**Abstract** (250 Words Max)

A high-resolution infrared spectrum of gaseous Carbon Monoxide (CO), taken at room temperature and atmospheric pressure, is examined for characteristic rotational structure between 2000 and 2200 wavenumbers. The rotational structure is assigned, and both quadratic and cubic functions are used comparatively to extract rotational constants of interest. The cubic function is found to have a stronger correlation to experimental data than the quadratic (through a comparison of residuals), likely because the $x^3$ term accounts for centrifugal distortion. Gathered constants are used to determine the equilibrium rotational constant, $B\_e$, as $1.9312(10)$, which is within experimental precision of the existing accepted value of $1.9313$ \cite{NIST}. The usefulness of Carbon Monoxide (and the determined values) to determine the temperature of astronomical bodies is discussed, and basic models using a Boltzmann distribution and experimental data are constructed.

**Introduction** (500 words max)

Carbon monoxide is a very useful compound for chemist and astronomers alike. As a diatomic molecule, its rotational structure is particularly well defined and easy to study, and unlike other common diatomic gasses like Nitrogen and Hydrogen gas ($\textnormal{H}\_2$ and $\textnormal{N}\_2$ respectively) it has a dipole meaning it is IR active. This allows carbon monoxide to be used as a reference point for various applications in cosmology, notably in the determination of the temperature of stellar objects like nebula.

This use case as a reference necessitates the precise analytical measurement of various properties of the molecule. These include, but are not limited to, the various rotational constants ($B\_v$) and bond lengths ($r\_v$), and by extension the equilibrium rotational constant and bond length ($B\_e$ and $r\_e$ respectively). It is through the precise measurement of these properties that we can effectively model the rotational structure of the IR spectrum as a function of temperature, and these models can be in turn applied to spectra gathered from interstellar bodies to predict their temperature.

\begin{equation}

\label{eqn:B}

B\_e = \frac{h}{8 \pi^2 c \mu r\_e^2}, \qquad \mu = \frac{m\_1 m\_2}{m\_1 + m\_2}

\end{equation}

In this experiment, a research grade spectrometer is used to take a precise IR spectrum of gaseous carbon monoxide (CO) at room temperature and pressure; the rotational structure of note (between about 2000 and 22000 wavenumbers) is then assigned, with P and R branches being identified (reference figure \ref{fig:transitions}). A curve is then fitted to the data to extract $B\_1$, $B\_0$ and $\omega$, which are then in turn used to calculate $B\_e$ and $r\_e$. These values are compared to published literature to gauge experimental accuracy and precision.

This process is repeated for quadratic and cubic fits, and the two are quantitively and qualitatively compared. The data is then used to make a basic model based on a Boltzmann distribution that can be used to predict the temperature of stellar bodies. This model is ‘sanity checked’ by using it to calculate what the temperature of the sample the spectra was gathered from and comparing this to expectations of room temperature.

**Experimental Methods**

Data was recorded using a {SPECTROMETER NAME} FT IR spectrometer, using a high resolution and by averaging 64 scans to ensure usable, high-resolution data.

In order to correctly model the global precession of the data, both a cubic and a quadratic function were used and compared. These functions were defined as follows in \ref{eqn:fit}, with the quadratic version simply emitting the cubic term, i.e., $ D = 0$. Note that $D$ is just an arbitrary constant, whose physical meaning will be discussed later.

Data processing was done largely in \textsc{Python 3}, with \textsc{Mathematica} being used for some algebra and unit conversions. \textsc{SciPy} ( and several of its daughter packages), \textsc{NumPy} and \textsc{Matplotlib} were used extensively. Python code, raw data , {\LaTeX} files and illustrations can be found on \textsc{GitHub}\cite{GitHub}. Error handling was done natively within these packages.

**Results** (1500 words Max with discussion)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **Experimental (x3)** | **Experimental (x2)** | **Literature [1][2][3]** | **Units** |
|  | 1.9224(10) | 1.8998(14) | 1.9225 | cm-1 |
|  | 1.9054 (10) | 1.9172(14) | 1.9051 | cm-1 |
|  | 1.9312(10) | 1.9260(14) | 1.9313 | cm-1 |
|  | 0.0174(15) | 0.0175(19) | 0.0175 | cm-1 |
|  | 2143.190(13) | 2143.192(32) | 2169.814 | cm-1 |
|  | 1.1282(15) | 1.1295(80) | 1.1283 | Angstrom |

**Sum of Residual Squares**

|  |  |
| --- | --- |
| **Cubic** | **Quadratic** |
| 0.0291099 | 0.302497 |

Peaks were assigned as shown in figure \ref{fig:spectra}. The function in \ref{eqn:fit} was then fitted to extract $B\_0$, $B\_1$ and $\omega$ for both the quadratic and cubic case, with uncertainties from the fitting. These values were then used to calculate $B\_e$ and $\alpha\_e$ by solving $B\_\nu = B\_e - \alpha\_e \left( \nu + 0.5 \right)$ for $\nu = 0$ and $1$ simultaneously, Then, equilibrium bond length was calculated using \ref{eqn:B}. More details can be found in the experimental notes\cite{notes}. The results are shown in table \ref{tab:results}, and the cubic fit is shown graphically in figure \ref{fig:Cubic}.

To further investigate the two models, it is rescissory to compare their accuracies by calculating their respective sum of residuals. We find that the cubic and quadratic fits have a residual sum of squares of $0.0291$ and $0.3025$ respectively, within the context of absorbance values within about $0.05$ and $0.35$. This is favourable to the cubic model, and this trend continues when we plot the residuals as in figure \ref{fig:Residuals}.

It should be clear that the residuals of the quadratic plot have a clear cubic pattern; this result suggests that adding a cubic term would be much more appropriate for this data. This conclusion concurs with the conclusions from both the residual comparison and with the relative accuracy of the cubic model with regards to data from literature.

Finally, it is useful to attempt to fit a Boltzmann distribution to the intensity of the R branch to extract thermal data. Fitting equation \ref{eqn:Boltz} to the R branch data exclusively yields the following plot (figure \ref{fig:Thermals}) and a thermal value of $289$ K, or $15.9$ C. This graph will be scrutinised more in the discussion , but for now just note that the fit is far from excellent.

{\it n.b.} in \ref{eqn:Boltz}, $\lambda$ is just some constant of proportionality.

**Discussion** (1500 words combined with results)

**Conclusions** (100 words max)

**References** (use this format)

[1] https://webbook.nist.gov/cgi/cbook.cgi?ID=C630080&Mask=1000#Diatomic

[2]

[3] J. S. Campbell, S. H. Kable, and C. S. Hansen, J. Chem. Phys. 155, 204303 (2021)

T. Engel, 2019*, Quantum Chemistry and Spectroscopy*, 4th edn, Pearson Education, Inc, New York, USA.

National Institute of Standards and Technology (NIST), U.S. Department of Commerce, 2021, *Carbon Monoxide*, NIST Chemistry WebBook, SRD 69, [accessed July 2022](https://webbook.nist.gov/cgi/cbook.cgi?ID=C630080&Mask=1000#Dia77).

[Rank](https://www.sciencedirect.com/science/article/abs/pii/0022285265900482" \l "!), D, [St Pierre](https://www.sciencedirect.com/science/article/abs/pii/0022285265900482#!), A & [Wiggins](https://www.sciencedirect.com/science/article/abs/pii/0022285265900482#!), T 1965, ‘Rotational and Vibrational Constants of CO’, *Journal of Molecular Spectroscopy*, vol. 18, no. 4, [pp. 418-427](https://www.sciencedirect.com/science/article/abs/pii/0022285265900482).

# Mina-Camilde, N, Manzanares, C & Caballero, J 1996, ‘Molecular Constants of Carbon Monoxide at v = 0, 1, 2, and 3: A Vibrational Spectroscopy Experiment in Physical Chemistry’, *Journal of Chemical Education*, vol. 73, no. 8, [pp. 695-826](https://doi.org/10.1021/ed073p804).

# https://doi.org/10.1021/ed073p804

**Appendix**