

A RE-EXAMINATION OF THE QUANTITATIVE INFRARED ABSORPTION CROSS-SECTIONS OF ISOBUTANE

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Recently published work^c has called into question the absolute infrared absorption cross-section values for isobutane presented in the Northwest Infrared (NWIR) database. As a result, we have remeasured these cross-sections. In all, four data sets were acquired, analyzed and compared to the original NWIR database with excellent agreement. All new data sets were measured with a nominal pathlength of 20 cm and sample temperature of 25.0 °C. Three data sets were acquired using a Bruker IFS 125HR spectrometer equipped with a HgCdTe detector. Spectra were first recorded between 600 and 5000 cm^{-1} at 0.112 cm^{-1} instrument resolution using thirteen burdens of isobutane (0.3 to 22 Torr), each pressure-broadened to one atmosphere using N_2 gas. The second and third data sets were recorded using thirteen burdens of isobutane (0.1 to 23 Torr), at an instrument resolution of 0.01 cm^{-1} . A spectrum of each sample was recorded neat and then recorded pressure-broadened to one atmosphere using N_2 gas, producing two data sets. A fourth data set, using eleven burdens of neat isobutane (0.5 to 23 Torr) was recorded using a Bruker IFS 66v/S with a DTGS detector. Spectra were recorded between 400 and 6500 cm^{-1} at 2 cm^{-1} instrument resolution. Each of the four data sets was fitted using a weighted linear least squares algorithm and resulted in a “composite” \log_{10} absorbance spectrum of isobutane with concentration-pathlength units of $\text{ppm}^{-1} \text{m}^{-1}$. The wavenumber axis is in units of cm^{-1} . For the 125HR data sets, the integrated band strengths for both the C-H stretch and CH_2 bend regions are within 2% of the original NWIR integrated band strengths, and the 66v/S integrated band strengths for both spectral regions are within 5% of the NWIR data. The agreement between the original and new cross-section data is close to the original experimental error, 3%, reported for the NWIR database.

^aRetired.

^bRetired.

^cDM Hewett, PF Bernath, BE Billinghurst. 2019 “Infrared absorption cross sections of isobutane with hydrogen and nitrogen as broadening gases.” *Journal of Quantitative Spectroscopy and Radiative Transfer* 227:226–229.