練習実験報告

肖宇笑

May 30, 2024

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Contents

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Galvano Sepctrum

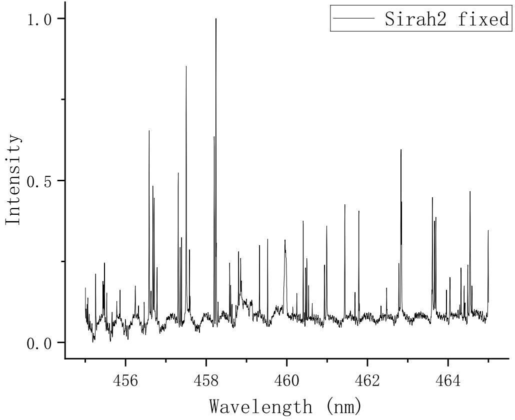

Fig. 1: Wavelen. correction

Galvano Sepctrum

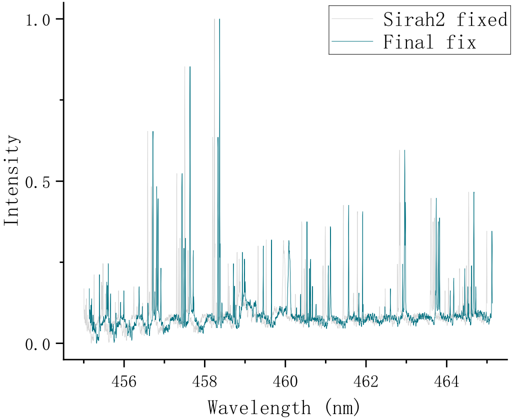

Fig. 1: Wavelen. correction

Galvano Sepctrum

Calibration

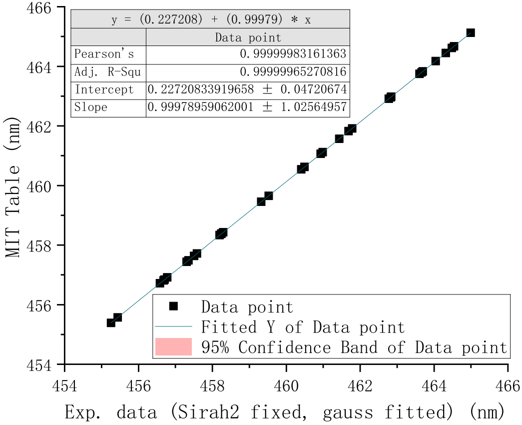

Fig. 2: Correction function

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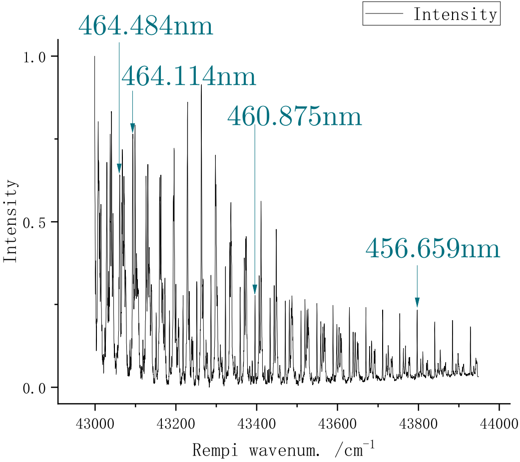
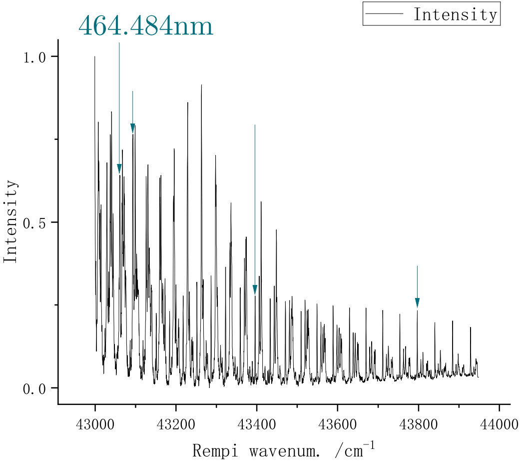
Selected peaks

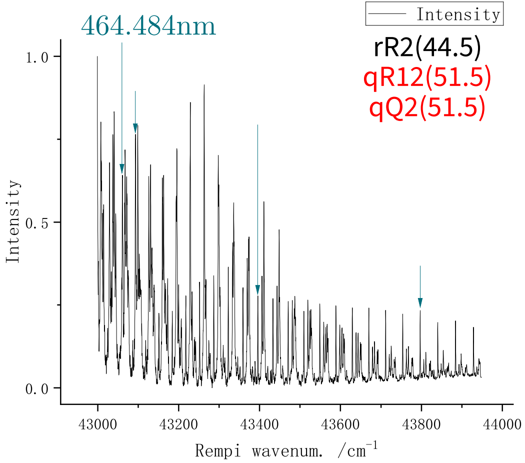


Peak 1



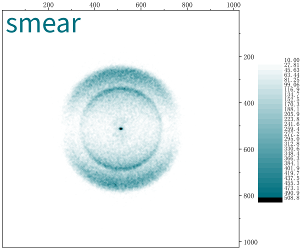
464.484nm
Intensity
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm-1

Peak 1

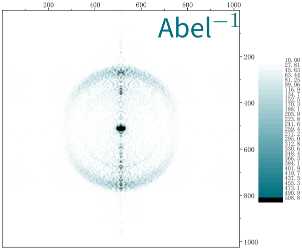


464.484nm
Intensity
rR2(44.5)
qR12(51.5)
qQ2(51.5)
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm-1

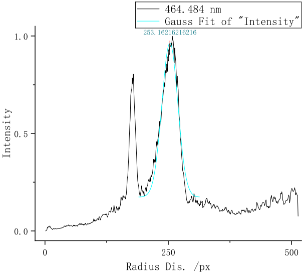
Peak 1



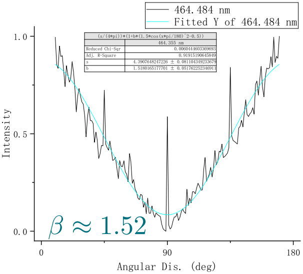
smear



Abel^{-1}

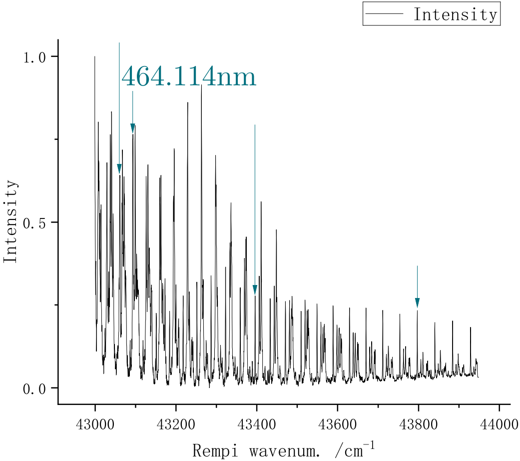


464.484 nm
Gauss Fit of "Intensity"
253.16216216216
Intensity
Radius Dis. /px



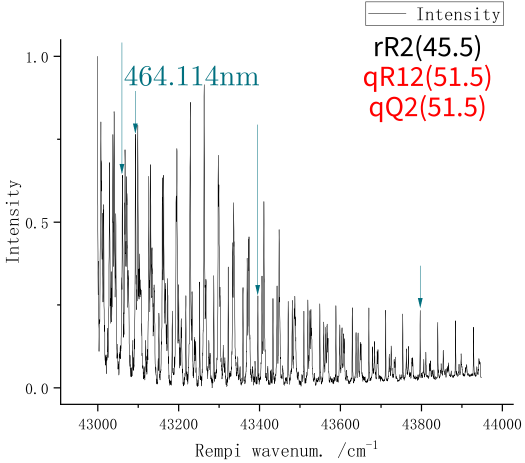
464.484 nm
Fitted Y of 464.484 nm
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
464.355 nm
Reduced Chi-Sqr 0.0060444603369693
Adj. R-Square 0.91915190645849
s 4.3907648247226 ± 0.081104349233679
b 1.5180165177701 ± 0.051762252346911
$\beta \approx 1.52$
Intensity
Angular Dis. (deg)

Peak 2



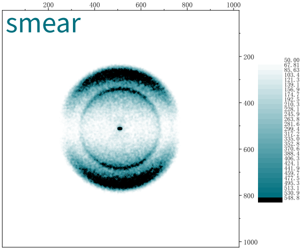
Intensity
464.114nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

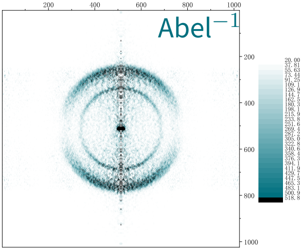
Peak 2

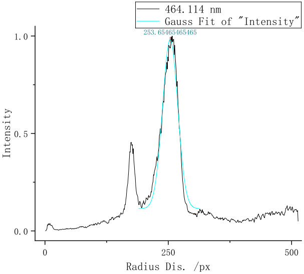


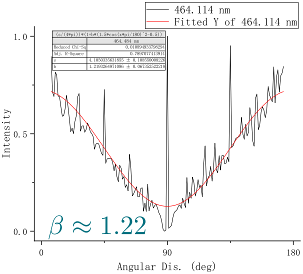
Intensity
rR2(45.5)
qR12(51.5)
qQ2(51.5)
464.114nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm-1

Peak 2

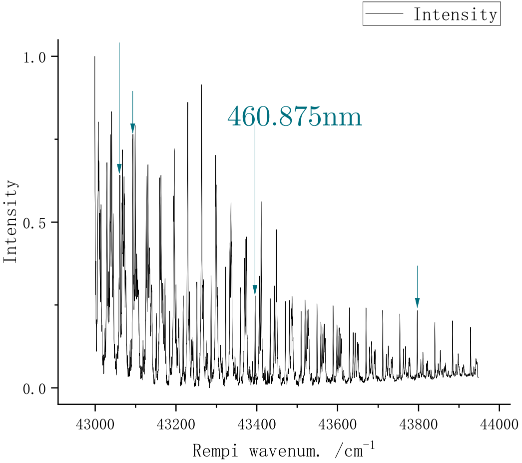

smear


Abel^{-1}


464.114 nm
Gauss Fit of "Intensity"
253.65465465465
Intensity
Radius Dis. /px

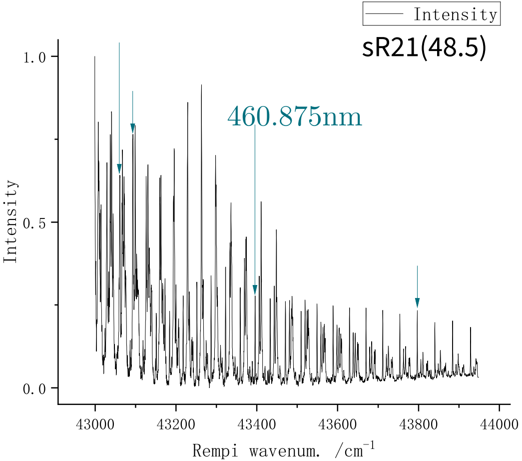

464.114 nm
Fitted Y of 464.114 nm
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
464.484 nm
Reduced Chi-Sq 0.010894933798294
Adj. R-Square 0.7897077413914
s 4.1050335631855 ± 0.108550008226
b 1.2193264971086 ± 0.067352522218
Intensity
Angular Dis. (deg)
$\beta \approx 1.22$

Peak 3



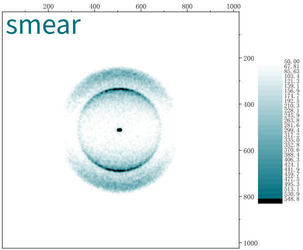
Intensity
460.875nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

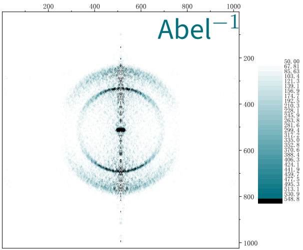
Peak 3

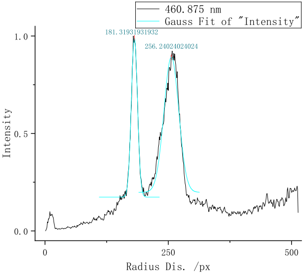


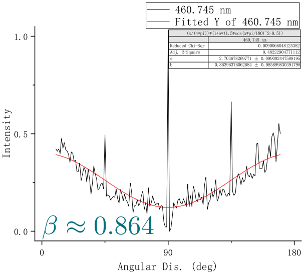
Intensity
sR21(48.5)
460.875nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm^{-1}

Peak 3

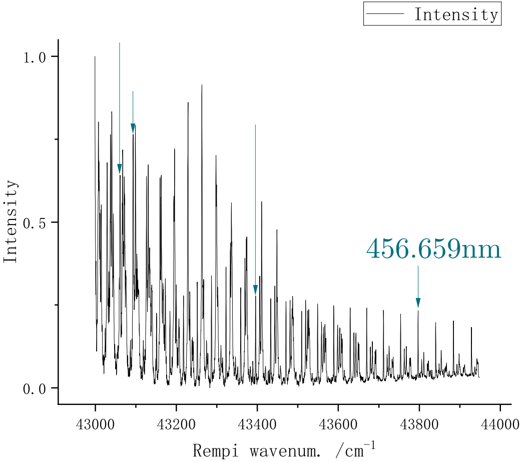

smear
200
400
600
800
1000


Abel^{-1}
200
400
600
800
1000


460.875 nm
Gauss Fit of "Intensity"
181.31931931932
256.24024024024
Intensity
1.0
0.5
0.0
0
250
500
Radius Dis. /px

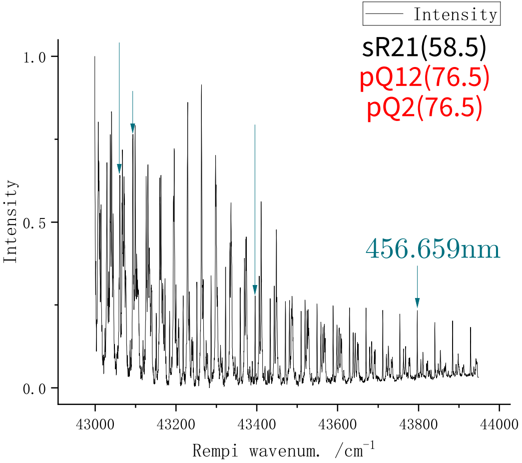

460.745 nm
Fitted Y of 460.745 nm
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
460.745 nm
Reduced Chi-Sqr 0.0090066048125382
Adj. R-Square 0.48222904771112
s 2.703678269771 ± 0.099002447588195
b 0.86396376062684 ± 0.085899830391798
Intensity
1.0
0.5
0.0
0
90
180
Angular Dis. (deg)
$\beta \approx 0.864$

Peak 4



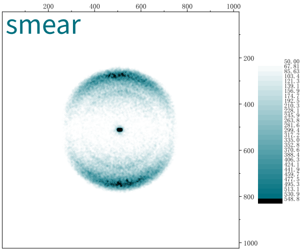
Intensity
1.0
0.5
0.0
Intensity
456.659nm
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm-1

Peak 4

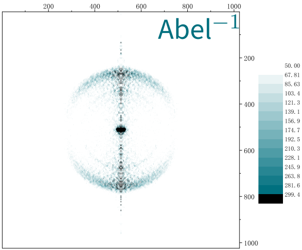


Intensity
sR21(58.5)
pQ12(76.5)
pQ2(76.5)
456.659nm
1.0
0.5
0.0
Intensity
43000
43200
43400
43600
43800
44000
Rempi wavenum. /cm-1

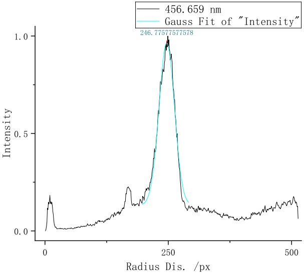
Peak 4



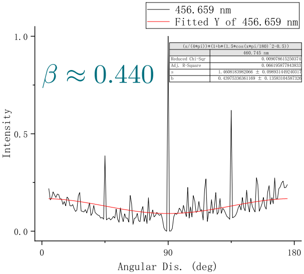
smear
200
400
600
800
1000
50.00
67.81
85.63
103.4
121.3
139.1
156.9
174.7
192.5
210.3
228.1
245.9
263.8
281.6
299.4
317.2
335.0
352.8
370.6
388.4
406.3
424.1
441.9
459.7
477.5
495.3
513.1
530.9
548.8



Abel^{-1}
200
400
600
800
1000
50.00
67.81
85.63
103.4
121.3
139.1
156.9
174.7
192.5
210.3
228.1
245.9
263.8
281.6
299.4



456.659 nm
Gauss Fit of "Intensity"
246.77577577578
Intensity
Radius Dis. /px
0
250
500
0.0
0.5
1.0



456.659 nm
Fitted Y of 456.659 nm
$\beta \approx 0.440$
(s/(4*pi))*(1+b*(1.5*cos(x*pi/180)^2-0.5))
460.745 nm
Reduced Chi-Sqr 0.009078615250374
Adj. R-Square 0.066195877843833
s 1.4608183982066 ± 0.098931449240317
b 0.43975336361169 ± 0.13583104587326
Intensity
Angular Dis. (deg)
0
90
180
0.0
0.5
1.0

Contents

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

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

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	$43\,058.49\text{cm}^{-1}$		$\Delta E_v(1 \to 0) + E(J = 44)$
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	$43\,796.34\text{cm}^{-1}$		$\Delta E_v(1 \to 0) + E(J = 58)$

[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}	$E_{\text{bond}}(\mathrm{O{-}NO})^2$	$E_{\text{int.}}(\mathrm{NO})$
Peak 1 $464.484\mathrm{nm}$	$43\,058.49\mathrm{cm}^{-1}$		$2341.932\,775\,0\mathrm{cm}^{-1} + E(J = 44)$
Peak 2 $464.114\mathrm{nm}$	$43\,092.81\mathrm{cm}^{-1}$		$2341.932\,775\,0\mathrm{cm}^{-1} + E(J = 45)$
Peak 3 $460.875\mathrm{nm}$	$43\,395.69\mathrm{cm}^{-1}$	$25\,128.57\mathrm{cm}^{-1}$	$2341.932\,775\,0\mathrm{cm}^{-1} + E(J = 48)$
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}	$E_{\text{bond}}(\mathrm{O-NO})$[3]	$E_{\text{int.}}(\mathrm{NO})$
Peak 1 $464.484\mathrm{nm}$	$43\,058.49\mathrm{cm}^{-1}$	$25\,128.57\mathrm{cm}^{-1}$	$5814.033\mathrm{cm}^{-1}$
Peak 2 $464.114\mathrm{nm}$	$43\,092.81\mathrm{cm}^{-1}$		$5965.969\mathrm{cm}^{-1}$
Peak 3 $460.875\mathrm{nm}$	$43\,395.69\mathrm{cm}^{-1}$		$6239.696\mathrm{cm}^{-1}$
Peak 4 $456.659\mathrm{nm}$	$43\,796.34\mathrm{cm}^{-1}$		$8004.278\mathrm{cm}^{-1}$

[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

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

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

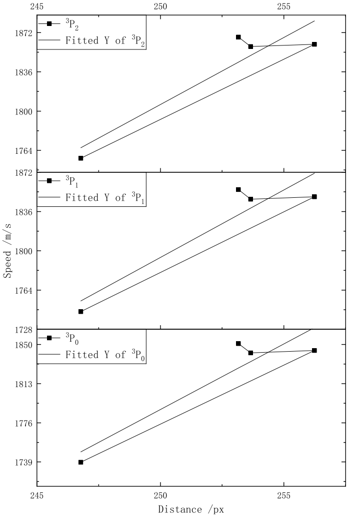
Speed correction

Trans. speed of NO

$E_{\text{int.}}(\mathrm{O})$	$v(\mathrm{NO}) = \sqrt{\frac{2E_{\text{trans}}(\mathrm{NO})}{m(\mathrm{NO})}}$	Δy
$^3P_2$ $(0\,\mathrm{cm}^{-1})$	$1867.845\,\mathrm{m\,s^{-1}}$	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
$^3P_1$ $(158.625\,\mathrm{cm}^{-1})$	$1856.033\,\mathrm{m\,s^{-1}}$	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
$^3P_0$ $(226.977\,\mathrm{cm}^{-1})$	$1850.920\,\mathrm{m\,s^{-1}}$	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 $\approx -1298 \mathrm{m\,s^{-1}}$

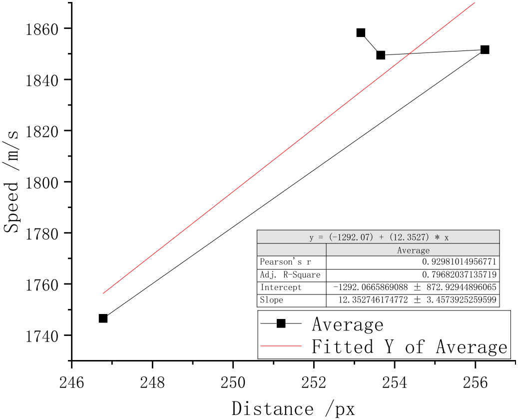
$^3P_0$

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

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

Speed correction

Trans. speed of NO



Average

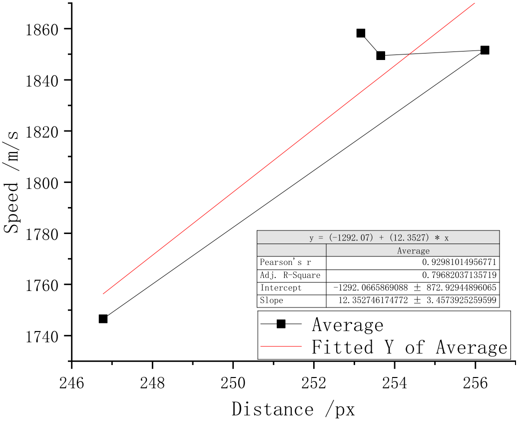
$12.35 \mathrm{m\,s^{-1}\,px^{-1}}$

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

Contents

Contents

Error



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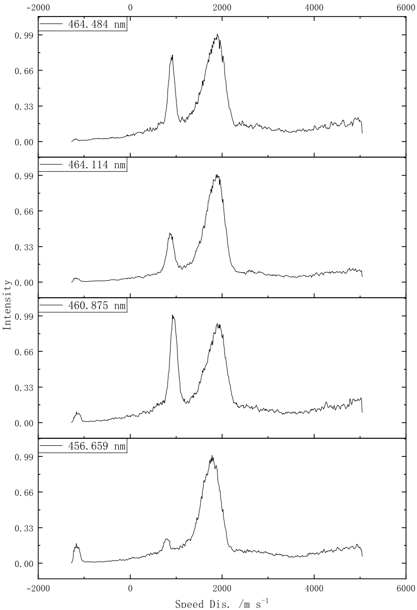

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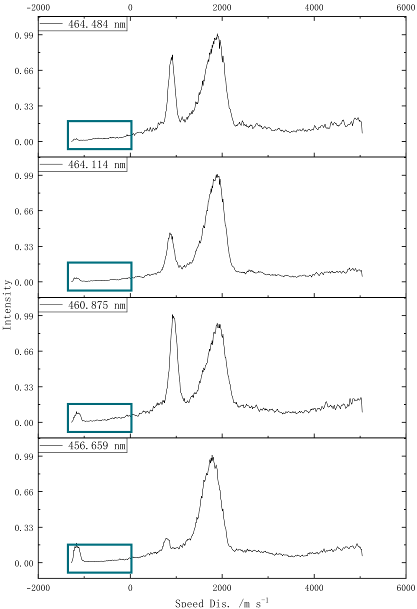
[a] Maybe a $\pm 5\,\mathrm{m\,s^{-1}}$-level intercept noise are permitted.

Error



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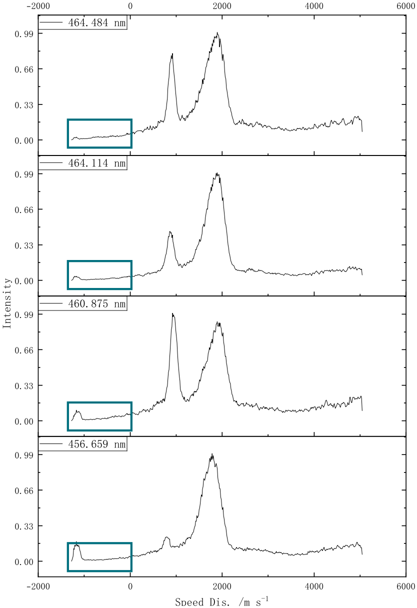

Average

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

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.

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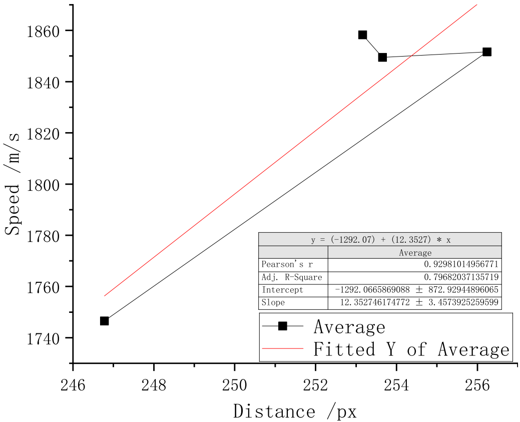
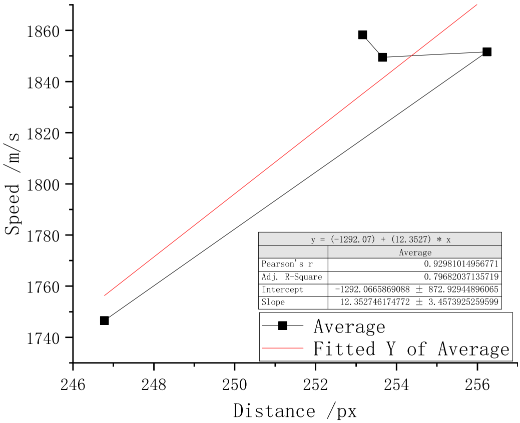

y = (-1292.07) + (12.3527) * x
Average
Pearson's r 0.92981014956771
Adj. R-Square 0.79682037135719
Intercept -1292.0665869088 ± 872.92944896065
Slope 12.352746174772 ± 3.4573925259599
Average
Fitted Y of Average
Speed /m/s
Distance /px
1740
1760
1780
1800
1820
1840
1860
246
248
250
252
254
256

Error



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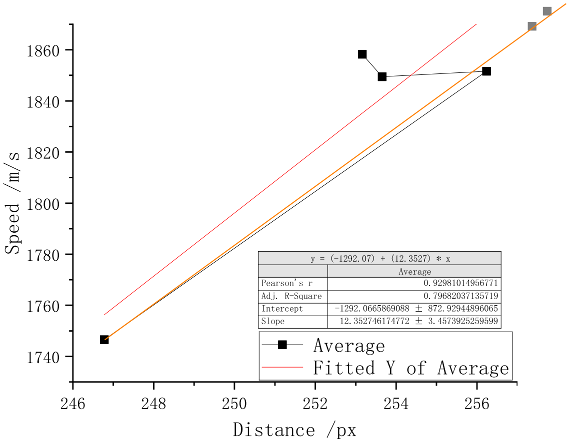

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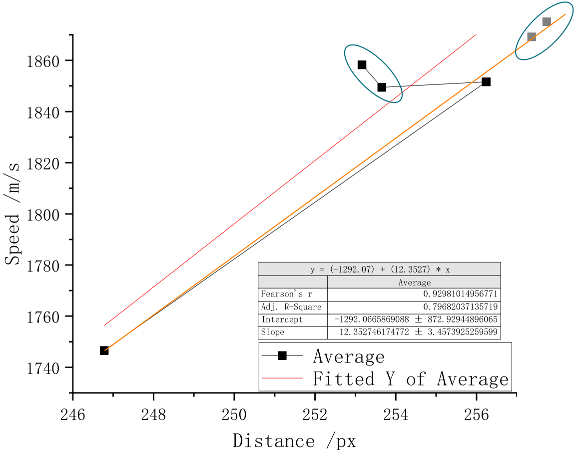

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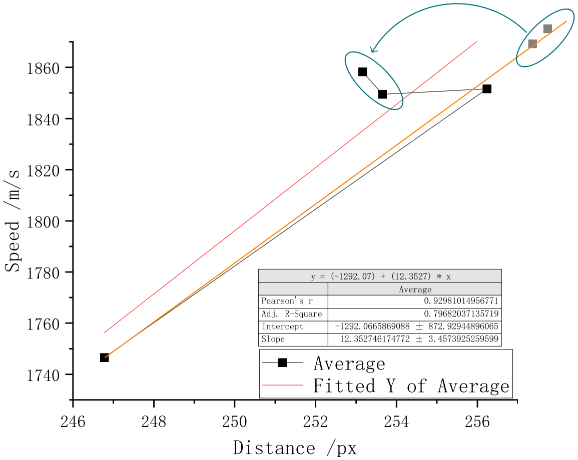

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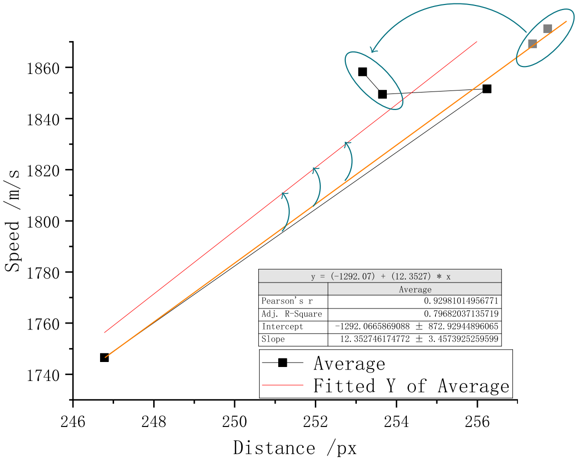
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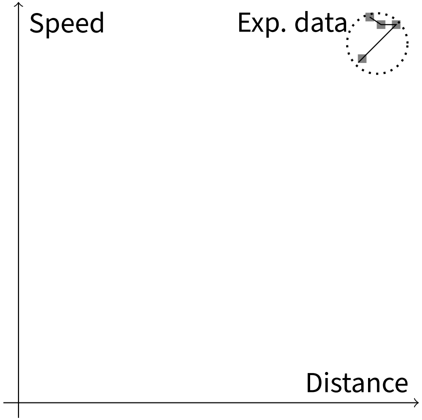

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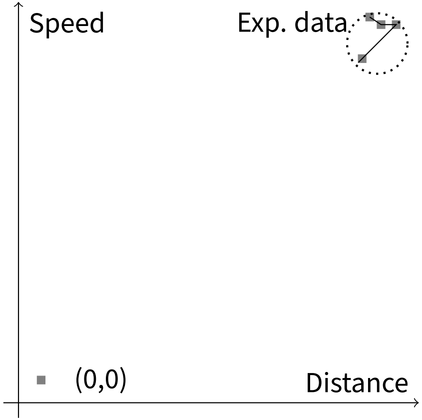

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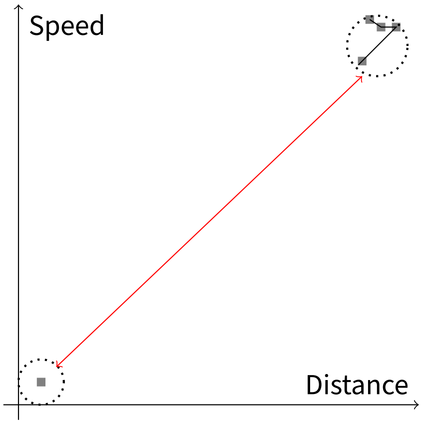
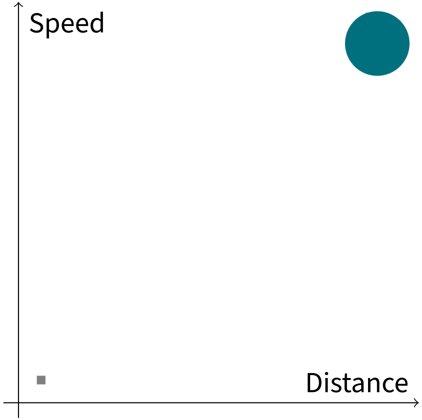


If we assume a virtual zero point:
The fake data obtains a huge weight!
Statistics tools always treat all data as proper indications.

Error



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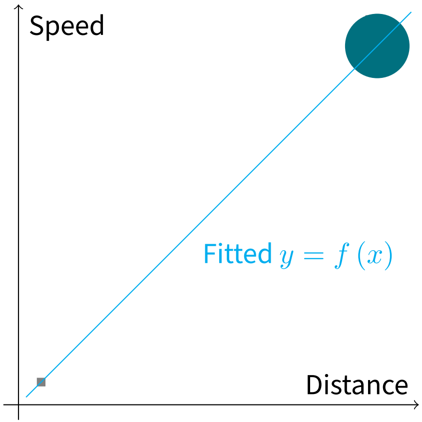

If we assume a virtual zero point:
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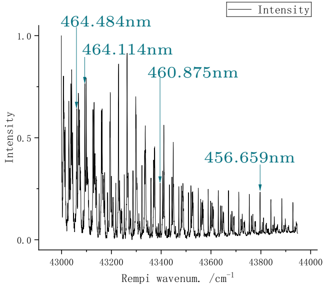
Statistics tools always treat all data as proper indications.

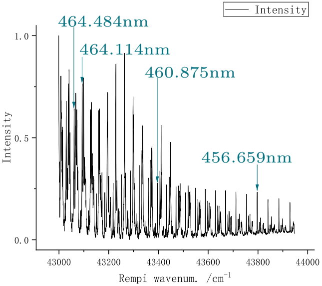
$\Longrightarrow$ After assignments, which are the points we should use?

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



+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 $\approx 43796.34\text{cm}^{-1}$
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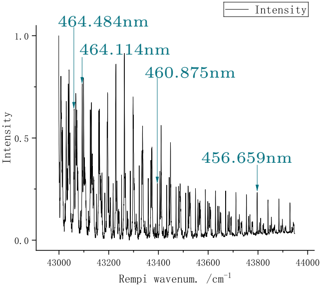

+1 peak | ??? | +10 peak

$44.5 \rightarrow 45.5$ | ¿¿¿ | $48.5 \rightarrow 58.5$

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 $\approx 43796.34\text{cm}^{-1}$
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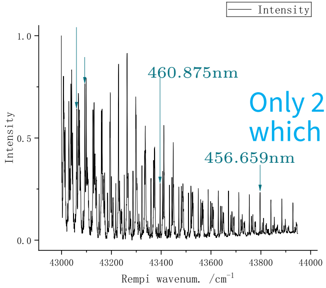

Only 2 peaks
which seem more valid.

+10 peak

48.5→58.5

	460.875nm $\approx$ 43395.69cm^{-1}	456.659nm $\approx$ 43796.34cm^{-1}
	px $=$ 256.240	px $=$ 246.776
	$sR21\,(48.5)$	$sR21\,(58.5)$

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.