

Ethane PSEUDO-LINELIST

There are two C₂H₆ pseudo linelists:

c2h6_2953_3018.101

c2h6_1350_1496.101

The former is a hodge-podge described in:

http://mark4sun.jpl.nasa.gov/report/c2h6_spectroscopy.pdf

Basically it consists of:

- a quantum-mechanically-derived linelist for the PQ3-branch at 2976 cm⁻¹ which was included in HITRAN2004
- linelists kludged by Linda Brown 20 years ago for ATMOS covering the 9 strongest PQ-branches from 2973-3001 cm⁻¹. These were in HITRAN2000 but not in HITRAN2004
- linelists kludged by Geoff Toon for the 2953-2973 and 3001-3018 cm⁻¹ regions containing weaker PQ-branches

The latter linelist is described below.

INTRODUCTION.

This document gives information on a C₂H₆ pseudo-linelist derived at JPL in May 2005. The linelist was created based on on 3 laboratory spectra taken at the Pacific Northwest National Laboratory (PNNL), provided by Steven Sharp, and one high-resolution spectrum recorded at Kitt Peak National Solar observatory by Linda Brown.

The pseudo-linelist covers the 1350-1496 cm⁻¹ region containing the nu₆ band, which is missing from HITRAN_2004.

[HITRAN_2004 contains C₂H₆ lines for the nu₁₂ (822 cm⁻¹), nu₁ (2954 cm⁻¹), and nu₁₀ (2985) bands, but not the nu₆ (1379 cm⁻¹)].

The measurement conditions for these spectra are tabulated below.

File	Temp	P_tot	P_c2h6	l_cell	spacing	res.
"c2h6pnnl_50C"	323.2	760.5	2.14	0.20	0.0603	0.1125
"c2h6pnnl_25C"	298.2	760.5	2.14	0.20	0.0603	0.1125
"c2h6pnnl_05C"	278.2	760.5	2.14	0.20	0.0603	0.1125
"r850530R0.017"	299.0	5.0	5.00	0.25	0.0029	0.0060

Temp - Temperature in K

P_tot - total pressure in torr

P_ch3cn - CH₃CN partial pressure in torr

l_cell - cell length in m

spacing - spectral point spacing in cm⁻¹

res. - spectral resolution in cm⁻¹

DESCRIPTION.

The laboratory transmittance spectra were simultaneously fitted (using the GFIT algorithm) by iteratively adjusting the strengths and ground-state energies of the pseudo-lines.

Due to the high resolution of the Kitt Peak spectrum

a pseudo-line spacing of 0.0025 cm⁻¹ was chosen.

An air broadened halfwidth of 0.068 cm⁻¹/atm and a

self broadened halfwidth of 0.300 cm⁻¹/atm

was assumed for all pseudolines.

The current version of the pseudo-linelist covers a frequency range between 1350 and 1496 cm^{-1} . This is only part of the ethane band around 1500 cm^{-1} . This region was chosen as the Kitt Peak spectrum was contaminated with a significant amount of water, blacking out several spectral regions beyond 1496 cm^{-1} .

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