VIBRATIONAL ENERGIES AND ROTATIONAL CONSTANTS OF $^{12}C^{16}O_2$

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The positions of about 5000 spectral lines of $^{12}C^{16}O_2$ have been accurately measured with a multispectrum nonlinear least squares fitting technique[a]. The spectra were obtained with the Fourier Transform Spectrometer at the McMath-Pierce facility of the National Solar Observatory at Kitt Peak at a resolution of 0.01 cm^{-1} with a natural carbon dioxide sample. These positions are from the 1830 to 4000 cm^{-1} spectral region and include about 100 vibration-rotation bands. The wavenumber scales of the spectra were carefully calibrated to the same standard, making the data set homogeneous. There are approximately 60 vibrational levels represented by the bands and over 50 of them are tied together by combinations of observed bands. All of the vibrational energies and rotational constants for these bands have been determined in one global solution. The individual positions were weighted according to the uncertainties of the positions as determined by the spectrum fits. For each band at least one of the vibrational levels is constrained by most or all of the other bands. As a result, this produces values superior to those from single band solutions. The uncertainties in the differences of the various combinations of parameters are also readily available using the derived uncertainties in the parameters and the correlations between parameters.

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