All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for CO_25T
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: 25.00 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 46.22, 9.9655, 182.76, 366.12, 0.56591, 0.32968, 1.9909, 0.90881, 0.78680 and 100.68 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, $\varepsilon$=530)
- 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 $T^2$ (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.68%, Type B ≤ 3%
- Frequency correction: V(corrected) = V(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 $7^{th}$-order polynomial.