Improved spectroscopic parameters of methane in the MIR for atmospheric remote sensing

D. Dubravica[a], M. Birk[b], F. Hase[a], J. Loos[b], M. Palm[c], A. Sadeghi[c], G. Wagner[b]

[a] KIT IMK-ASF BOD, Hermann-von-Helmholtz-Platz 1, 76344 Leopoldshafen, Germany
Tel.: +49 721 608-22434, Fax: +49 721 608-24742, E-mail: darko.dubravica@kit.edu
[b] German Aerospace Center (DLR), [c] University of Bremen

In support of atmospheric remote sensing within NDACC (Network for the Detection of Atmospheric Composition Change), improved spectroscopic data for CH4 have been derived, covering the 2400 to 3000 cm^{-1} spectral region. Laboratory molecular absorption spectra were recorded with the DLR Bruker IFS125HR FTIR spectrometer in combination with a globar source and a long path absorption cell. A first set of measurements with pure methane and low pressures (0.02 – 5.00 mbar) was performed to improve the transition wavenumber, the line intensity and the self-broadened half-width. The second set of measurements was made with a defined air-methane mixture at total pressures (30 – 1000 mbar) relevant for atmospheric observations for fitting air-broadened half-widths and air induced pressure shifts. A retrieval software based on the method of least squares has been developed to adjust the spectroscopic parameters of the methane HITRAN 2012 line list [1]. A few parts of the energy term scheme resulting from the HITRAN 2012 lower state energy and the associated transition wavenumber were replaced by values predicted by the MIRS software [2,3] in order to improve first-guess values.

The fitting routine performs multi-spectra fits, and handles line parameters of several lines at a time. The spectra and residuals of two exemplary microwindows used by the NDACC are presented to compare the original HITRAN values with the modified line list. The current fits are based on a simple Voigt lineshape model.

[1] http://www.cfa.harvard.edu/hitran/
[2] A. V. Nikitin et al., JQSRT **2003**, 82, 239-249
[3] http://xeon.univ-reims.fr/MIRS/