Update the broadening coefficients for CH_3Cl

First, a couple of issues that have been identified in the 3 μm region of CH_3Cl in HITRAN2012 were fixed. In particular, the air-broadening temperature dependencies of the lines around 3 μm used to be negative while they are supposed to be positive. And all of the lines in the 3 μm band had a shift of -0.02 cm^{-1}/atm. We compared the calculated spectra from the HITRAN database with the PNNL database and the results shows that such a strong shift of the lines appears to be incorrect. Therefore; we set the shift to be 0.00 and n_{air} to be positive around 3 μm. In a similar fashion we removed the shift of -0.02 cm^{-1}/atm in the $\nu_2+\nu_6$ band around 5 μm.

Both experimental measurements and calculations have been made of the self- and air-broadening coefficients of CH3Cl recently. The available results have been collected and evaluated to update the database for CH3Cl.

The details of the updated values for line shape parameters are described as follows:

For self-broadening coefficients of CH_3Cl:

1. The $CH_3{}^{35}Cl$ self-broadening coefficients at reference temperature 296K for the R-branch ($\Delta K=0$) are computed by a semi-empirical(SE) method[1]. We use these semi-empirical calculations for R-branch and P-branch (for all ΔK values) lines in all of the bands of the two isotopologues $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ considered in the database. The average value of RMS-deviations of the SE CH_3Cl self-broadening coefficients from the experimental data of Ref.[2] is 0.0408cm^{-1}/atm. We used the ratio of the individual half-widths to this value to estimate the uncertainties and determine a corresponding error code.
   Only R-branch transitions for quantum numbers of $0\leq J\leq 70$ and $0\leq K\leq 20$ are available from Ref. [1]. The empirical relation enables evaluation of the P-branch and Q-branch broadening coefficients from those of the R-branch.
   $$\gamma_P(J,K) \approx \gamma_R(J-1,K) \approx \gamma_Q(J,K)$$
2. Then we also use the experimental results collected from papers to the same J- and K-transitions.
   (a) Experimental results from Ref.[3] have been used for the same ISO, (J',K'-J",K") transitions in all of the bands.
   error_code = 5 and ref_code = 4

   (b) Experimental results from Ref.[2] are for both pure rotational (J= 6, 31, 37, 40, 45, 50) and ν_1 bands of CH_3Cl. The measured self-broadening coefficients for pure rotational transitions have been used for the corresponding transitions in the database. We also use the experimental results of the ν_1 band for the transitions sharing the same quantum numbers.

For air-broadening coefficients of CH_3Cl:

1. The air-broadening coefficients and associated temperature exponents for both $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ rovibrational transitions of R-branches($\Delta K=0$) are calculated by a semi-classical(SC) approach[4]. We use the SC calculation for R-branch and P-branch (for all ΔK values) lines in all of the bands.

$$\gamma_P(J,K) \approx \gamma_R(J-1,K) \approx \gamma_Q(J,K)$$

2. Experimental results from Ref.[5] and Ref.[6] have also been used for the transitions sharing the same quantum numbers.

For air-broadening temperature dependencies of CH_3Cl:

The air-broadening temperature exponents have also been updated from the SC calculations of Ref.[4]. Only the rovibrational transitions of R-branches and P-branches are calculated. The values for Q-branches were kept at the constant value of 0.70.

$$N_P(J,K) \approx N_R(J-1,K)$$

Update line lists for CH_3Cl in the 1900-2600 cm^{-1} spectral region

There are 43147 line parameters for which were calculated based on the recently analyzed [7] Fourier transform spectra in the range of 1900-2600 cm^{-1}. The data is taken from the supplementary file of Ref.[7]. The statistics of the line positions analysis were 4~10 × 10^{-4} cm^{-1} and the RMS of intensity fitting was 7.4% for $CH_3{}^{35}Cl$ and 6.6% for $CH_3{}^{37}Cl$. Therefore, the error code 4 was given for line positions and the error code 5-for line intensities.

The total results are divided into two parts for 36068 lines which has already in the HITRAN2012 and 7079 new lines which need to be added into the database. We also recalculated the Einstein coefficients for the lines which had intensities changed. The broadening parameters of the new lines were calculated the same new algorithm described above.

[1] A.S. Dudaryonok, N.N. Lavrentieva, J.V. Buldyreva, J. Quant. Spectrosc. Radiat. Transf. 130 (2013) 321–326.

[2] C. Bray, D. Jacquemart, N. Lacome, M. Guinet, A. Cuisset, S. Eliet, F. Hindle, G. Mouret, F. Rohart, J. Buldyreva, J. Quant. Spectrosc. Radiat. Transf. 116 (2013) 87–100.

[3] A. Barbouchi Ramchani, D. Jacquemart, M. Dhib, H. Aroui, J. Quant. Spectrosc. Radiat. Transf. 120 (2013) 1–15.

[4] J. Buldyreva, J. Quant. Spectrosc. Radiat. Transf. 130 (2013) 315–320.

[5] M. Guinet, F. Rohart, J. Buldyreva, V. Gupta, S. Eliet, R. a. Motiyenko, L. Margulès, a. Cuisset, F. Hindle, G. Mouret, J. Quant. Spectrosc. Radiat. Transf. 113 (2012) 1113–1126.

[6] J. Buldyreva, L. Margulès, R.A. Motiyenko, F. Rohart, J. Quant. Spectrosc. Radiat. Transf. 130 (2013) 304–314.

[7] A.V. Nikitin, T.A. Dmitrieva, I.E. Gordon, J. Quant. Spectrosc. Radiat. Transf. (2016).

The new HITRAN ref table for CH_3Cl:

Positions

[GlobRef 1038] 8. A.V. Nikitin, T.A. Dmitrieva, I.E. Gordon, "Improved spectroscopic line list of methyl chloride in the 1900-2600 cm-1 spectral region", JQSRT in press (2016).

Intensities

[GlobRef 1038] 9. A.V. Nikitin, T.A. Dmitrieva, I.E. Gordon, "Improved spectroscopic line list of methyl chloride in the 1900-2600 cm-1 spectral region", JQSRT in press (2016).

Half-widths (air)

[GlobRef 1011] 4. J. Buldyreva, "Air-broadening coefficients of $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ rovibrational lines and their temperature dependence by a semi-classical approach", *J Quant Spectrosc Radiat Transf*, **130**, 315-320(2013)

[GlobRef 1012] 5. M. Guinet, F. Rohart, J. Buldyreva, V. Gupta, S. Eliet, R.A. Motiyenko, L. Margul ès, A. Cuisset, F. Hindle, G. Mouret, "Experimental studies by complementary terahertz techniques and semi-classical calculations of N_2- broadening coefficients of $CH_3{}^{35}Cl$", *J Quant Spectrosc Radiat Transf*, **113**, 1113-1126(2012)

[GlobRef 1013] 6. J. Buldyreva, L. Margul ès, R.A. Motiyenko, F. Rohart, "Speed dependence of CH_3 ^{35}Cl–O_2 line-broadening parameters probed on rotational transitions: Measurements and semi-classical calculations", *J Quant Spectrosc Radiat Transf*, **130**, 304-314(2013)

Half-widths (self)

[GlobRef 1014] 3. A.S. Dudaryonok, N.N. Lavrentieva , J.V. Buldyreva, "CH3Cl self-broadening coefficients and their temperature dependence", *J Quant Spectrosc Radiat Transf*, **130**, 321-326(2013)

[GlobRef 1015] 4. A. Barbouchi Ramchani, D. Jacquemart, M. Dhib, H. Aroui, "Line positions, intensities and self-broadening coefficients for the ν_5 band of methyl chloride", *J Quant Spectrosc Radiat Transf*, **120**, 1-15(2013)

[GlobRef 1016] 5. C. Bray, D. Jacquemart, N. Lacome, M. Guinet, A. Cuisset, S. Eliet, F. Hindle, G. Mouret, F. Rohart, J. Buldyreva, " Analysis of self-broadened pure rotational and rovibrational lines of methyl chloride at room temperature", *J Quant Spectrosc Radiat Transf*,

116, 87-100(2013)

Temperature dependence of air-broadened half-width
[GlobRef 1011] 2. J. Buldyreva, "Air-broadening coefficients of $CH_3{}^{35}Cl$ and $CH_3{}^{37}Cl$ rovibrational lines and their temperature dependence by a semi-classical approach", *J Quant Spectrosc Radiat Transf*, **130**, 315-320(2013)