

Absorption spectrum of Iodine vapour and Emission spectra of metals using constant deviation spectrometer

Aryan Shrivastava*

School of Physical Sciences, National Institute of Science Education and Research

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Emission spectra of metals were recorded using a constant deviation spectrometer and the observed lines were calibrated with a mercury lamp. The absorption spectrum of iodine vapour was analyzed to determine vibronic energy levels, bond dissociation energy, and the molecular force constant. The dissociation energy in the excited state was obtained as $D_0 = (0.346 \pm 0.001)$ eV, and the force constant as $f = (32.4 \pm 2.4)$ N m⁻¹. The results illustrate the use of optical spectroscopy in studying both atomic and molecular structure.

I. OBJECTIVE

1. Calibrate the C.D.S using a calibration source
2. Determine the wavelength of the unknown spectra of the given metals in the arc lamp source.
3. To study the absorption spectrum of iodine vapour with a Constant Deviation spectrometer and then to determine:
 - (a) the energy level diagram of iodine molecule
 - (b) the electronic energy gap and vibrational energies
 - (c) bond dissociation limit.
 - (d) force constant for the excited state

II. THEORY

A. Emission Spectra of Metals

Atoms possess discrete electronic energy levels, and electronic transitions between these levels result in the emission or absorption of photons with energy

$$E = h\nu = \frac{hc}{\lambda} \quad (1)$$

where h is Planck's constant, c is the speed of light, and λ is the photon wavelength. When a metal is excited in an electric arc, its atoms emit radiation at characteristic wavelengths that appear as bright lines in the emission spectrum. These lines serve as unique spectral "finger-prints" for each element.

B. Absorption Spectrum of Iodine Vapour

In molecules, the electronic states are further split into vibrational levels. The potential energy of a diatomic

molecule such as iodine is well described by the anharmonic Morse potential [1]:

$$U(r) = D_e \left(1 - e^{-a(r-r_e)}\right)^2, \quad (2)$$

where D_e is the depth of the potential well, r_e is the equilibrium bond length, and a is a molecular constant given by the following equation.

$$a = \bar{\nu}_e \sqrt{\frac{\pi c \mu}{h D_e}} \quad (3)$$

Solving the Schrödinger equation yields vibrational energy levels, approximately given by

$$E_\nu = \left(\nu + \frac{1}{2}\right) \bar{\nu}_e - \bar{\nu}_e x_e \left(\nu + \frac{1}{2}\right)^2 \quad (4)$$

with vibrational quantum number ν , wavenumber corresponding to harmonic vibrational frequency $\bar{\nu}_e$, and anharmonicity constant x_e .

When white light passes through iodine vapour, specific wavelengths are absorbed due to transitions from the ground electronic state X to the first excited state B (as shown in fig. 1).

$$(X, \nu'') \rightarrow (B, \nu') \quad (5)$$

where ν'' and ν' are vibrational quantum numbers in the ground and excited states, respectively. The resulting absorption bands correspond to vibronic transitions (coupled electronic and vibrational excitations). The observed band structure provides information on vibrational spacings, the electronic energy gap, and the dissociation energy of the molecule.

Assuming a harmonic oscillator approximation, the force constant f of the iodine molecule can be estimated from the average difference in wavenumbers $\Delta\nu_{\text{avg}}$ between adjacent absorption lines. The relation is

$$f = 4\pi^2 \mu (c \Delta\nu_{\text{avg}})^2 \quad (6)$$

where μ is the reduced mass of the iodine molecule and c is the velocity of light. The determination of f thus gives insight into the stiffness of the molecular bond in the excited state and is an important parameter in characterizing the molecular potential energy curve.

* aryan.shrivastava@niser.ac.in

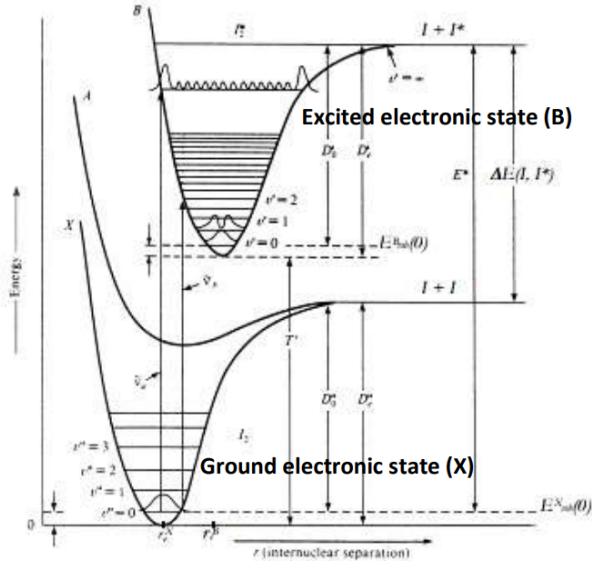


FIG. 1. Schematic energy level diagram for Iodine

C. Constant Deviation Spectrometer

In an ordinary prism spectrometer, the condition for minimum deviation is reached when the angle of incidence equals the angle of emergence. At this point, the ray inside the prism is symmetric and parallel to the base, and the angle of deviation is minimized.

The constant deviation prism (Pellin–Broca prism) is designed such that, for a suitable angle of incidence θ_i , the emergent ray is always deviated by a fixed angle of 90° irrespective of wavelength. Geometrically, it can be shown that for the prism system

$$\theta_r = \theta_i, \quad (7)$$

and the emergent ray becomes perpendicular to the incident ray. The effective deviation angle is

$$\delta = 90^\circ. \quad (8)$$

The spectrometer using this prism is called a Constant Deviation Spectrometer (CDS). The advantage of this arrangement is that the collimator and telescope are fixed at right angles, and the prism table alone is rotated. The wavelength λ corresponding to a spectral line is obtained directly from the drum calibration, which is performed using a standard source (such as a mercury lamp).

If λ_{given} denotes the known wavelength of the calibration source and λ_{obs} the corresponding observed value, the calibration curve

$$\lambda_{\text{given}} \sim \lambda_{\text{obs}} \quad (9)$$

is used to determine the corrected wavelength λ_{corr} for an unknown spectral line.

III. EXPERIMENTAL APPARATUS

The experimental setup consists of a Constant Deviation Spectrometer (CDS) equipped with a Pellin–Broca prism, a collimator, and a telescope fixed at right angles. The prism table is rotatable and connected to a calibrated drum for wavelength measurement.

For calibration, a mercury vapour lamp is used as the reference source. In the emission experiment, the source is a DC arc lamp with replaceable metal electrodes (such as copper and brass). In the absorption experiment, an incandescent lamp (60–100 W) serves as the white light source, and a sealed glass tube containing iodine crystals provides iodine vapour when heated.

A regulated DC power supply, arc stand, and spirit level are used to ensure alignment. The complete arrangement is shown schematically in Fig. 2.

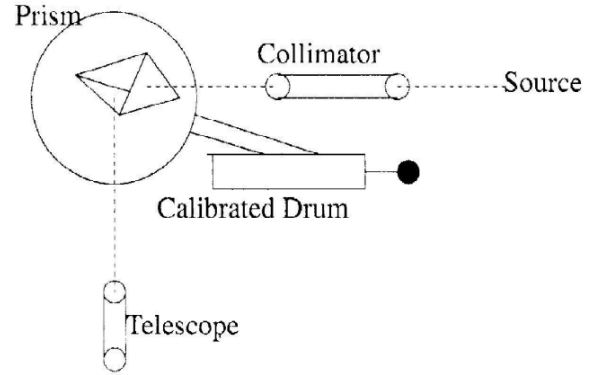


FIG. 2. Schematic diagram of the experimental setup using Constant Deviation Spectrometer.

IV. OBSERVATIONS

The observations in this experiment consist of two parts: calibration of the Constant Deviation Spectrometer using the mercury lamp, followed by measurement of the spectral lines of metals (emission) and iodine vapour (absorption).

For calibration, the observed drum readings (λ_{obs}) corresponding to known mercury spectral lines (λ_{given}) are recorded. A calibration curve is plotted between λ_{given} and λ_{obs} , and the fitted relation is used to obtain the corrected wavelength λ_{corr} of any unknown spectral line.

For the absorption spectrum of iodine vapour, narrow dark absorption bands are observed. The positions of these absorption bands are noted as λ_{obs} , corrected using calibration to λ_{corr} , and then converted into wavenumbers ($\tilde{\nu} = 1/\lambda$). Consecutive differences in wavenumber ($\Delta\tilde{\nu}$) are used to estimate vibrational spacing and the force constant of the molecule.

TABLE I. Calibration data for Hg source.

S. No.	$\lambda_{\text{given}} (\text{\AA})$	$\lambda_{\text{observed}} (\text{\AA})$
1	5460	5460
2	5790	5750
3	5790	5780
4	5960	5950
5	6150	6100
6	6200	6150
7	6230	6210
8	6910	6870

V. DATA ANALYSIS

A. Least square fitting

We analyze the experimental data by fitting a straight line of the form

$$Y = aX + b,$$

where a is the slope and b is the intercept. Applying the least squares method [2] yields the best-fit values of a and b that minimize the squared deviations between the observed and fitted data. The complete computational implementation, including the least-squares routine and error analysis, is provided in the code repository [3].

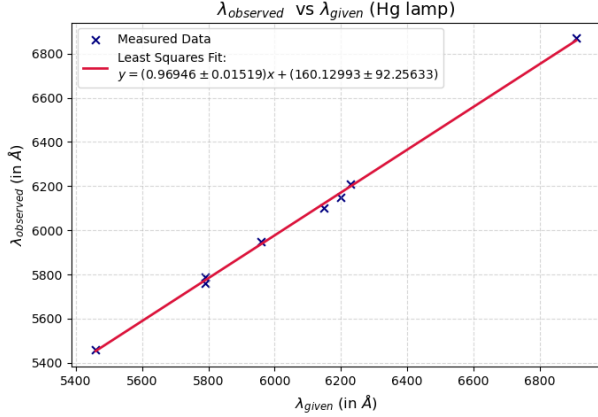


FIG. 3. Least-squares fit for calibration Hg source

The uncertainties in slope and intercept obtained from the graph is calculated as follows:

$$\delta Y = \sqrt{\frac{\sum (Y_n - Y_i)^2}{N - 2}}, \quad (10)$$

$$\delta a = \delta Y \sqrt{\frac{\sum X^2}{(N \sum X^2) - (\sum X)^2}}, \quad (11)$$

$$\delta b = \delta Y \sqrt{\frac{N}{(N \sum X^2) - (\sum X)^2}}, \quad (12)$$

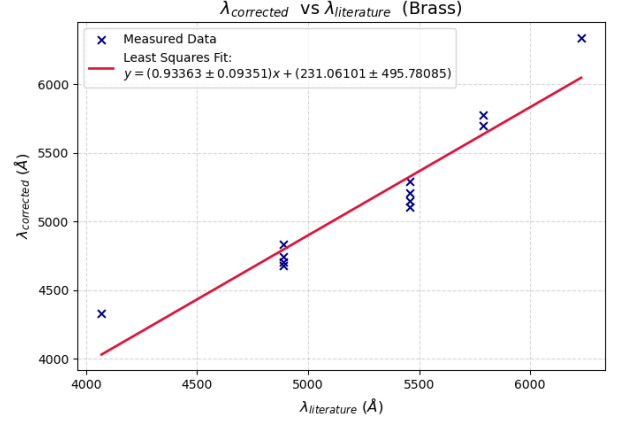


FIG. 4. Least-squares fit for Brass metal.

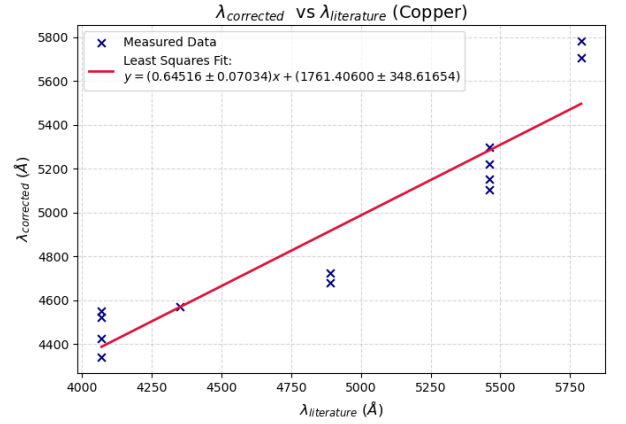


FIG. 5. Least-squares fit for Copper metal

B. Calculation of bond dissociation energy and force constant

1. Bond dissociation energy in the excited state.

From the absorption series, we take the band origin (first observed vibronic line) as $\tilde{\nu}_{\min} = 15979.0 \text{ cm}^{-1}$ and the observed convergence/limit as $\tilde{\nu}_{\max} = 18771.0 \text{ cm}^{-1}$. The approximate dissociation energy measured from the $v' = 0$ level in the excited electronic state (in wavenumbers) is

$$\begin{aligned} D_0(\text{cm}^{-1}) &= \tilde{\nu}_{\max} - \tilde{\nu}_{\min} \\ &= 18771.0 - 15979.0 \\ &= 2792.0 \text{ cm}^{-1}. \end{aligned}$$

Converting to electron volts using $1 \text{ eV} = 8068 \text{ cm}^{-1}$ (manual),

$$D_0(\text{eV}) = \frac{2792.0}{8068} = 0.3461 \text{ eV}.$$

TABLE II. Corrected Wavelengths and Calculated Quantities for Iodine Absorption Spectrum

Sn. No.	$\lambda_{\text{observed}}$ (Å)	$\lambda_{\text{corrected}}$ (Å)	$\bar{\nu}_e$ (cm ⁻¹)	$\Delta \bar{\nu}_e$ (cm ⁻¹)	Energy (eV)
1	6290	6258.0	15979.0	N/A	1.981
2	6250	6219.0	16079.0	100	1.994
3	6220	6190.0	16155.0	76	2.003
4	6180	6151.0	16256.0	102	2.016
5	6140	6113.0	16360.0	103	2.030
6	6090	6064.0	16490.0	131	2.045
7	6050	6025.0	16597.0	106	2.058
8	6010	5987.0	16704.0	108	2.071
9	5970	5948.0	16813.0	109	2.085
10	5940	5919.0	16896.0	83	2.095
11	5890	5870.0	17035.0	140	2.109
12	5860	5841.0	17120.0	85	2.123
13	5820	5802.0	17234.0	114	2.137
14	5790	5773.0	17321.0	87	2.148
15	5750	5735.0	17438.0	117	2.162
16	5730	5715.0	17497.0	59	2.169
17	5700	5686.0	17587.0	89	2.180
18	5670	5657.0	17677.0	90	2.192
19	5640	5628.0	17769.0	91	2.203
20	5610	5599.0	17861.0	92	2.214
21	5580	5570.0	17954.0	93	2.226
22	5550	5541.0	18048.0	94	2.238
23	5520	5512.0	18144.0	95	2.250
24	5490	5482.0	18240.0	96	2.261
25	5470	5463.0	18305.0	66	2.272
26	5440	5434.0	18403.0	98	2.282
27	5420	5415.0	18469.0	66	2.290
28	5400	5395.0	18535.0	66	2.299
29	5370	5366.0	18635.0	100	2.310
30	5350	5347.0	18703.0	68	2.319
31	5330	5327.0	18771.0	68	2.327

TABLE III. For metal Brass

S. No.	$\lambda_{\text{observed}}$ (Å)	$\lambda_{\text{corrected}}$ (Å)	$\lambda_{\text{literature}}$ (Å)
1	6370	6336	6230
2	5790	5773	5790
3	5710	5696	5790
4	5290	5289	5460
5	5210	5211	5460
6	5150	5153	5460
7	5100	5104	5460
8	4820	4832	4890
9	4730	4746	4890
10	4690	4706	4890
11	4660	4678	4890
12	4300	4329	4070

TABLE IV. For metal copper

S. No.	$\lambda_{\text{observed}}$ (Å)	$\lambda_{\text{corrected}}$ (Å)	$\lambda_{\text{literature}}$ (Å)
1	6370	6336	6230
2	5790	5773	5790
3	5710	5696	5790
4	5290	5289	5460
5	5210	5211	5460
6	5150	5153	5460
7	5100	5104	5460
8	4820	4832	4890
9	4730	4746	4890
10	4690	4706	4890
11	4660	4678	4890
12	4300	4329	4070

TABLE V. Calibration least squares fit

i	x	y	x ²	xy
1	5460.0	5460.0	29811600.0	29811600.0
2	5790.0	5760.0	33524100.0	33350400.0
3	5790.0	5790.0	33524100.0	33524100.0
4	5960.0	5950.0	35521600.0	35462000.0
5	6150.0	6100.0	37822500.0	37515000.0
6	6200.0	6150.0	38440000.0	38130000.0
7	6230.0	6210.0	38812900.0	38688300.0
8	6910.0	6870.0	47748100.0	47471700.0
Σ	48490.0	48290.0	295204900.0	293953100.0

TABLE VI. least square fitting for Brass

i	x	y	x ²	xy
1	6230.0	6336.0	38812900.0	39473280.0
2	5790.0	5773.0	33524100.0	33425670.0
3	5790.0	5696.0	33524100.0	32979840.0
4	5460.0	5289.0	29811600.0	28877940.0
5	5460.0	5211.0	29811600.0	28452060.0
6	5460.0	5153.0	29811600.0	28135380.0
7	5460.0	5104.0	29811600.0	27867840.0
8	4890.0	4832.0	23912100.0	23628480.0
9	4890.0	4746.0	23912100.0	23207940.0
10	4890.0	4706.0	23912100.0	23012340.0
11	4890.0	4678.0	23912100.0	22875420.0
12	4070.0	4329.0	16564900.0	17619030.0
Σ	63280.0	61853.0	337320800.0	329555220.0

TABLE VII. Copper least squares fit

i	x	y	x ²	xy
1	4070.0	4338.0	16564900.0	17655660.0
2	4070.0	4426.0	16564900.0	18013820.0
3	4070.0	4523.0	16564900.0	18408610.0
4	4070.0	4552.0	16564900.0	18526640.0
5	4350.0	4571.0	18922500.0	19880350.0
6	4890.0	4679.0	23912100.0	22880130.0
7	4890.0	4726.0	23912100.0	23110140.0
8	5460.0	5104.0	29811600.0	27867840.0
9	5460.0	5153.0	29811600.0	28135380.0
10	5460.0	5186.0	29811600.0	28284960.0
11	5460.0	5298.0	29811600.0	28927080.0
12	5790.0	5705.0	33524100.0	33031950.0
13	5790.0	5783.0	33524100.0	33483570.0
Σ	63830.0	64079.0	319309000.0	318431510.0

2. Average vibrational spacing and force constant.

From the table of consecutive wave-number differences $\Delta\tilde{\nu}_i$ (excluding the first N/A entry) the mean spacing is

$$\Delta\tilde{\nu}_{\text{avg}} = 93.03 \text{ cm}^{-1}.$$

We know, μ is the reduced mass of I_2 . Using the atomic

mass of iodine

$$\begin{aligned} m_{\text{I}} &= 126.90447 \text{ u} \\ (1 \text{ u} &= 1.660539 \times 10^{-27} \text{ kg}) \\ \mu &= \frac{m_{\text{I}}}{2} = \frac{126.90447 \times 1.660539 \times 10^{-27}}{2} \\ &= 1.05365 \times 10^{-25} \text{ kg}. \end{aligned}$$

Treating the excited-state vibrational motion approximately as harmonic, the (angular) vibrational frequency is $\omega = 2\pi c \Delta\tilde{\nu}_{\text{avg}}$ where c is the speed of light (m s^{-1}) and $\Delta\tilde{\nu}_{\text{avg}}$ must be converted to m^{-1} by multiplying by 100. Substituting numerical values,

$$\begin{aligned} f &= 4\pi^2 (1.05365 \times 10^{-25}) (3 \times 10^8 \times (93.03 \times 100))^2 \\ &\approx 32.36 \text{ N m}^{-1}. \end{aligned}$$

3. First Vibrational Energy

The first vibrational energy is given by the energy difference in the first and second absorption spectral line.

$$E = 1.994 - 1.981 = 0.013 \text{ eV}$$

C. Error analysis

The uncertainty in the vibrational spacings can be estimated directly from the scatter of the measured differences $\Delta\tilde{\nu}_i$. Instead of using the instrument least count, we calculate the statistical spread of the observed values. The standard deviation of the set of N measurements is

$$\sigma_{\Delta} = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (\Delta\tilde{\nu}_i - \Delta\tilde{\nu}_{\text{avg}})^2},$$

where $\Delta\tilde{\nu}_{\text{avg}}$ is the average spacing. Since the force constant depends on the mean spacing, the relevant uncertainty is the *standard error of the mean* (SEM), defined as

$$\sigma_{\Delta\tilde{\nu}_{\text{avg}}} = \frac{\sigma_{\Delta}}{\sqrt{N}}.$$

From the data we obtain $\Delta\tilde{\nu}_{\text{avg}} = 93.1 \text{ cm}^{-1}$, $\sigma_{\Delta} = 19.1 \text{ cm}^{-1}$, and hence

$$\sigma_{\Delta\tilde{\nu}_{\text{avg}}} \approx \frac{19.1}{\sqrt{30}} \approx 3.5 \text{ cm}^{-1}.$$

1. Uncertainty in dissociation energy.

The dissociation energy was obtained as $D'_0 = \tilde{\nu}_{\text{limit}} - \tilde{\nu}_0 = 2792 \text{ cm}^{-1}$. Assuming independent errors for the two limiting wavenumbers, the uncertainty is

$$\sigma_{D'_0} \approx \sqrt{2} \sigma_{\Delta\tilde{\nu}_{\text{avg}}} \approx \sqrt{2} \times 3.5 \approx 5.0 \text{ cm}^{-1}.$$

In electron volts, using $1 \text{ eV} = 8068 \text{ cm}^{-1}$,

$$D'_0 = (0.346 \pm 0.001) \text{ eV}.$$

2. Uncertainty in the force constant.

Propagating the error in force constant, we obtain

$$\begin{aligned} \sigma_f &= f \times \frac{2\sigma_{\Delta\tilde{\nu}_{\text{avg}}}}{\Delta\tilde{\nu}_{\text{avg}}} = 32.4 \times \frac{2 \times 3.5}{93.1} \\ &\approx 2.4 \text{ N m}^{-1} \end{aligned}$$

Thus,

$$f = (32.4 \pm 2.4) \text{ N m}^{-1}.$$

3. Conclusion

The standard error of the mean provides a good estimate for uncertainty in difference in consecutive wavenumbers. The dissociation energy is determined with a small error bar ($\pm 0.001 \text{ eV}$), while the force constant is obtained with a moderate relative uncertainty ($\sim 7.5\%$).

VI. RESULTS

The emission spectra for Brass and Copper were observed using the constant deviation spectrometer calibrated to a known Hg source. These plots depict the emission spectra for the metals.

The absorption spectrum of iodine vapour was recorded and analyzed. From the data, the average vibrational spacing was found to be:

$$\Delta\tilde{\nu}_{\text{avg}} = (93.1 \pm 3.5) \text{ cm}^{-1}$$

The bond dissociation energy in the excited state was determined as:

$$D_0 = (0.346 \pm 0.001) \text{ eV}$$

and the force constant as

$$f = (32.4 \pm 2.4) \text{ N m}^{-1}$$

Plots of the calibration curve, the energy level diagram, and the absorption bands were obtained to support these results.

VII. CONCLUSION

The experiment demonstrated the quantized nature of vibrational levels within an electronic state and the convergence of these levels towards the dissociation limit. The obtained plots of the absorption bands and energy level diagram illustrate the concept of vibronic transitions and anharmonicity. The results are consistent with the theoretical expectations outlined in the Morse potential model, thereby validating the spectroscopic method used in this experiment.

In addition, the emission spectra of metals were also recorded using a constant deviation spectrometer, and the characteristic spectral lines of the given samples were observed.

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- [1] National Institute of Science Education and Research (NISER). *Emission Spectra of Metals and Absorption Spectrum of Iodine Vapour*. NISER, 2024. Laboratory Manual for Modern Physics Experiments.
- [2] John R. Taylor. *An Introduction to Error Analysis: The*

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- [3] Aryan Shrivastava. P343—modern-physics-lab. <https://github.com/crimsonpane23/P343---Modern-Physics-lab.git>, 2025.