N91-13336

Analysis of Pressure-Broadened Ozone Spectra in the 3-μm Region

Eleanor S. Prochaska
Western Carolina University
Cullowhee, N.C.

The presence of a layer of photochemically produced ozone in the stratosphere has been recognized for some time. This ozone layer is vital to life on earth, as it provides a shield from harmful ultraviolet radiation that is a normal component of sunlight. During the mid 1980's, a deficit in the ozone layer was observed over the Antarctic continent. Since that time, the need to observe and monitor the ozone content in the stratosphere has been the motivation of considerable scientific effort. More recently, the effects of increased atmospheric ozone amounts at the earth's surface have been found to be of significant environmental concern. Spectroscopic methods are the basis for remote sensing techniques to measure atmospheric content of many species, including ozone, on global and regional scales. As technology continues to improve, the understanding of the spectra of these species becomes increasingly important in allowing accurate retrieval of data obtained by remote sensing techniques.

The Molecular Spectroscopy Lab at NASA-Langley has been involved in a long term effort to carefully and fully characterize the infrared spectra of small molecules of atmospheric interest, including methane, water vapor, ozone, and their isotopic counterparts. High resolution gas phase infrared spectra are obtained using both a tunable diode laser system, and the McMath Fourier transform spectrometer at the Kitt Peak Solar Observatory. Spectra are obtained at various pressures and temperatures for pure gas samples, and for samples containing mixtures of the species of interest in nitrogen, oxygen, or air. From these spectra, using a non-linear least squares fitting technique, spectral parameters of position, intensity and half-width have been determined for varying laboratory conditions that approximate atmospheric conditions experienced in remote sensing situations. These parameters are of interest in theoretical studies of these species, as well as in allowing more accurate interpretation of remote sensing data.

The current work in the lab involves the analysis of a series of McMath FTIR spectra of ozone broadened by mixing with air, nitrogen or oxygen. Each spectrum covers the region from 2396 to 4057 cm^{-1}. Each vibrational band is analysed by first dividing its region into small (0.5 to 2.0 cm^{-1}) intervals containing a few well isolated absorption lines of reasonable intensity. Each of these small intervals is "fit" by multiple iterations of the non-linear least squares program until residuals (difference between calculated and observed spectrum, as percent of the strongest intensity in the interval) are minimized to a "reasonable" value which corresponds to the noise level of the measured spectrum. Position, intensity and half-width are recorded for later analysis. Half-widths are normalized for each pressure and a pressure broadening coefficient is determined for each absorption line.

This summer, intervals for the $3\nu_3$ ozone band in the region from 3000 to 3060 wavenumbers are being examined. In particular, analysis of the region from 3000 to 3030 wavenumbers has been completed for all ten experimental conditions, and broadening coefficients have been found for over 200 lines of the $3\nu_3$ region for the three broadening gases. The remaining 3030 to 3060 wavenumber region remains to be fitted before a final analysis of line broadening in the $3\nu_3$ ozone band can be completed.

Appendices:

1. Ozone Broadening Experimental Conditions
2. Comparison of Halfwidths for O_3 Line at 3010.9152 cm^{-1}. (comparable results have been obtained for each line that has been studied in the ozone $3\nu_3$ region)

OZONE BROADENING

EXPERIMENTAL CONDITIONS

Gas Mixture	Volume Mixing Ratio	Pressure
O_3 in Air	4.16%	105.0 torr
	2.13	204.9
	1.43	305.0
	1.08	405.3
O_3 in N_2	4.54	105.1
	2.33	205.1
	1.57	304.2
O_3 in O_2	5.18	106.3
	2.67	206.2
	1.80	306.4

All spectra were recorded using a 2.39 m cell at 26 ± 1°C, and 0.01 cm^{-1} resolution.

COMPARISON OF HALFWIDTHS FOR O_3 LINE AT 3020.9152 CM^{-1}