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The abundance of H_2O-O_2 complex in the Earth's atmosphere

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The absorption of solar radiation by collision complex of oxygen is small but significant part of the total budget of incoming short-wave radiation [S. Solomon, et al, 1998]. Equally, the emission and absorption by the van der Waals complexes in the Earth atmosphere may have an impact on the total budget of the earth long-wave radiation if these abundances are high enough. Recently, it has been reported the first observation to observe van der Waals molecule in the Earth's atmosphere [K. Pfeilsticker et al, 2003]. It is difficult to estimate the global distribution of these complexes by observation, because there are only a few spectroscopic data, especially, for the complex including water vapor.

In this paper, we estimated the abundance of the H_2O-O_2 van der Waals complex in the Earth's atmosphere. Oxygen and water vapor are one of most important molecule in earth atmosphere. Recently, Kasai et al. succeeded to record the microwave spectrum of H_2O-O_2 by Fourier-Transform Microwave Spectroscopy combined with the pulsed nozzle super-sonic jet technique [Kasai et al, 2004]. The abundance of H_2O-O_2 van der Waals complex is given by the equilibrium equation with H_2O and O_2 in the Earth's atmosphere.

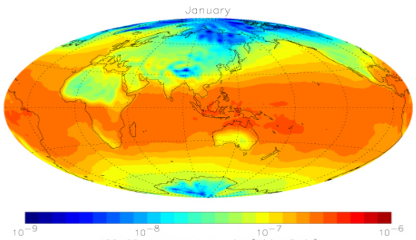
$$[H_2O] + [O_2] <=> [H_2O\text{-}O_2] \qquad (1)$$

The equilibrium constant, $K_p(T)$, is given in the following expression, [Vaida et al, 2000]

$$\frac{\left\{ [P_{\mathrm{H2O\text{-}O2}}] / [P_0] \right\}}{\left\{ [P_{\mathrm{H2O}}] / [P_0] \right\} \left\{ [P_{\mathrm{O2}}] / [P_0] \right\}} = e^{-\Delta G/RT} = K_p(T) \qquad (2)$$

,where $K_p(T)$ is the temperature-dependent equilibrium constant, $P_{H2O\text{-}O2}$, P_{H2O} and P_{O2} are the pressures of the H_2O-O_2 complex, water vapor, and oxygen. P_0 is the reference pressure at each altitude. Hence $[P_{H2O\text{-}O2}]$ / $[P_0]$ is the partial pressure of the complex. ΔG is the Gibbs's free energy. $K_p(T)$ is given by $e^{-\Delta G/RT}$. $\Delta G = \Delta H - T\Delta S$. The ΔH is the function of the binding energy of H_2O and O_2 molecules. ΔS is calculated from the ro-viblational, electronic states of H_2O, O_2 and H_2O-O_2. Accordingly the partial pressure of the H_2O-O_2 is calculated in the way $[P_{H2O\text{-}O2}]/[P_0] = K_p(T)\{[P_{H2O}]/[P_0]\}*\{[P_{O2}]/[P_0]\}$. The water vapor volume mixing ratio vertical profiles, temperature, and pressure were obtained from NCEP data to calculate global distribution of H_2O-O_2 van der Waals complex. The seasonal variations are calculated. One example of the global distribution is shown in Figure. The vmr abundance of H_2O-O_2 van der Waals complex at ground level shows the 10^{-6} order in the equator region and 10^{-8} order in the polar winter region.

The estimated abundance of H_2O-O_2 van der Waals complex



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