

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams: sw.sharpe@pnl.gov

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Composite spectrum for 23BUTDI_25T

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

Equivalent concentration x path-length of composite spectrum: 3.5443×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2,3-Butanedione; Biacetyl; Butane-2,3-dione; Butanedione; Diacetyl; Dimethyl diketone; Dimethyl glyoxal; 2,3-Butadione; 2,3-Diketobutane; (CH₃CO)₂; Glyoxal, dimethyl-; Butadione; UN 2346; 2,3-Dioxobutane; 2,3-butandione; 2,3 Butandione (Diacetyl); 2,3-butanedione (diacetal); 2,3-Butanedione (Diacetyl); 2,3-butanodione; Butan-2,3-dione; butane-2,3-dione (diacetyl); Butanedione (diacetyl) C₄H₆O₂: [431-03-8]
- Physical properties: MW=86.0892 g/mole, mp= -2.4. C, bp=88.0° C, Density (25 C) 0.975 g/cm³.
- Supplier and stated purity: Aldrich 97 %
- Sample class: I (PNNL scale).
- Temperature of sample: 24.99 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr.
- Individual samples at 1.22644, 2.1878, 4.7350, 3.2420, 0.56633, 32.50, 16.17, 8.3000, 25.60 and 12.1710 Torr. Path length= 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 580 cm⁻¹ (1.538 to 17.24 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 10 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =0.60%, Type B \leq 3%

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000135+8.5741\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide, water and 0.56% ethyl acetate features were removed via spectral subtraction and the composite spectrum was corrected by a rescaling multiplier of 1.005582.
- Baseline correction via 7th order polynomial subtraction.