

All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, February, 2000

Composite spectrum for CO_50T

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

Sample Conditions-

- Chemical name and CAS number: Carbon monoxide, CO : [630-08-0]
- Physical properties: M.W. 28 amu, F.P. -207C, B.P. -190C
- Supplier and stated purity: Air Products and Chemicals, Inc., 99.99%
- Sample class: I (PNNL scale).
- Temperature of sample: 50.03 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.3200, 0.44193, 0.95435, 153.11, 51.59, 9.6671 and 2.1065 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, temperature controlled environment, evacuated optics bench
- Spectral range: 6,500 to 600 cm^{-1} (1.534 to 16.667 microns)
- Instrumental resolution (interferogram): 0.112 cm^{-1}
- Spectral intervals after 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: 9 (Bruker arbitrary)
- 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 ($\alpha = 0.85$, $\beta = 530$)
- Composite spectrum created from 7 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 = 0.92%, Type B = 3%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide removed by spectral subtraction. Baseline straightened by subtraction of 7th-order polynomial.