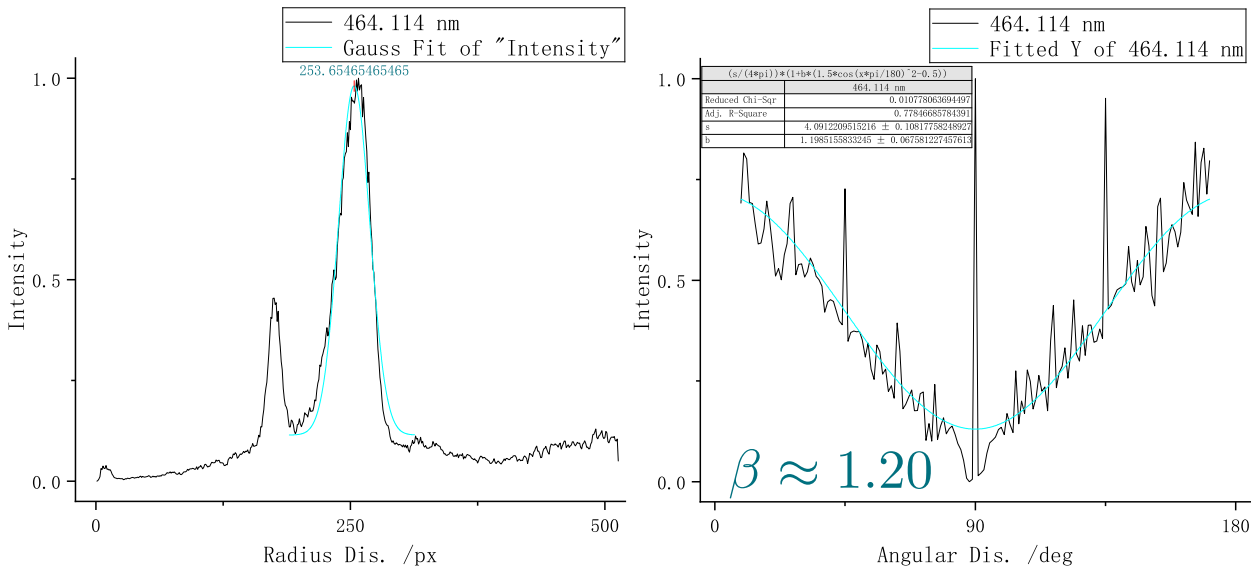

Intensity
464.114nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 2

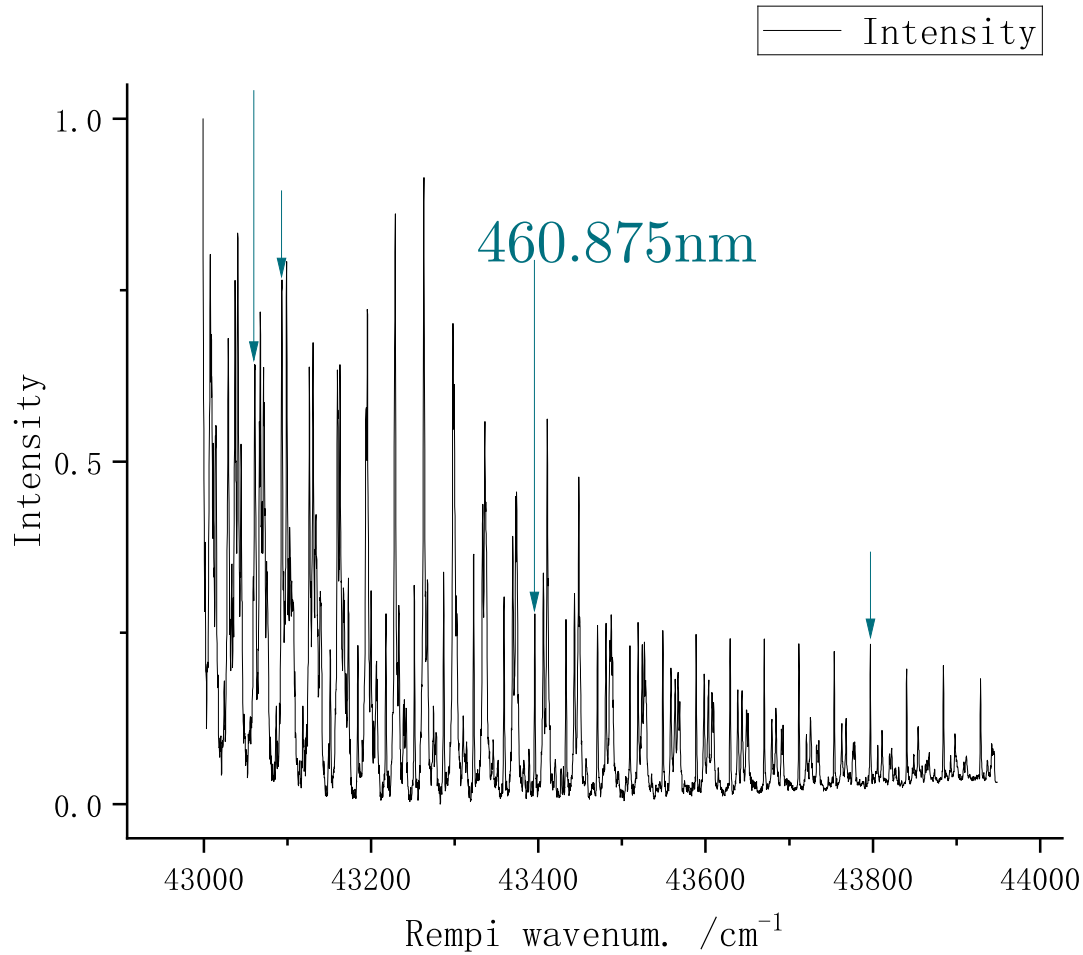

Intensity
464.114nm
rR2(45.5)
qR12(51.5)
qQ2(51.5)
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 2

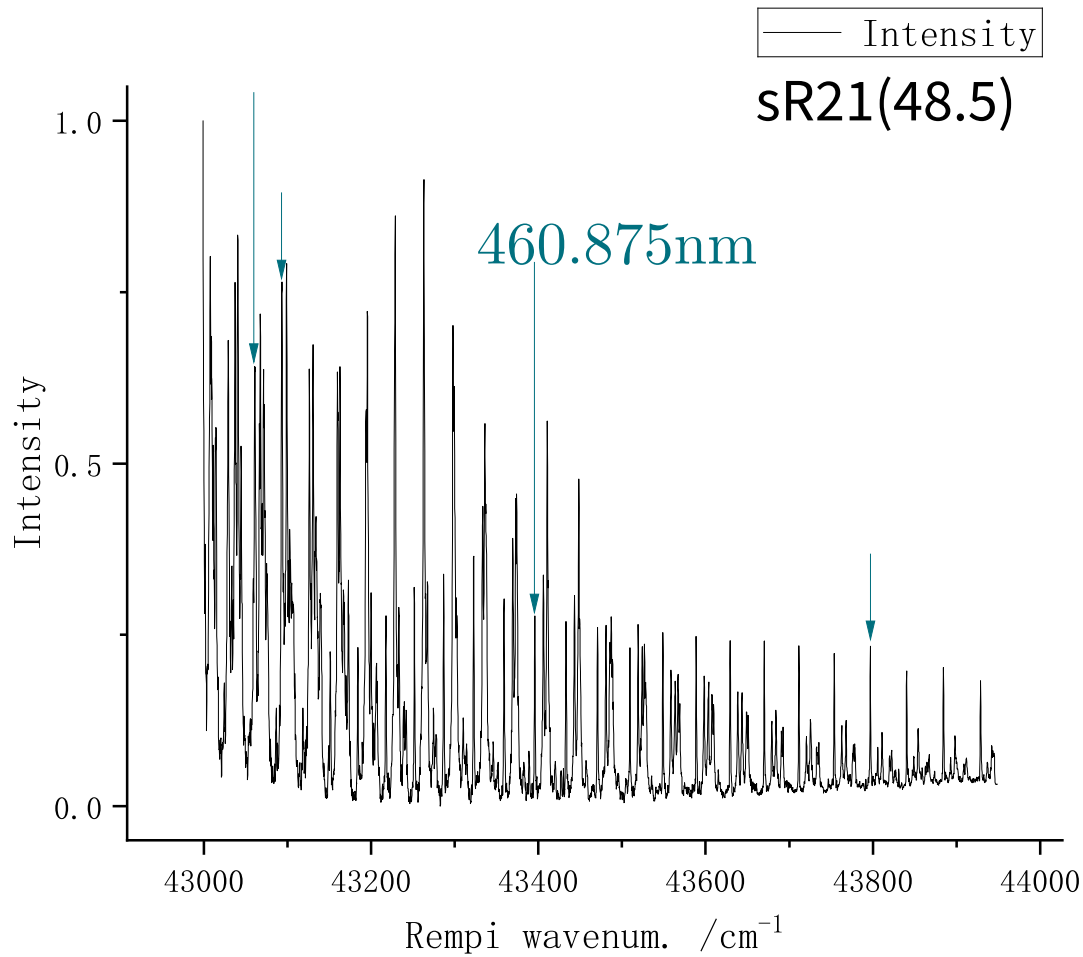

smear
Abel^{-1}


464.114 nm
Gauss Fit of "Intensity"
253.65465465465
Intensity
Radius Dis. /px
464.114 nm
Fitted Y of 464.114 nm
Intensity
Angular Dis. /deg
$\beta \approx 1.20$

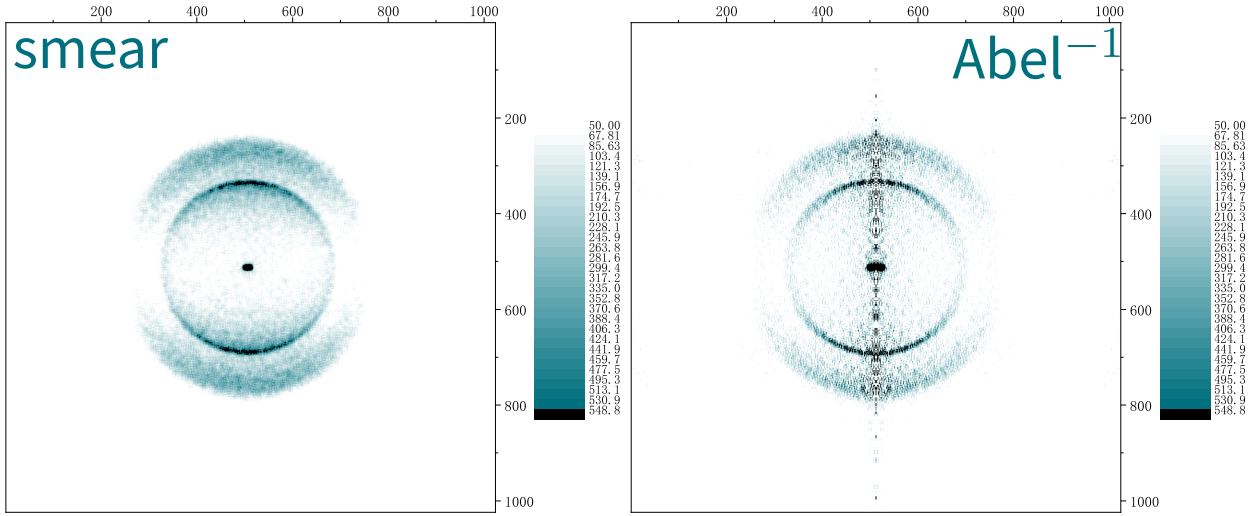
Peak 3

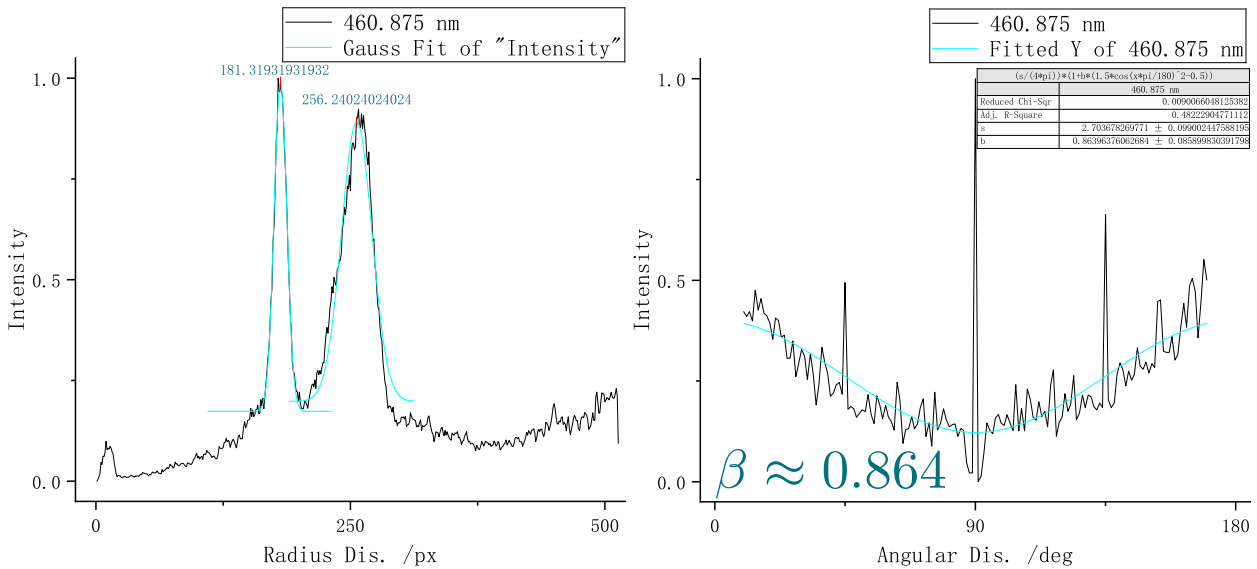

Intensity
460.875nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 3

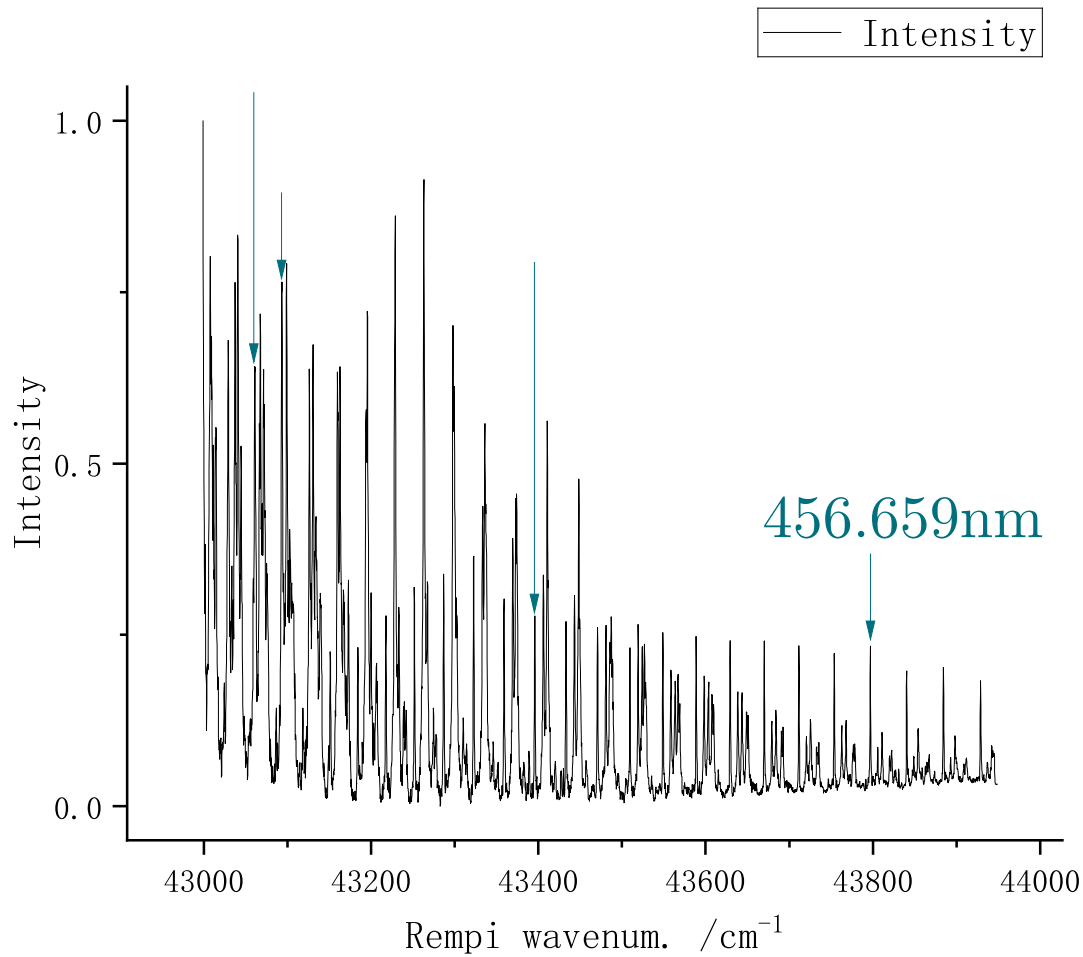

Intensity
sR21(48.5)
460.875nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 3

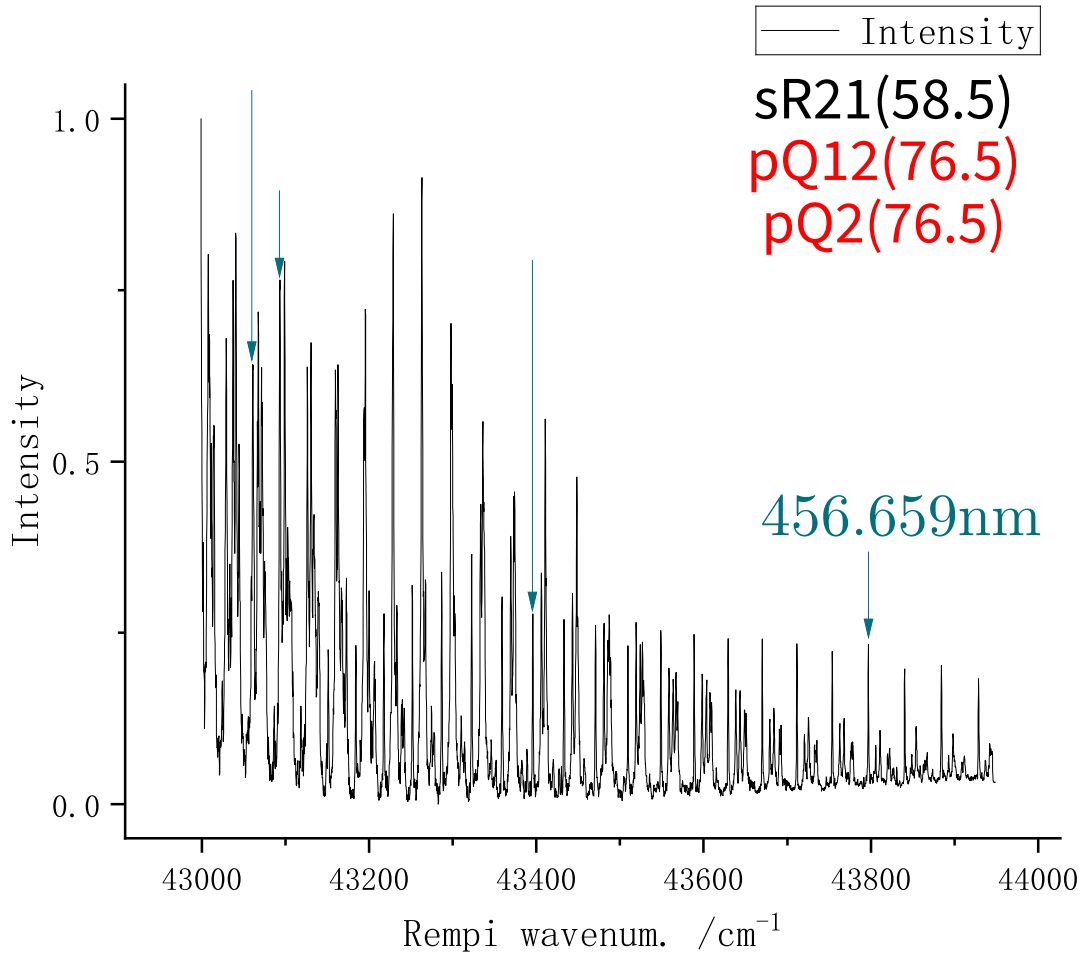

smear
Abel^{-1}


460.875 nm
Gauss Fit of "Intensity"
181.31931931932
256.24024024024
Intensity
Radius Dis. /px
460.875 nm
Fitted Y of 460.875 nm
Intensity
Angular Dis. /deg
$\beta \approx 0.864$

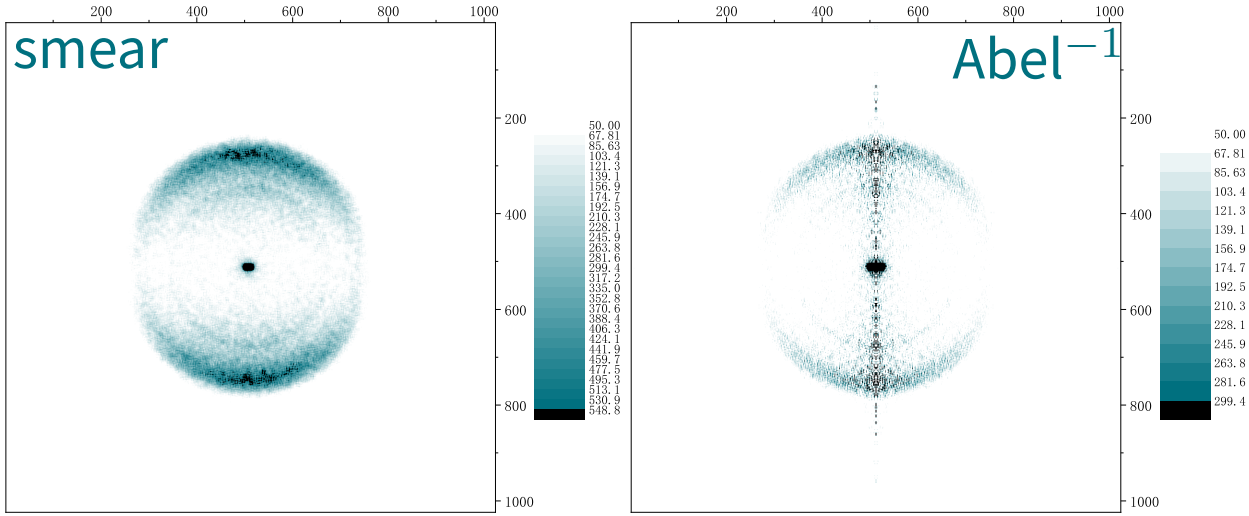
Peak 4

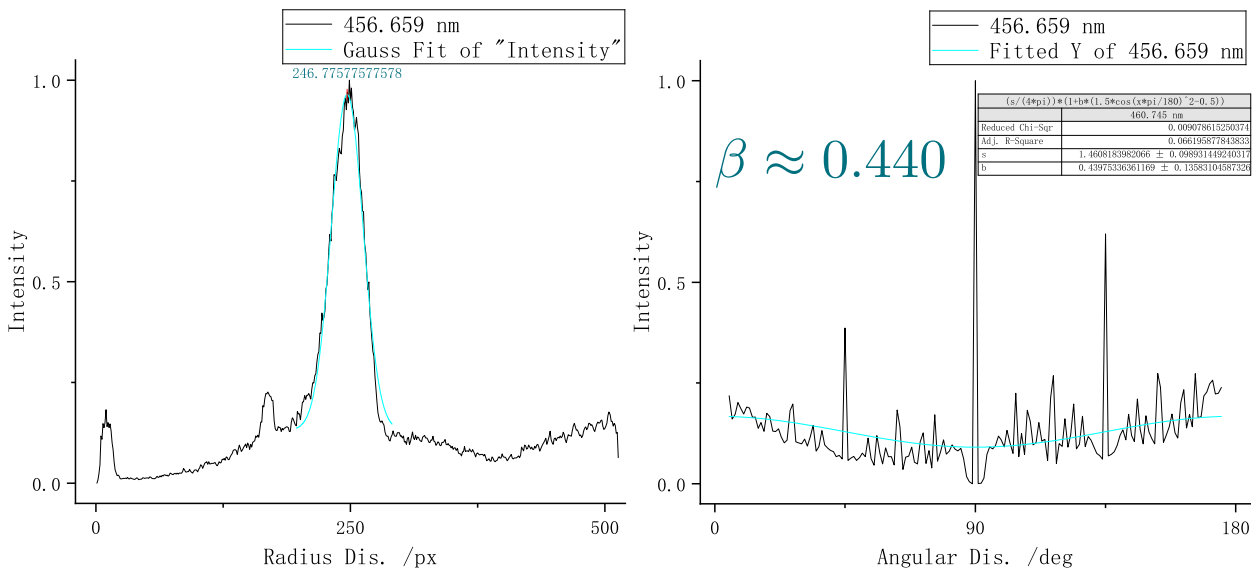

Intensity
1.0
0.5
0.0
Intensity
456.659nm
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 4


Intensity
sR21(58.5)
pQ12(76.5)
pQ2(76.5)
456.659nm
Intensity
1.0
0.5
0.0
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 4


smear
Abel^{-1}


456.659 nm
Gauss Fit of "Intensity"
246.77577577578
Intensity
Radius Dis. /px
456.659 nm
Fitted Y of 456.659 nm
$\beta \approx 0.440$
Angular Dis. /deg

Contents

Contents

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

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.

Contents

Contents

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	$43\,058.49\text{cm}^{-1}$	$25\,128.57\text{cm}^{-1}$	$\Delta E_v(1 \to 0) + E(J = 44)$
Peak 2 464.114nm	$43\,092.81\text{cm}^{-1}$		$\Delta E_v(1 \to 0) + E(J = 45)$
Peak 3 460.875nm	$43\,395.69\text{cm}^{-1}$		$\Delta E_v(1 \to 0) + E(J = 48)$
Peak 4 456.659nm	$43\,796.34\text{cm}^{-1}$		$\Delta E_v(1 \to 0) + E(J = 58)$

[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 $456.659\mathrm{nm}$	$43\,796.34\mathrm{cm}^{-1}$		$2341.932\,775\,0\mathrm{cm}^{-1} + E(J = 58)$

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

Speed correction

Trans. energy of NO

	E_{total}	$E_{\text{bond}}\,(\text{O}-\text{NO})^2$	$E_{\text{int.}}\,(\text{NO})$
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

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

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

[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_{total}	$E_{\text{bond}}(\text{O}-\text{NO})$[3]	$E_{\text{int.}}(\text{NO})$
Peak 1 464.484nm	$43\,058.49\text{cm}^{-1}$	$25\,128.57\text{cm}^{-1}$	5814.033cm^{-1}
Peak 2 464.114nm	$43\,092.81\text{cm}^{-1}$		5965.969cm^{-1}
Peak 3 460.875nm	$43\,395.69\text{cm}^{-1}$		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]	$E_{\text{trans}}(\text{total}) \approx 2.875464 E_{\text{trans}}(\text{NO})$ $= E_{\text{total}} - E_{\text{bond}}(\text{O}-\text{NO}) - E_{\text{int.}}(\text{O}) - E_{\text{int.}}(\text{NO})$	$E_{\text{trans}}(\text{NO})$ $= \frac{1}{2} m(\text{NO}) v^2(\text{NO})$
$^3P_2$	11081.356cm^{-1}	4375.588cm^{-1}
	10964.609cm^{-1}	4334.685cm^{-1}
(0cm^{-1})	10794.143cm^{-1}	4344.824cm^{-1}
	9398.766cm^{-1}	3870.489cm^{-1}
$^3P_1$	10922.731cm^{-1}	4320.423cm^{-1}
	10805.984cm^{-1}	4279.520cm^{-1}
(158.625cm^{-1})	10635.518cm^{-1}	4289.659cm^{-1}
	9240.141cm^{-1}	3815.324cm^{-1}
$^3P_0$	10854.379cm^{-1}	4296.653cm^{-1}
	10737.632cm^{-1}	4255.749cm^{-1}
(226.977cm^{-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.

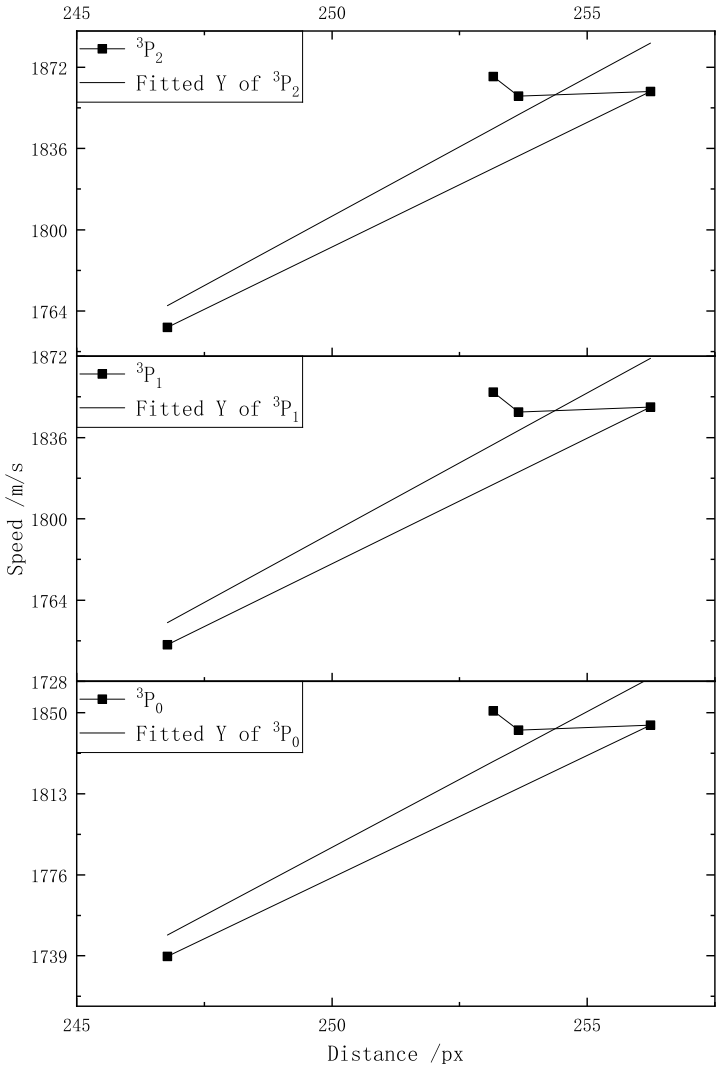
Speed correction

Trans. speed of NO

$E_{\text{int.}}(\mathrm{O})$	$v(\mathrm{NO}) = \sqrt{\frac{2E_{\text{trans}}(\mathrm{NO})}{m(\mathrm{NO})}}$	Δy
${}^3P_2$	$1867.845\,\mathrm{m\,s^{-1}}$	253.177
	$1859.094\,\mathrm{m\,s^{-1}}$	253.650
$(0\,\mathrm{cm^{-1}})$	$1861.267\,\mathrm{m\,s^{-1}}$	256.147
	$1756.732\,\mathrm{m\,s^{-1}}$	246.776
${}^3P_1$	$1856.033\,\mathrm{m\,s^{-1}}$	253.177
	$1847.226\,\mathrm{m\,s^{-1}}$	253.650
$(158.625\,\mathrm{cm^{-1}})$	$1849.413\,\mathrm{m\,s^{-1}}$	256.148
	$1744.168\,\mathrm{m\,s^{-1}}$	246.776
${}^3P_0$	$1850.920\,\mathrm{m\,s^{-1}}$	253.177
	$1842.089\,\mathrm{m\,s^{-1}}$	253.650
$(226.977\,\mathrm{cm^{-1}})$	$1844.282\,\mathrm{m\,s^{-1}}$	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 $\approx -1298\mathrm{m\,s^{-1}}$

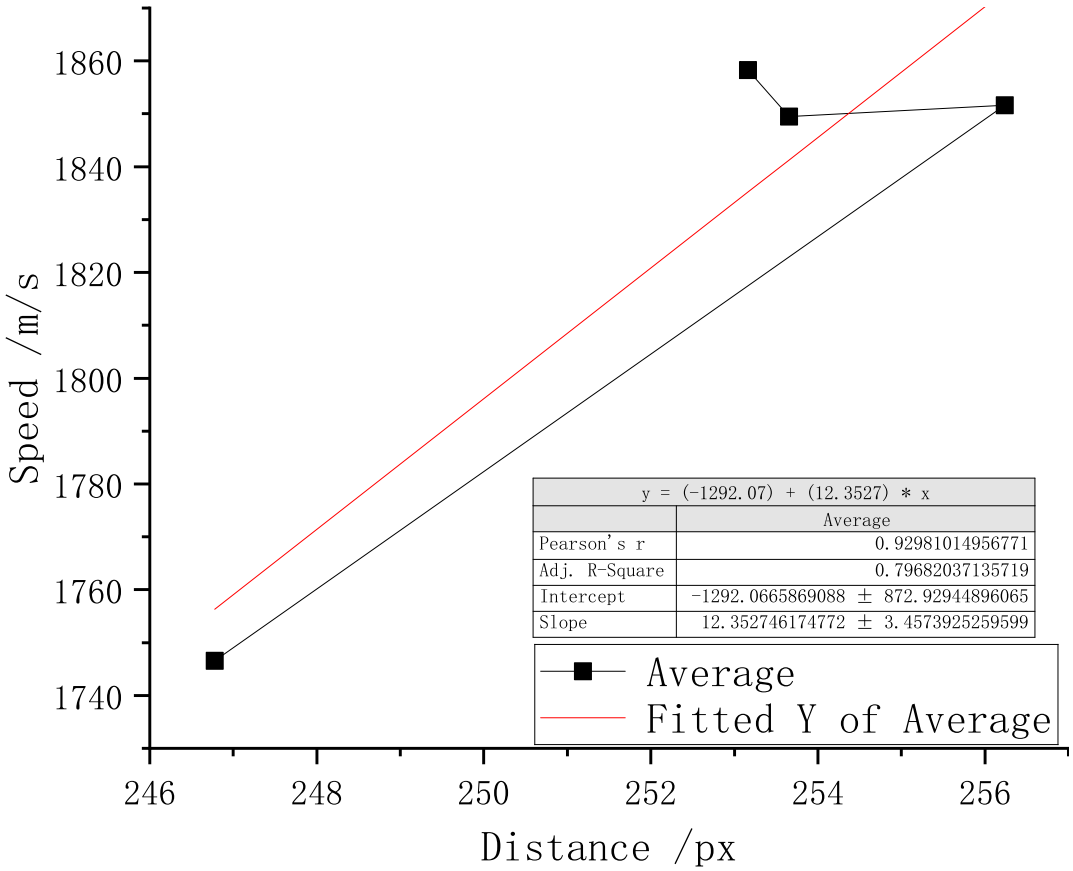
$^3P_0$

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

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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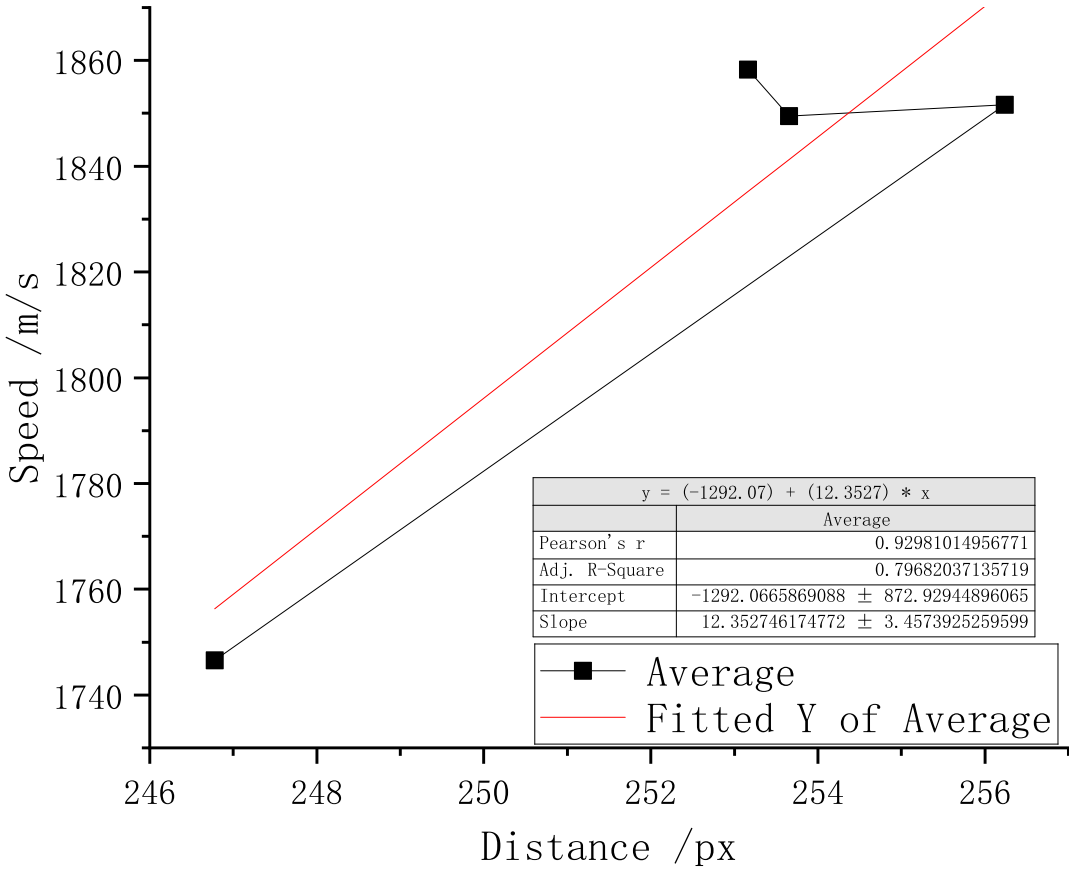
Error

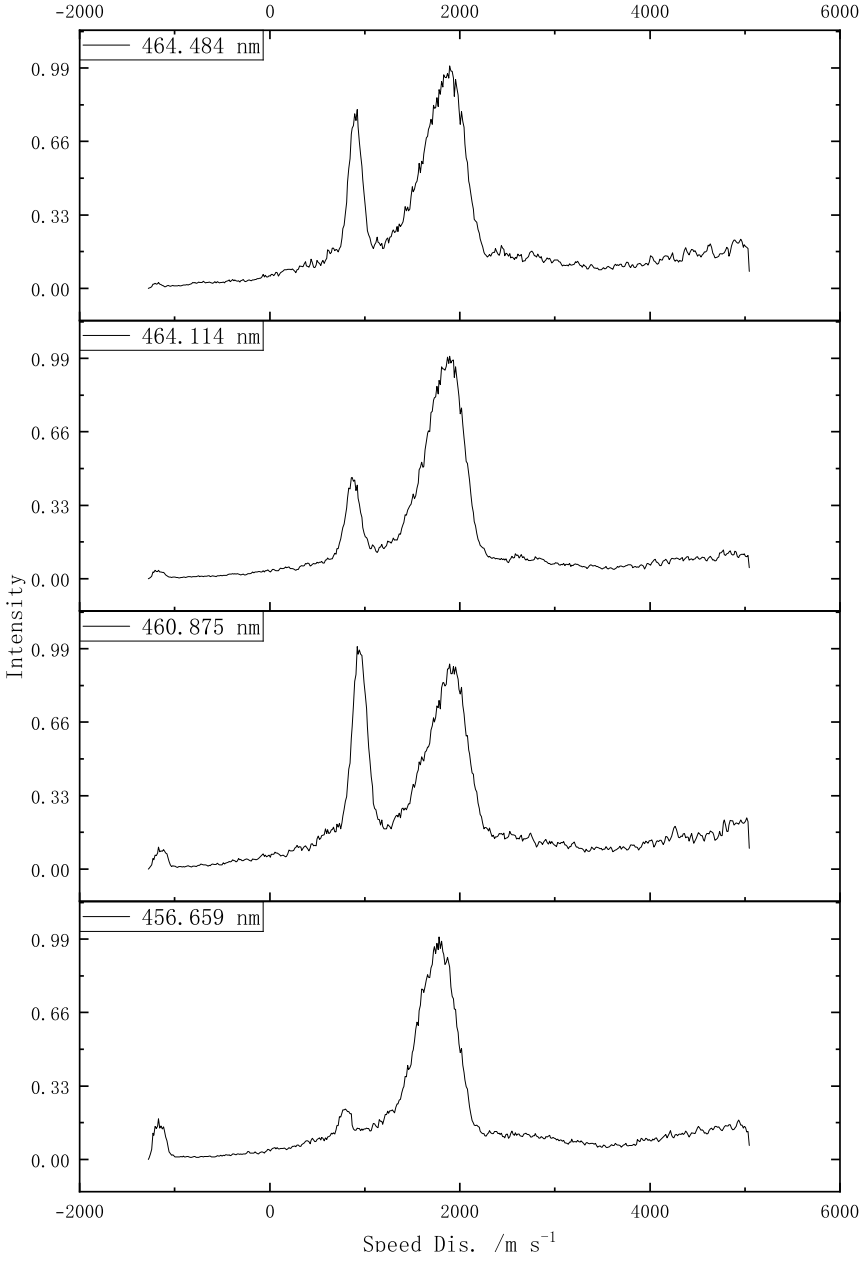


Average

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

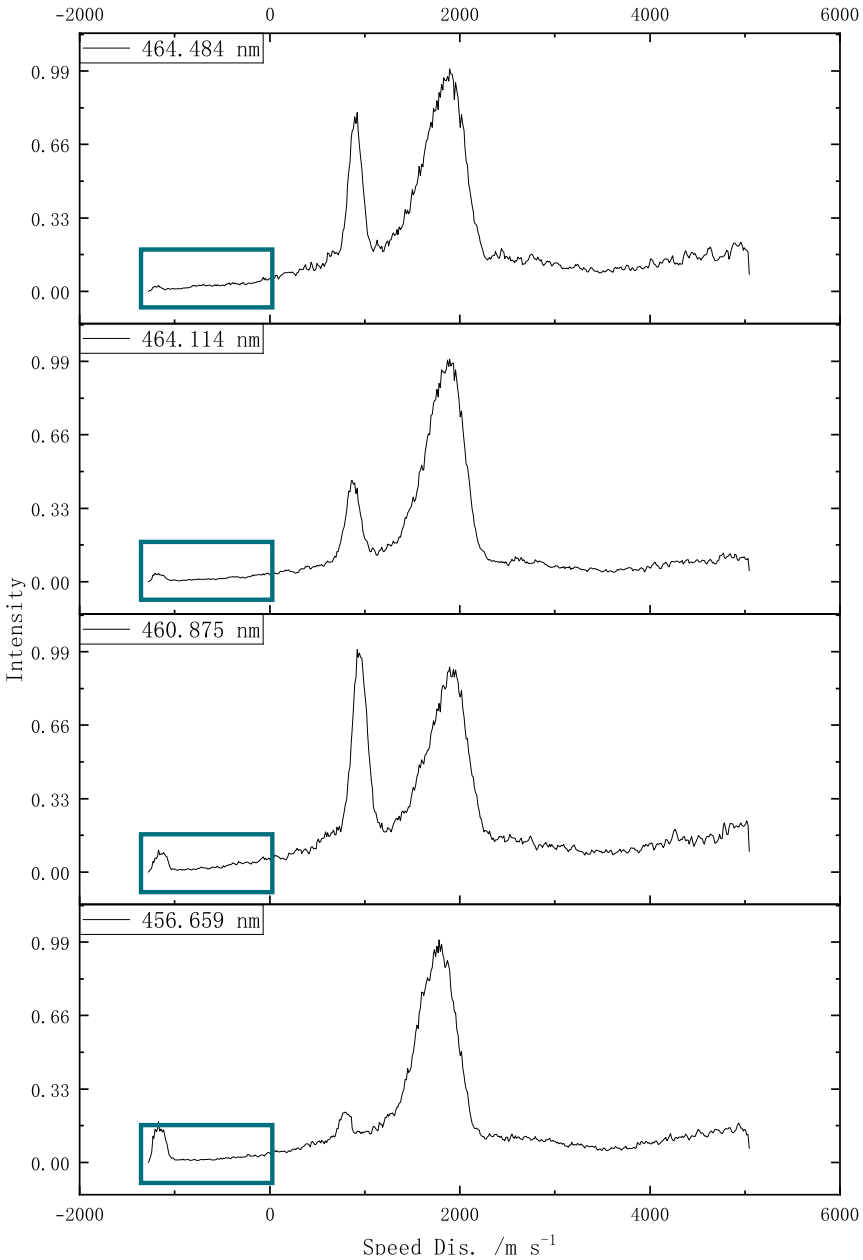
Intercept $\approx -1292\mathrm{m\,s^{-1}}$

Error



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

Error



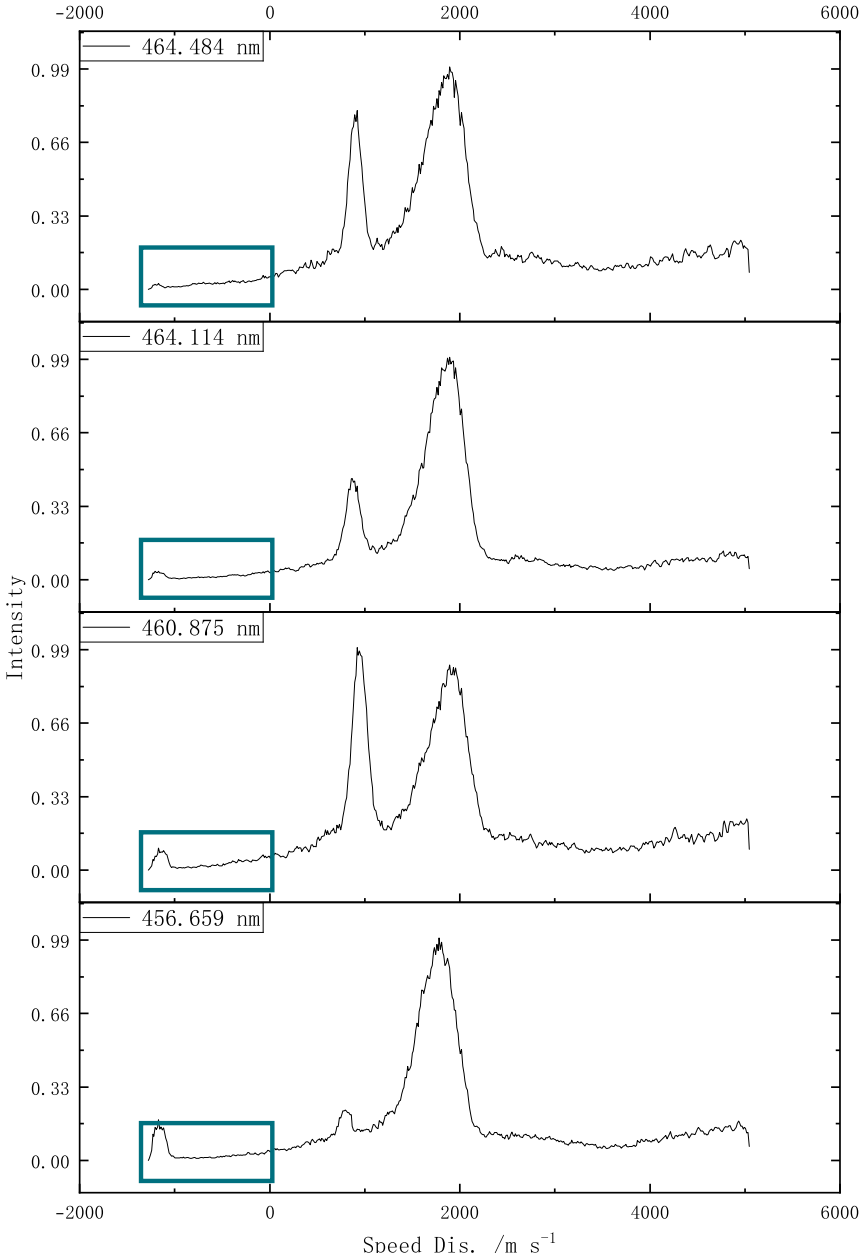
Average

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

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

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

Error



Average

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

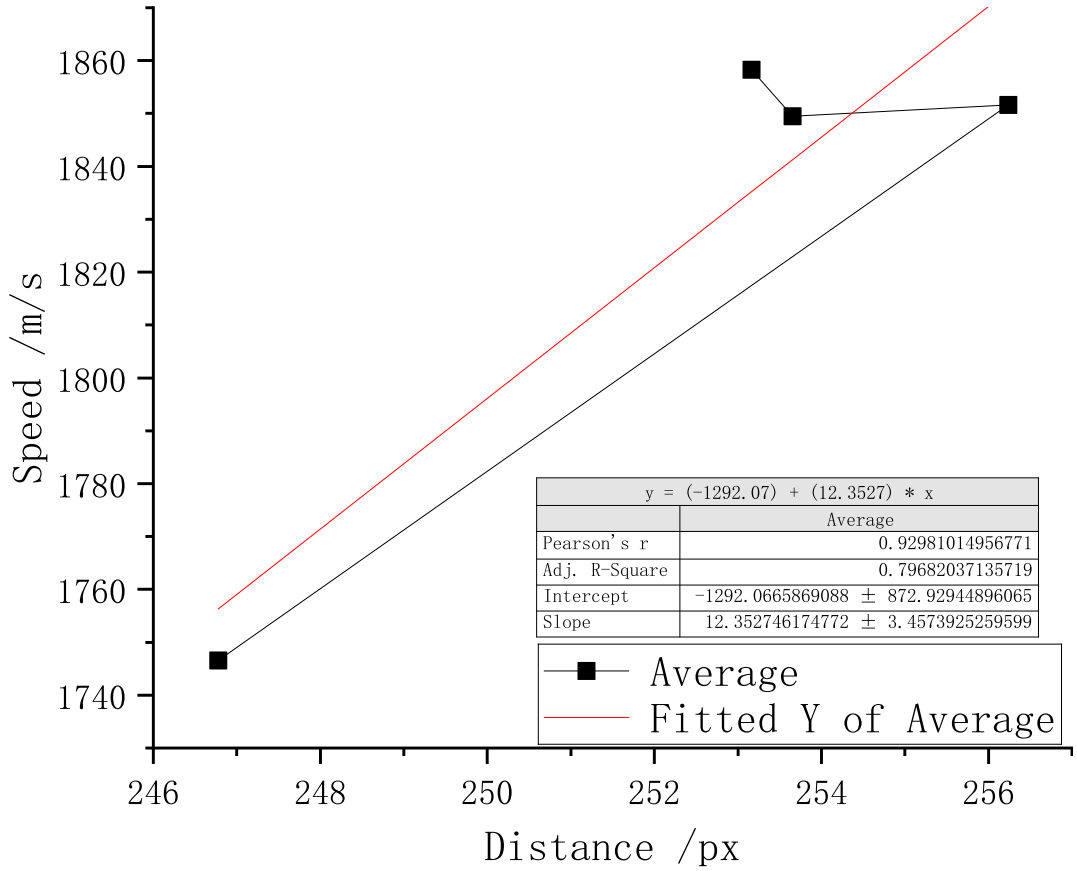
Intercept $\approx -1292\mathrm{m\,s^{-1}}$

Notice

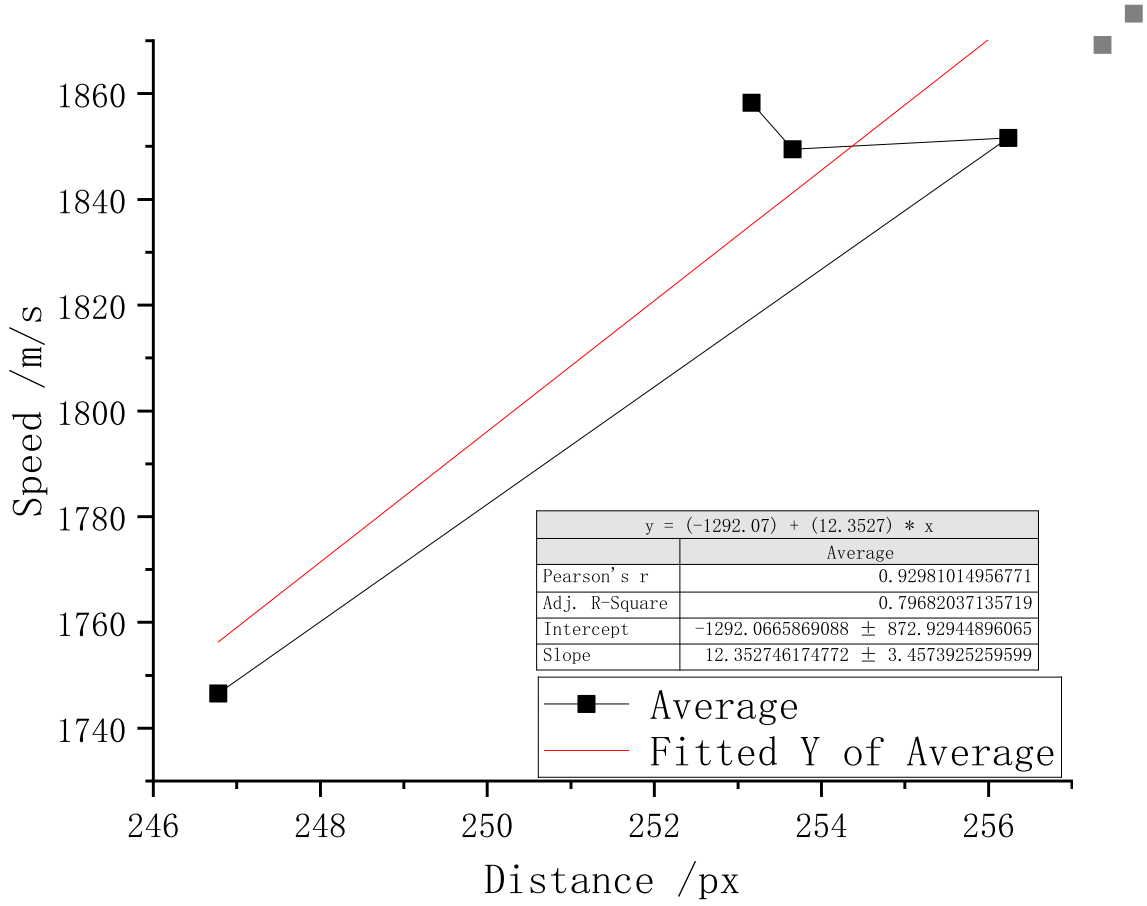
What we are calculating here are actually $|\mathbf{v}_{\mathrm{NO}}|$, which are not supposed to be minus [a].

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

Error


1860
1840
1820
1800
1780
1760
1740
Speed /m/s
246
248
250
252
254
256
Distance /px
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

Error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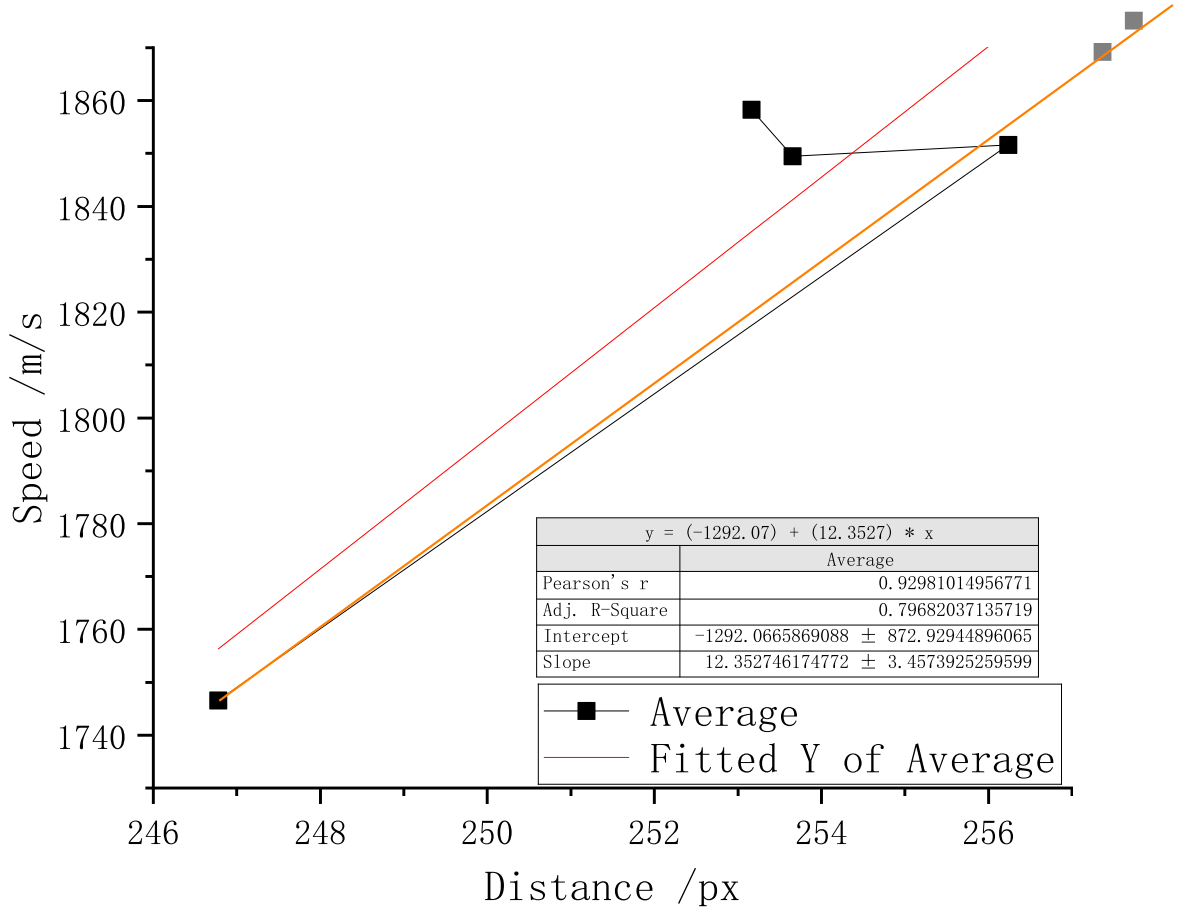
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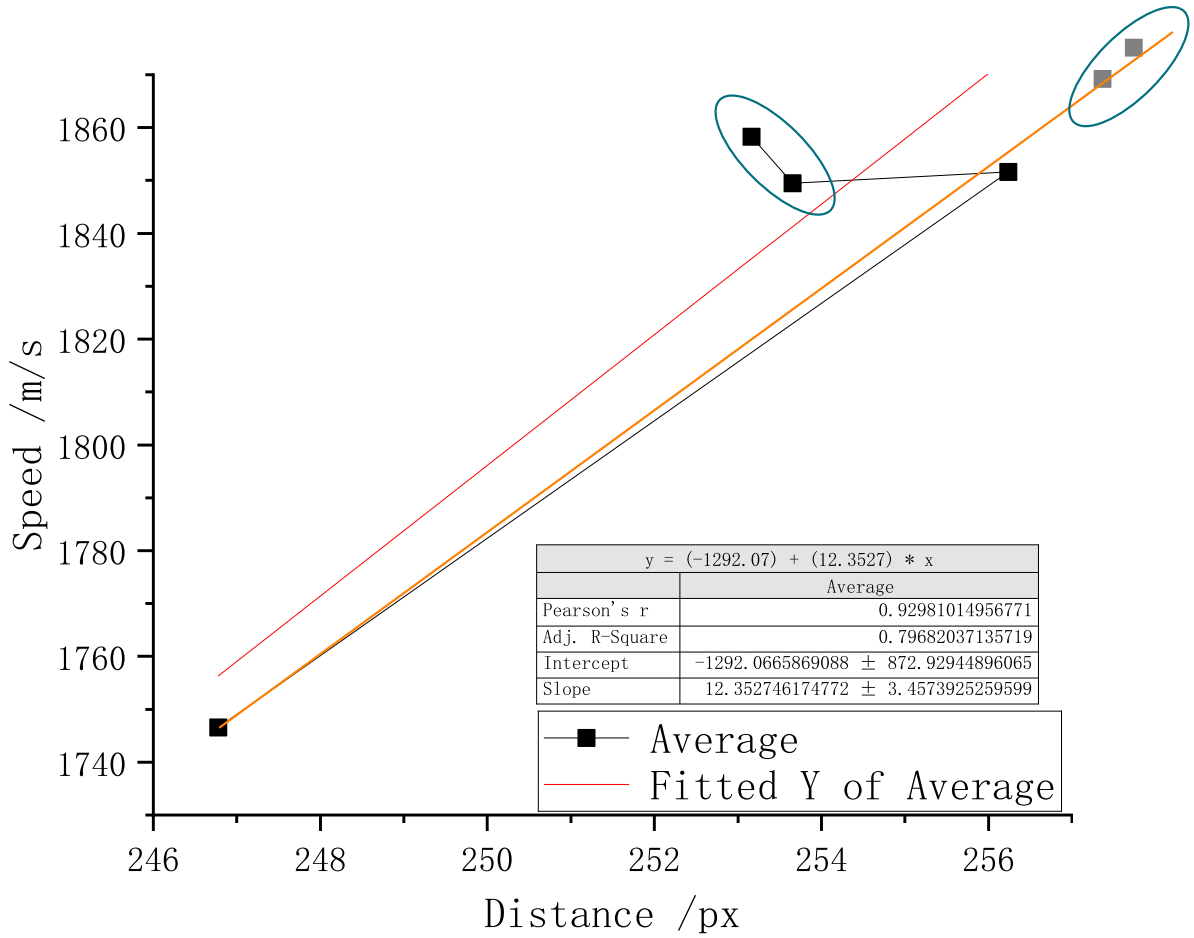
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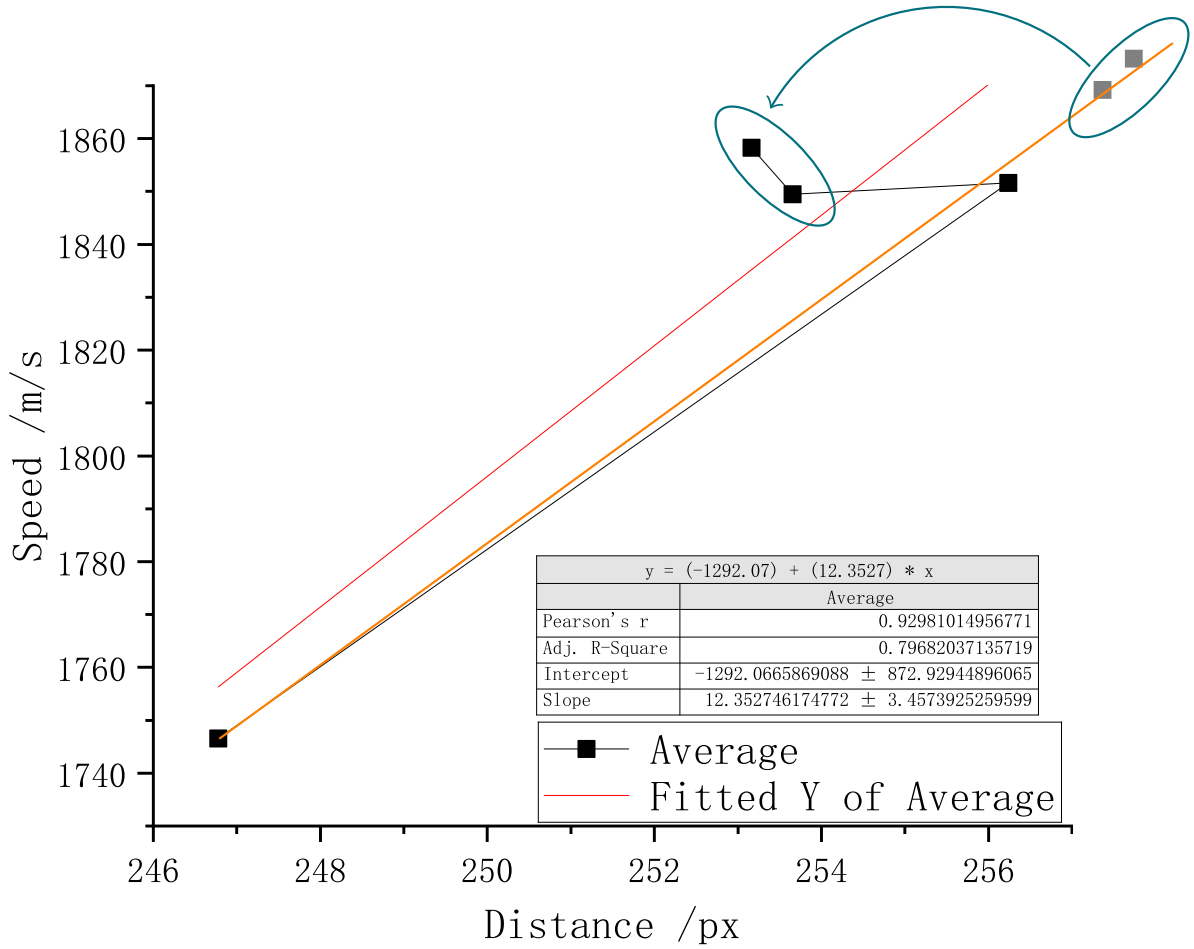
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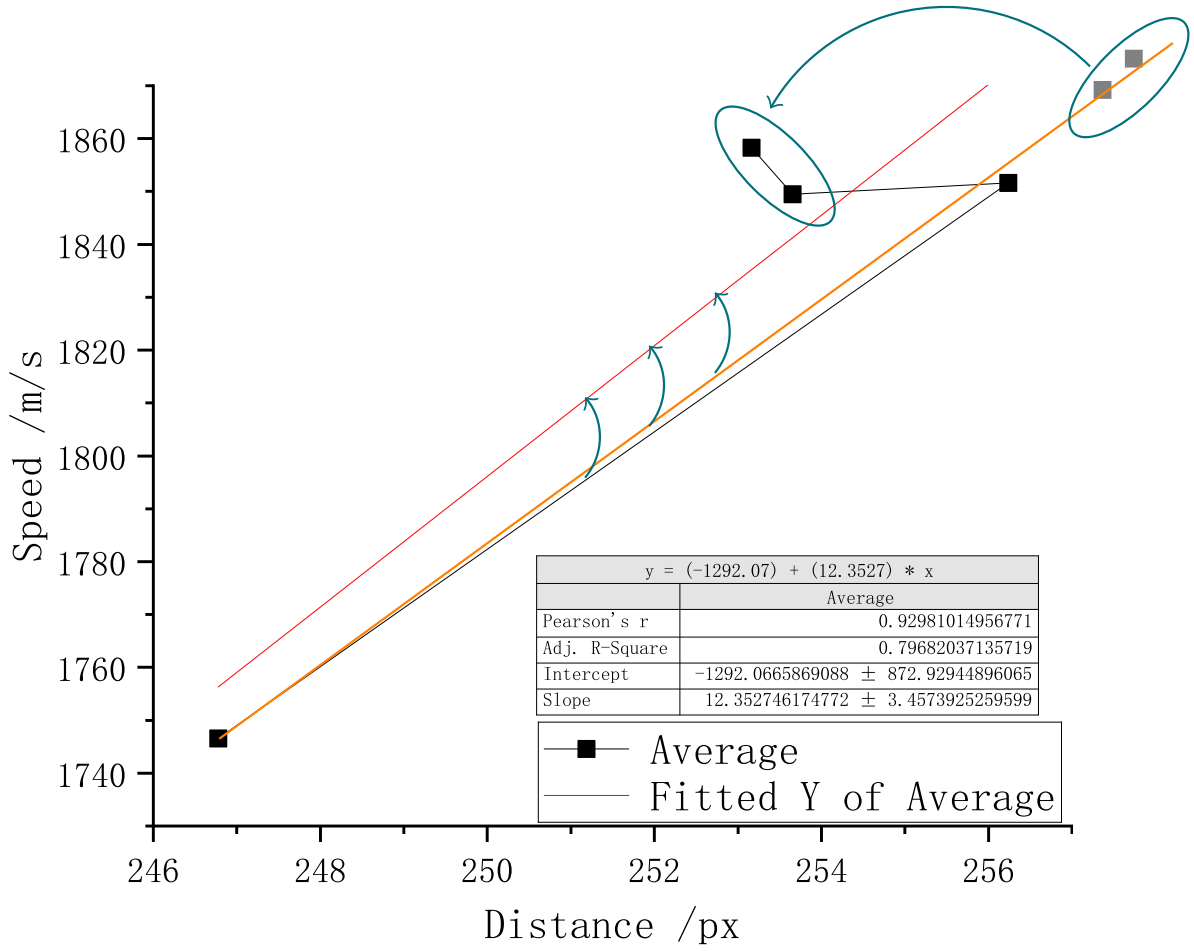
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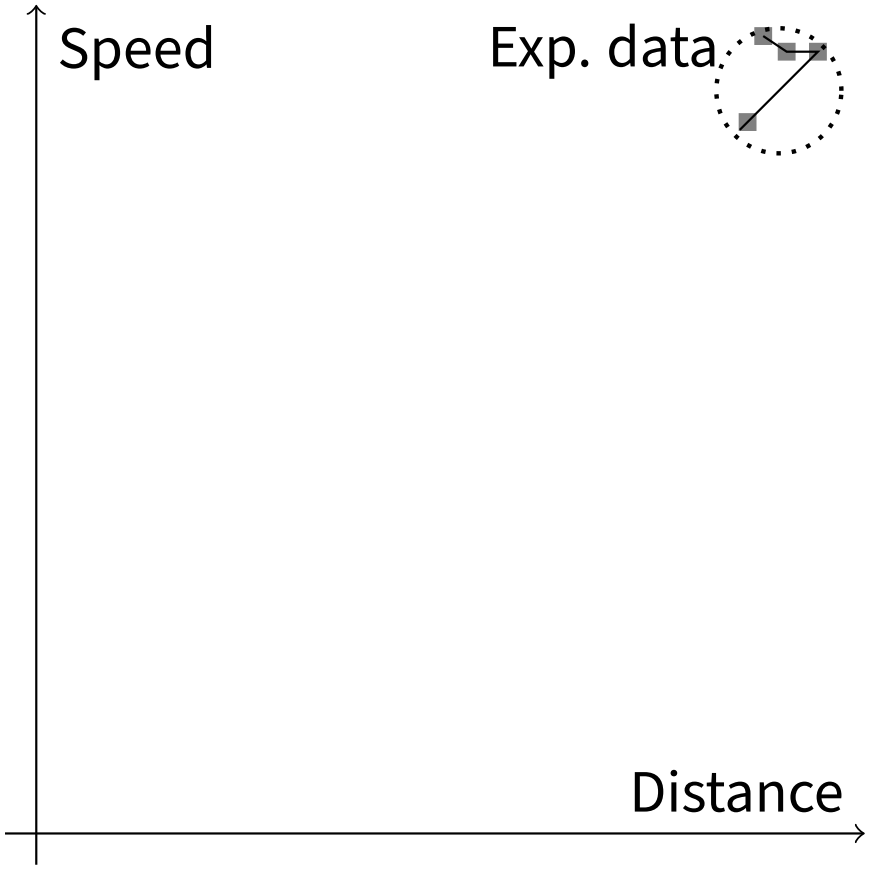
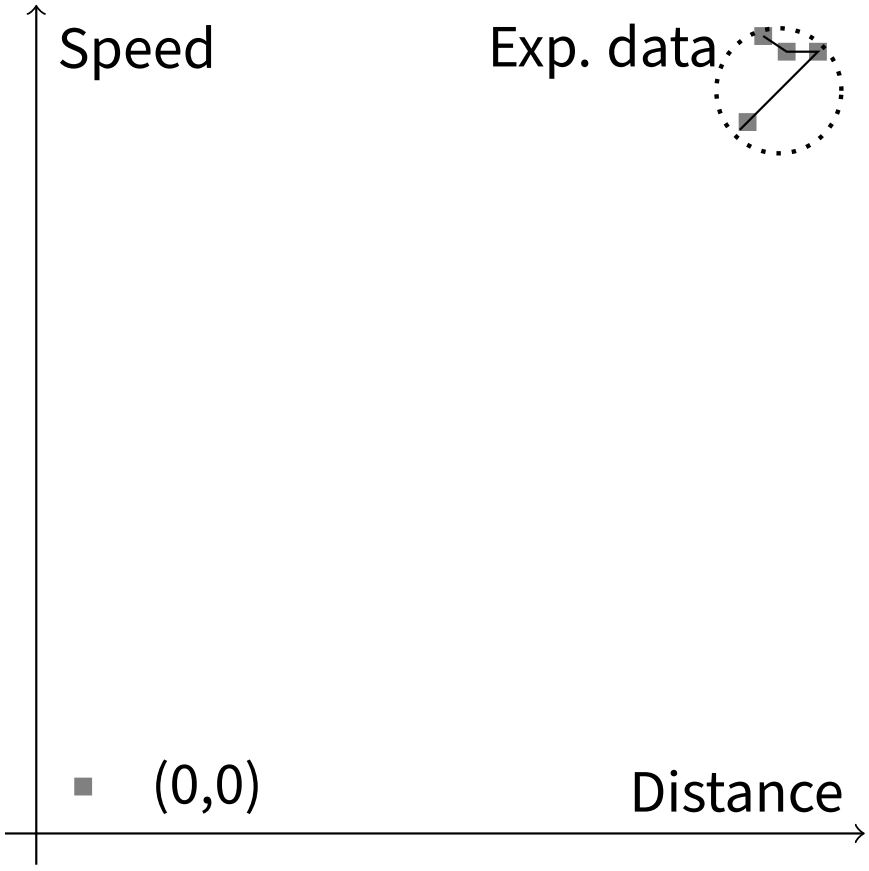
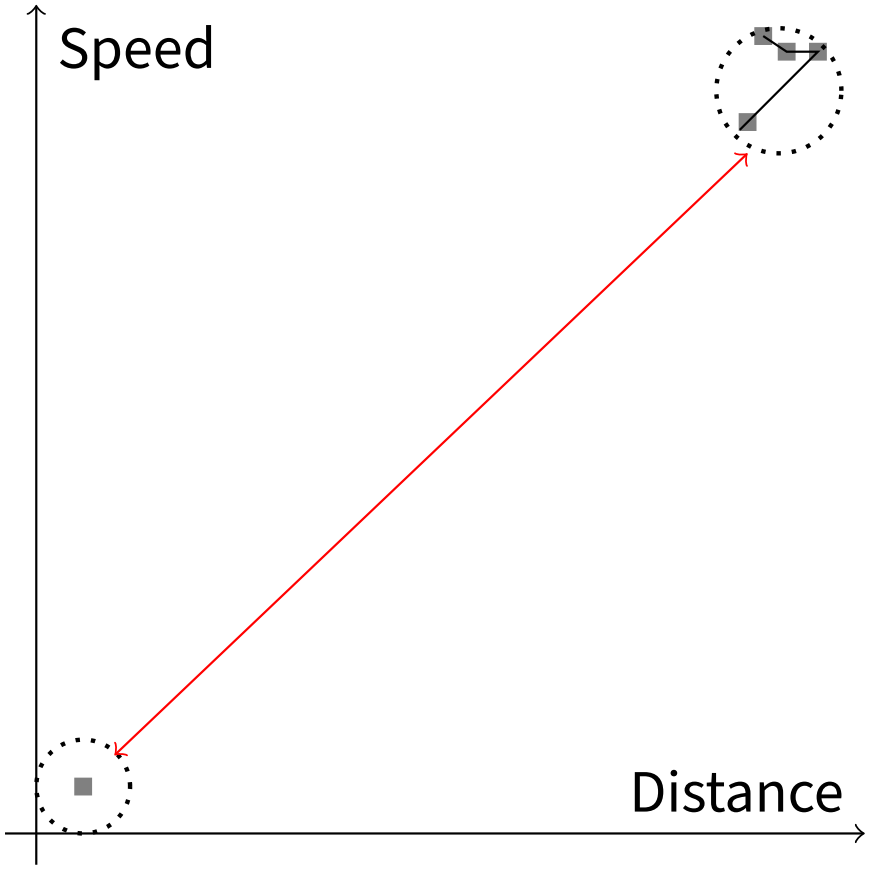


Error



Error

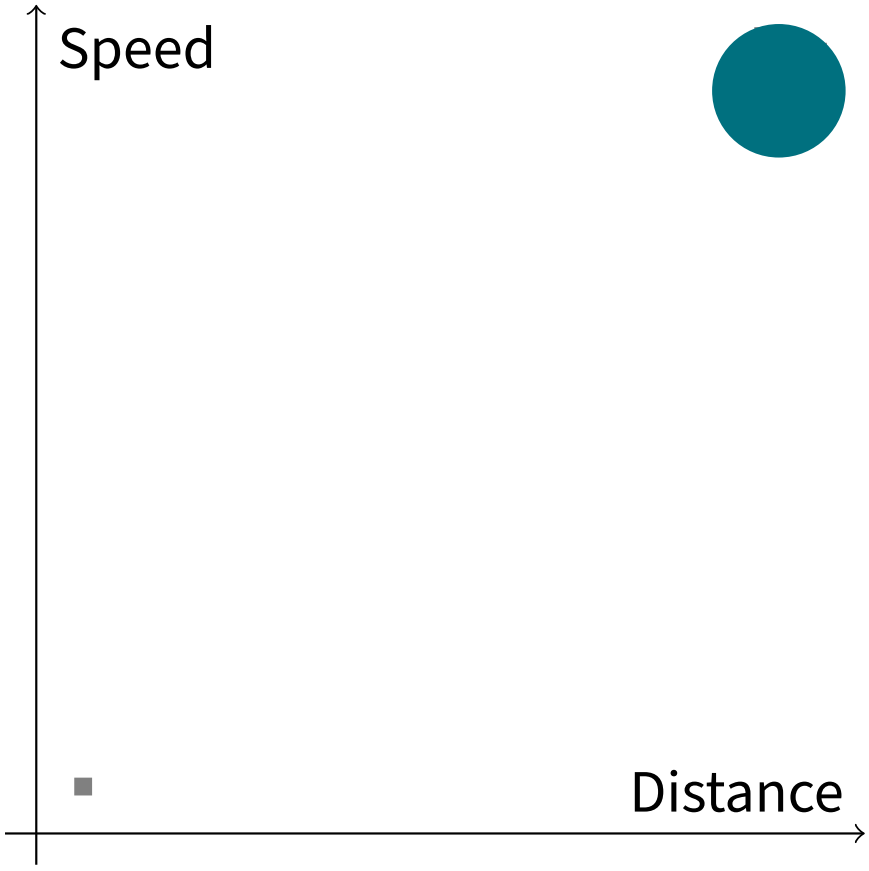


If we assume a virtual zero point:

The fake data obtains a huge weight!

Statistics tools always treat all data as proper indications.

Error



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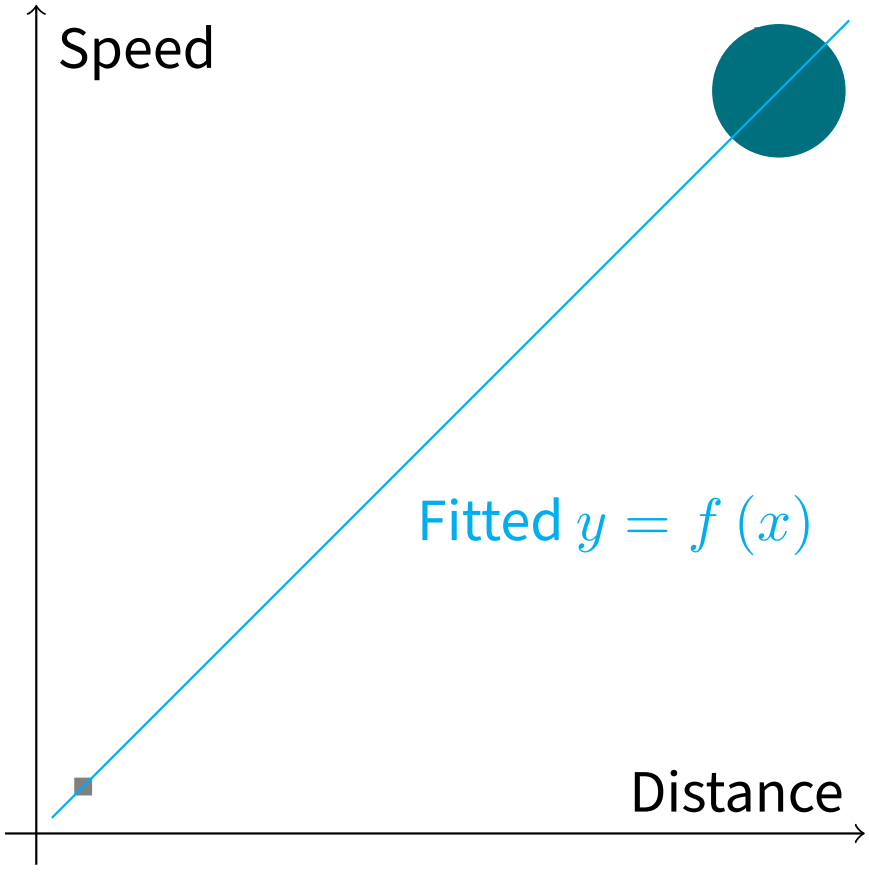
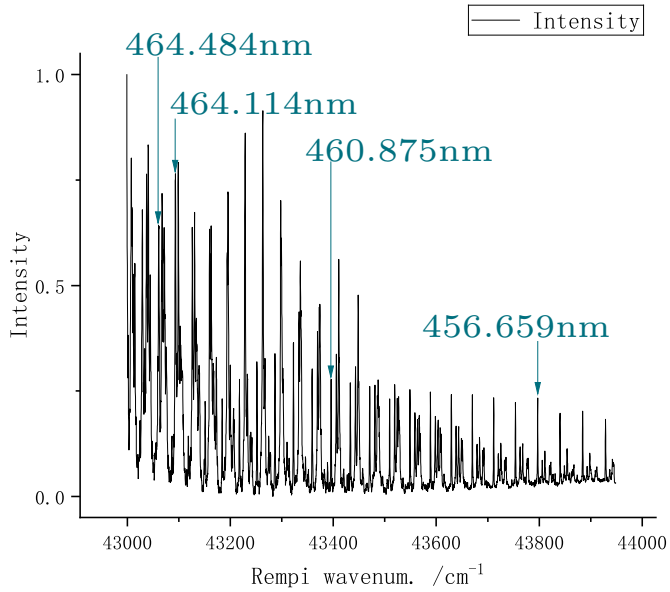


If we assume a virtual zero point:
The fake data obtains a huge weight!
Statistics tools always treat all data as proper indications.

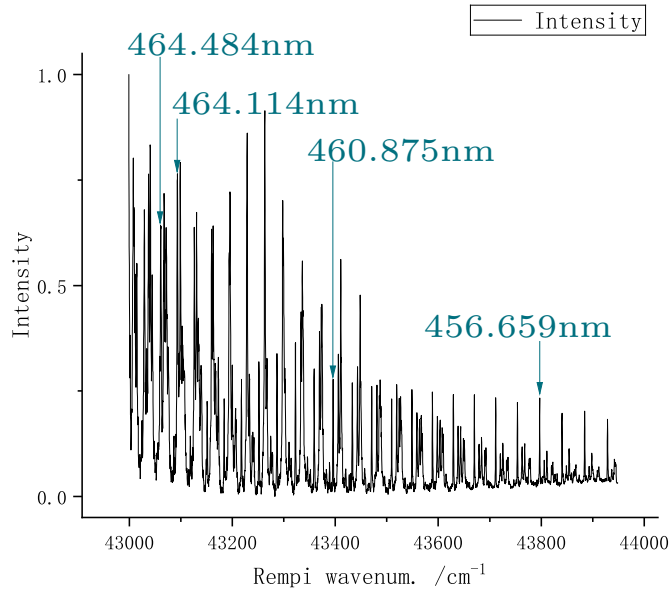
$\Longrightarrow$ After assignments, which are the points we should use?

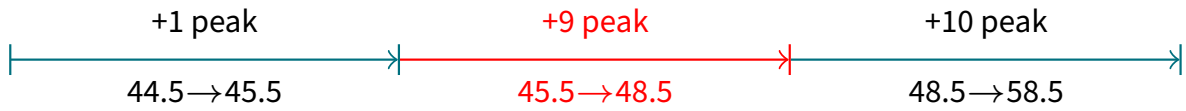
Assignment for Assignment



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

Assignment for Assignment





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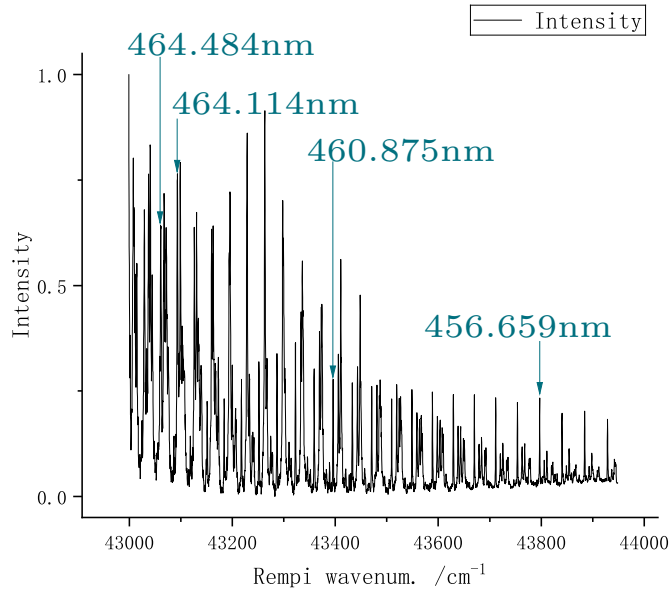

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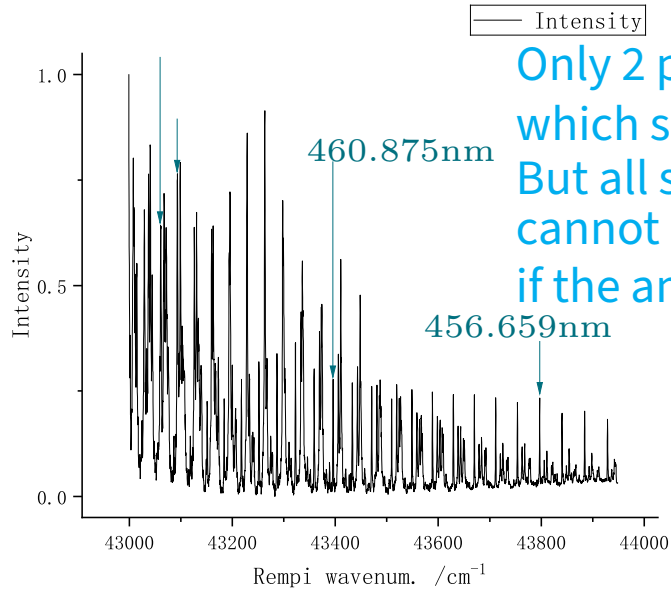

Only 2 peaks
which seem more valid.
But all statistics tools
cannot be properly applied
if the amount of data $\leqslant 3$.

+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 $= 246.776$
	$sR21\ (48.5)$	$sR21\ (58.5)$

Reference

[1] J. Danielak et al. *Journal of Molecular Spectroscopy* **181**.2 (1997), pp. 394–402.

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

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

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