

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for H2O2_25T

Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K

Equivalent concentration x path-length of composite spectrum: 1.4004×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Hydrogen Peroxide; H2O2; Albone; Albone DS; Dihydrogen dioxide; Elawox; Hydrogen dioxide; Hydrogen oxide; Hydrogen peroxide (H2O2); Inhibine; Lensept; Perhydrol; Perossido di idrogeno; Peroxaan; Peroxyde d'hydrogene; Superoxol; T-Stuff; Wasserstoffperoxid; Waterstofperoxyde; Albone 35; Albone 50; Albone 70; Hydrogen peroxide solution; Interrox; Kastone; Perone 30; Perone 35; Perone 50; UN 2014; HOOH; Dioxogen; Genoxide; Glycozone; High-strength hydrogen peroxide; Hioxy; Hioxyl; Hydroperoxide; Hydrozone; Lensan A; Mirasept; Oxogen; Oxydol; Oxysept; Oxzone; Pegasyl; Percarbamid; Perone; Peroxal; Peroxan; Peroxide; Peroxol; Peroxyl; Proxy; Pyrozone; Truzone
H₂ O₂ : [7722-84-1]
- Physical properties: MW=34.0147 g/mole, mp= -0.89° C, bp=150.2° C, Density (25 C) = 1.454 g/cm³
- Supplier and stated purity: Aldrich, 50%. Distilled to 82.78% by weight in house.
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 6.000, 1.000, 7.000, 2.500, 4.500, 1.500, 5.500 and 3.500.
- Individual samples at equivalent pressures of 0.062651, 0.187954, 0.031326, 0.219164, 0.078252, 0.140854, 0.046964, 0.172178 and 0.109568 Torr. Final data is a composite spectrum.
- Preparation: 50% hydrogen peroxide was distilled in house to 82.78% by weight which is 70.698% by volume.

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 7,500 to 510 cm⁻¹ (1.3333 to 19.61 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm⁻¹
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm⁻¹
- Interferogram zero-fill: 2X
- Apodization: Boxcar
- Phase correction: Mertz
- Beam splitter: Potassium bromide (KBr)
- IR source: Carbide glowbar (22 V)
- Scanner velocity: 60KHz (HeNe crossing frequency)

- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: 15798 to 0 cm^{-1}

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 9 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =8.13%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.0000016 + 3.59034 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and 37.95% water features were removed via spectral subtraction and the composite spectrum was corrected by rescaling of 1.61166.
- Baseline correction via 7th order polynomial subtraction