

An IR investigation of the CO dipole direction and other properties

Author: Kieran Fergus LIM

Practical:

Abstract

The infrared absorption spectra of gaseous carbon monoxide and atmospheric air (background containing carbon dioxide and water vapour) are recorded. The carbon monoxide spectrum is analysed in terms of molecular vibrations and rotations, various molecular properties and parameters, including the carbon-oxygen bond length, are determined from the spectrum.

The novel feature of this exercise is that the spectroscopic information are used to discuss the CO bond order, molecular dipole direction and other properties. An unusual feature is that the first overtone is measured, in addition to the fundamental vibrational transition.

This laboratory exercise illustrates that spectroscopy is a direct probe of molecular properties, which have practical applications. (Spectroscopy is not just an academic exercise in quantum theory.) The observed gas-phase spectra provide direct evidence of quantisation and the bond order. This exercise is the only occasion when students make a measurement of any molecular bond length in the Deakin University undergraduate chemistry program. It is one of the few occasions where a bond binding energy (the "bond strength") is determined. Furthermore, this laboratory exercise gives students the opportunity to gain "hands-on" experience with a Fourier-transform infrared (FT-IR) spectrometer, which is a common analytical technique in industrial and forensic laboratories.

Intended academic level

Undergraduate 3

Duration

1.5 hr reading and pre-lab exercise, 1.5 hr laboratory, 2 hr analysis of results

Outcomes

Students should be able to relate spectroscopic information and concepts to bonding and reactivity concepts in other parts of the chemistry syllabus.

Students will learn to operate a FTIR spectrometer.

Students will learn to transfer gases from gas cylinders to sample cells.

Students will learn to collate, display and analyse data using a spreadsheet.

Students should understand that each rovibrational spectrum in this exercise corresponds to a "single peak" in the more extended IR spectra, which are encountered in the typical synthetic laboratory.

Students should appreciate that molecular energy levels are quantised.

Students should understand that absorption of a photon results in a transition

from a lower-energy level to a higher-energy level. The quantised changes in molecular energy result in spectral peaks. The increase in molecular energy corresponds to the absorbed photon's energy.

Students should understand that symmetry constraints ("selection rules") determine which energy gaps can correspond to an "allowed" transition.

Materials

FT-IR spectrometer

10 cm gas cell (salt windows)

Carbon monoxide gas

Costs

Major cost is FT-IR spectrometer of between USD\$7000-15000.

Ongoing costs is minimal

Further comments

Detailed student notes, technical notes, demonstrator notes, evaluation of teaching and learning outcomes are available.

Reading

N/A

Contact details

Dr Kieran F Lim ()

School of Biological and Chemical Sciences, Deakin University, Geelong
3217 AUSTRALIA

E-mail: lim@deakin.edu.au; Telephone: int+[61]-(3)-5227-2146; Fax: int+[61]-(3)-5227-1040