Asymmetry of 118 GHz oxygen line in the Earth atmosphere: Pressure shift as a new element in atmospheric lines

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[1] Asymmetry of the atmospheric oxygen 118 GHz line due to the air pressure shift of the center frequency of this line is predicted, and estimations are given for some observation modes. The observability of this atmospheric line asymmetry by the appropriate instruments is shown. The necessity of considering the pressure shift in atmosphere propagation models such as the well-known millimeter wave propagation model (MPM) is demonstrated. Line shift as a new source of information is discussed. At the moment, 183 GHz water and 118 GHz oxygen lines are the only known microwave lines with appreciable air pressure frequency shift that are used for atmosphere sounding. The possible directions of further studies are outlined. *INDEX TERMS:* 6964 Radio Science: Radio wave propagation; 6904 Radio Science: Atmospheric propagation; 6969 Radio Science: Remote sensing; 0994 Exploration Geophysics: Instruments and techniques; 3360 Meteorology and Atmospheric Dynamics: Remote sensing; *KEYWORDS:* millimeter waves, remote sensing, atmospheric oxygen, microwave spectrum, pressure line shift, line asymmetry

1. Introduction

[2] Remote sensing of the Earth atmosphere by ground-based, aircraft-based, and satellite-based microwave sensors is a now widely used practice of great importance for atmosphere studies and weather prediction [e.g., *Schwartz et al.*, 1996; *Klein and Gasiewski*, 2000]. Interpretation of the data obtained from observations is based on the models of wave propagation through atmosphere (the most widely used is the millimeter wave propagation model (MPM) [*Liebe*, 1989; *Liebe et al.*, 1992]) and models of atmosphere. Until recently, only the intensity of the lines and line broadening caused by pressure were taken into account in microwave propagation models and were used as sources of information on temperature, pressure, and atmospheric composition in microwave sounding. Finding the pressure shift of the center frequency of the water 183 GHz [*Pumphrey and Buehler*, 2000] and oxygen 118 GHz [*Tretyakov et al.*, 2001] lines introduces some new elements in the description of the atmosphere lines (as it was not considered, e.g., in the well-known MPM atmosphere propagation model) and gives a new source of information in remote sensing. Oxygen line shift measurements [*Tretyakov et al.*, 2001] have been made in the laboratory using ordinary ambient air under normal atmospheric conditions by the modern methods of resonator spectroscopy [*Krupnov et al.*, 2000]. As for the water vapor line [*Pumphrey and Buehler*, 2000], its shift parameter was obtained by processing the data of microwave limb sounding by Microwave Limb Sounder (MLS) on UARS and Millimeter-wave Atmospheric Sounder (MAS)/Atmospheric Laboratory for Applications and Science (ATLAS) on board the space shuttle.

[3] Pressure shift of atmospheric gas microwave transition should lead to the asymmetry of the shape of emission and absorption atmospheric lines observed by upward and downward remote sensing. This paper is devoted to the estimation of such asymmetry effects for the 118 GHz oxygen line, possibilities of its observation, and some discussion of the air pressure shift as a new element of microwave atmospheric lines.

2. Estimation of Atmospheric Line Asymmetry

[4] Estimations of asymmetry of the atmospheric 118 GHz oxygen line produced by air pressure shift were done for some different remote sensing methods. We consider in this paper the simplest cases of zenith/nadir sounding modes that give the possibility of evaluating the order of magnitude of the effect without unnecessary complications. Calculations may be well adapted to the concrete mode of observation when needed. As the effect

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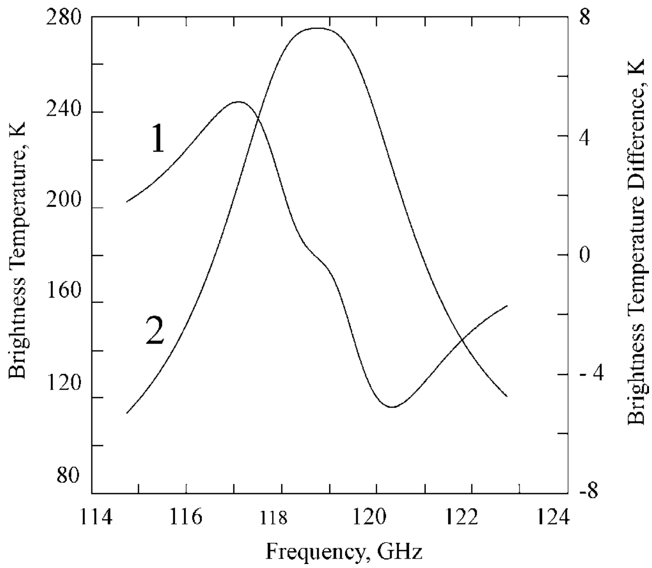

Figure 1. Difference between the brightness temperature of the downward atmosphere radiation calculated for the shifted and nonshifted lines $T^d_{bs}(f) - T^d_{bn}(f)$ as a function of the frequency f (curve 1, right scale). For comparison, the whole line as observed from the Earth is presented (curve 2, left scale).

mentioned is collisional, only the part of the atmospheric line where collisional broadening is prevailing is considered.

[5] Calculations were done using millimeter wave propagation model MPM-89 [*Liebe*, 1989] with inclusion of the pressure line shift. The standard model of the midlatitude atmosphere with linear descending temperature, exponentially decreasing humidity, ground level temperature equal to 15°C, and 7.5 g/m^3 ground level humidity up to an altitude of 10 km has been used. The summer middle atmosphere reference model [*Banett and Corney*, 1985] and water vapor profile [*Clough et al.*, 1986] have been employed for higher altitudes. Room temperature broadening and shift parameters were used, as the temperature dependence of the shift parameter is unknown at the moment. Commonly, both parameters are increasing with the cooling; thus the present estimation corresponds rather to the lower limit of asymmetry to be observed. Values of parameters measured by *Tretyakov et al.* [2001] are 2.14 ± 0.07 MHz/torr (16.1 MHz/kPa) for broadening and −0.19 ± 0.08 MHz/torr (−1.43 MHz/kPa) for the shift.

2.1. Passive Radiometric Sensing From the Ground

[6] Passive radiometric sensing from the ground corresponds to the downward atmospheric emission. Only zenith emission has been considered. In Figure 1 the difference between the brightness temperature of downward atmospheric emission is presented for the shifted line $T^d_{bs}(f)$ and for the nonshifted line $T^d_{bn}(f)$ (curve 1, right scale) as a function of the frequency. For comparison, the whole line as observed from the Earth is presented (curve 2, left scale). In Figure 2 the brightness temperature asymmetry is presented for shifted $T^d_{bs}(f_0 + \Delta f) - T^d_{bs}(f_0 - \Delta f)$ (curve 1) and nonshifted $T^d_{bn}(f_0 + \Delta f) - T^d_{bn}(f_0 - \Delta f)$ (curve 2) line models as a function of the frequency detuning Δf from the line center frequency $f_0 \approx 118.750$ GHz. Asymmetry of the nonshifted line is mostly the known Van Vleck-Weisskopf profile asymmetry. Asymmetry of the shifted line is also accounted for by the pressure shift of negative sign.

2.2. Nadir Satellite-Based Passive Radiometric Sensing

[7] This case corresponds to the upward atmosphere emission observed by satellite-based apparatus. In Figure 3 the brightness temperature asymmetry calculated for the upward atmosphere emission for shifted $T^u_{bs}(f_0 + \Delta f) - T^u_{bs}(f_0 - \Delta f)$ (curve 1) and nonshifted $T^u_{bn}(f_0 + \Delta f) - T^u_{bn}(f_0 - \Delta f)$ (curve 2) line models as function of the frequency detuning Δf from the center frequency $f_0 \approx 118.750$ GHz is presented.

2.3. Active Sounding of the Atmosphere

[8] Pressure shift of the line central frequency can cause not only atmospheric emission line asymmetry

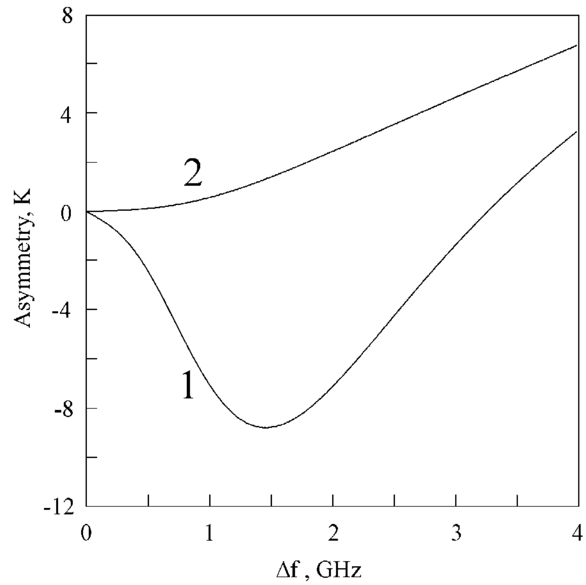

Figure 2. Brightness temperature asymmetry of the downward atmosphere radiation for shifted T^{d}_{bs} $(f_0 + \Delta f) - T^{d}_{bs}$ $(f_0 - \Delta f)$ (curve 1) and nonshifted T^{d}_{bn} $(f_0 + \Delta f) - T^{d}_{bn}$ $(f_0 - \Delta f)$ (curve 2) line models as a function of the frequency detuning Δf from the line center frequency $f_0 \approx 118.750$ GHz.

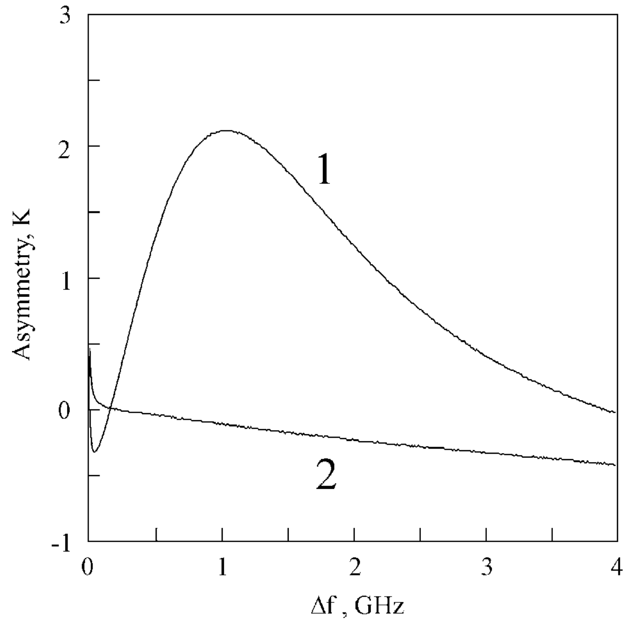

Figure 3. Brightness temperature asymmetry of upward atmosphere radiation calculated for the case of shifted T^{u}_{bs} $(f_0 + \Delta f) - T^{u}_{bs}$ $(f_0 - \Delta f)$ (curve 1) and nonshifted T^{u}_{bn} $(f_0 + \Delta f) - T^{u}_{bn}$ $(f_0 - \Delta f)$ (curve 2) line models as a function of the frequency detuning Δf from the center frequency $f_0 \approx 118.750$ GHz.

but also absorption line asymmetry. This feature could be detected by active sounding of the Earth atmosphere. It might be done by using natural sources (the Sun for the ground-based observation) or an artificial one (space-based or ground-based tunable microwave oscillator). The receiver can be mounted on the ground or on the satellite, respectively. This case corresponds to the observation of the absorption profile of the line. In Figure 4 the calculated zenith attenuation difference $A_s(f) - A_n(f)$ of shifted $A_s(f)$ and nonshifted $A_n(f)$ attenuation line models is presented as a function of the frequency f.

[9] The absorption asymmetry calculated for shifted $A_s(f_0 + \Delta f) - A_s(f_0 - \Delta f)$ (curve 1) and nonshifted $A_n(f_0 + \Delta f) - A_n(f_0 - \Delta f)$ (curve 2) models is presented in Figure 5 as a function of the frequency detuning Δf from the centerline frequency $f_0 \approx 118.750$ GHz.

[10] The estimations shown in Figures 1–5 suggest the possibility of observing the asymmetry of the 118 GHz atmospheric line produced by air pressure shift at the existing level of instrumentation (this question is considered in section 3 in more detail). These estimations also add evidence of the necessity of considering the line shifts in atmosphere propagation models. Quite possibly, this new source of information can be used to improve the existing methods of atmosphere parameter recovery,

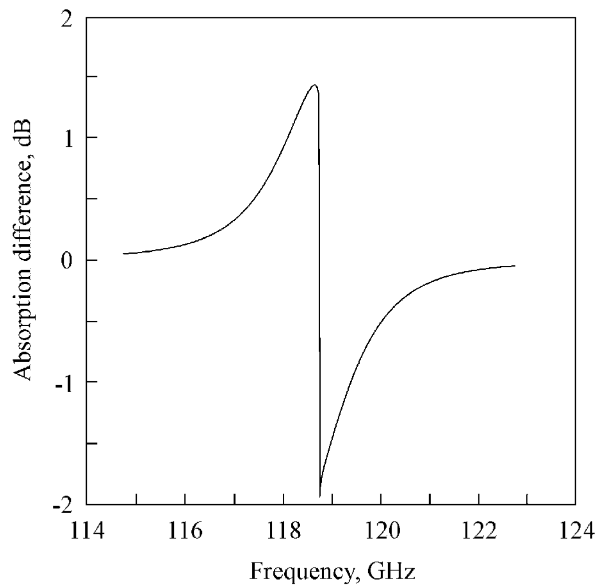

Figure 4. Calculated zenith atmosphere attenuation difference $A_s(f) - A_n(f)$ of shifted $A_s(f)$ and nonshifted $A_n(f)$ line models as a function of the frequency f.

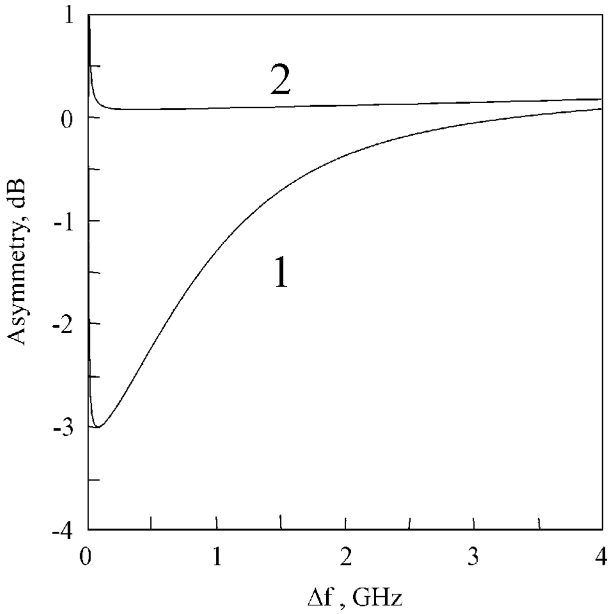

Figure 5. Atmosphere absorption asymmetry calculated for shifted $A_s(f_0 + \Delta f) - A_s(f_0 - \Delta f)$ (curve 1) and nonshifted $A_n(f_0 + \Delta f) - A_n(f_0 - \Delta f)$ (curve 2) line models as a function of the frequency detuning Δf from the centerline frequency $f_0 \approx 118.750$ GHz.

as did the introduction of the 183 GHz line shift by *Pumphrey and Buehler* [2000].

3. Discussion

[11] In this section we will point out the observability of asymmetry of the 118 GHz atmospheric line, the desirability of line shift studies of the lines of the 60 GHz oxygen band for better description of absorption in atmosphere, the principal possibility for extracting information about temperature from the shift-to-broadening ratio, and some possible directions for further studies.

[12] Estimations presented in Figures 1–5 suggest observability of the 118 GHz oxygen line asymmetry at the present level of instrumentation. The effect reaches about 8 K (Figure 2) for passive sounding from the ground and about 2 K for nadir mode observations from the high-altitude aircraft or satellite (Figure 3). Sensitivity of existing radiometers [e.g., *Lange et al.*, 1999; *Erickson et al.*, 1999], assuming 100 MHz bandwidth, is better than 0.05 K even for 1 s time constant. Observability of 118 GHz oxygen line asymmetry is strongly supported also by the recent observation of the same effect on the 183 GHz water line [*Pumphrey and Buehler*, 2000]. Pressure shift parameters for both lines are similar, and broadening of the 118 GHz oxygen line is about 2 times less than the same for 183 GHz water line, thus giving for the 118 GHz line about 2 times larger shift-to-broadening ratio. Tuned to the oxygen 118 GHz line frequency is a radiometer with low-noise cooled HEMT preamplifier installed on the recently (in February 2001) launched Odin satellite (information available from the Swedish Space Corporation at http://www.ssc.se/ssd/ssat/odin.html). The single sideband radiometer mounted on board the Odin satellite, now in action, might be possibly used for an attempt of observation of the asymmetry of the 118 GHz oxygen line though it is relatively narrow-banded. Its bandwidth constitutes 118.25 to 119.25 GHz, i.e., stretches 500 MHz on each side of the nonshifted center of the line. This bandwidth is not enough for covering the whole oxygen line (half width on half magnitude for this line at the sea level atmospheric pressure is about 1.6 GHz [*Tretyakov et al.*, 2001]), but possibly permits the first observation of the line asymmetry (as follows from Figure 3 considering the high sensitivity of the Odin radiometer). The authors suppose that it would be interesting to process sounding data from the Odin satellite to search for an asymmetry of the 118 GHz oxygen line in the frequency band and at the observation angles acceptable for this apparatus (and, of course, to get other data in broader frequency range).

[13] Up to the moment the 118 GHz oxygen line is the only line among lines of the magnetic fine structure spectrum of oxygen (the rest of which is confined around 60 GHz) with known appreciable air pressure shift. Quite possibly, at least some of the other fine structure lines of oxygen also are experiencing the air pressure shifts, but these lines are closely situated and their wings begin to overlap at pressures lower than the atmospheric one [see, e.g., *Liebe et al.*, 1992], which makes difficult the observation of the pressure shift effect by the method used by us for single 118 GHz line [*Krupnov et al.*, 2000]. Study at lower pressures, though, e.g., by spectrometer [*Krupnov*, 1979], searching for possible shifts of the lines of 60 GHz band could be of interest for further understanding and improvement of the description of the atmosphere absorption in the 60 GHz oxygen band.

[14] Worth noting is the physical possibility to know the temperature of the gas from shift and broadening of the line only, first mentioned by *Markov* [1994]. *Markov* [1994] pointed out that difference in temperature exponents of broadening and shift parameters gives the method of measurements of the gas temperature. The shift-to-broadening ratio for a given line in a given gas mixture is a universal function depending only on the temperature of the gas and independent of pressure (both broadening and shift are proportional to the pressure within the validity of the binary collisions assumption). In particular, such a function was measured by *Markov* [1994] for the self-perturbed water line

at 439 GHz. It is important to note that this function can be measured in laboratory experiment at convenient pressure in a gas mixture needed and then extended to the whole range of pressures where binary collisions prevail (i.e., up to the pressures exceeding the normal atmospheric one). In this method any absolute intensity measurements are not necessary, and obtaining the line shape in arbitrary units (without amplitude calibration) is sufficient. In application to the atmospheric lines exhibiting air pressure shift it could mean that observation of the atmospheric line asymmetry with sufficient signal-to-noise ratio gives principal possibility of atmosphere temperature measurements.

[15] Now two atmospheric lines exhibiting noticeable air pressure shifts are known. However, temperature dependencies of the shifts of these lines are unknown for both lines, demanding fine laboratory studies. The general considerations of temperature dependencies of the broadening and shift for known types of molecular interactions, though, were presented by *Pickett* [1980]. Temperature dependencies of the shift and broadening appear through relative collisional velocity of the molecules. Considerations of *Pickett* [1980] concern the temperature exponents of velocity for broadening, n, and for shift, s, in the terms of *Pickett* [1980]. The results of *Pickett* [1980] are that n ranges from 0 to 1 as the potential goes from dipole-dipole to a hard sphere, while s goes from $-3/2$ to 0 for the same progression of potential. So different temperature dependencies for broadening and shift of the lines discussed can be expected, but this subject needs further study.

[16] Since temperature dependence of pressure shift is unknown at the moment, it is impossible to estimate sensitivity of this method. Also, further developments both in the choice of the proper spectral line and in the finding of an optimal observation method are very desirable. In this paper we would like just to point out the existence of the physical effect permitting, in principle, independent temperature measurement of the atmosphere. The possibility of independent verification is always important, e.g., for finding out systematic errors of different methods. It seems that active sounding can give the first possibility of measurements of the most part of the atmospheric absorption line profile with large enough signal-to-noise ratio. The difference in atmosphere zenith/nadir opacity (i.e., in power of incoming signal) reaches about 2 times at proper frequencies (Figure 5), so it is large enough from the point of view of microwave measurements. Exclusion of the instrumental effects (frequency dependencies of transmitter and receiver) can be done by the well-known method of path variation (variation of the angle of observation through the atmosphere). Even significant efforts aimed at use of this new possibility of almost direct measurement of the temperature profile of atmosphere seem to be justified.

[17] Further directions of studies of interest include laboratory investigations of temperature dependencies of the shift for known lines 118 and 183 GHz, consideration of appropriate sounding instruments and technique, and search for the air pressure shifts of the other lines of other constituents of atmosphere molecules and also molecules present in the atmospheres of other planets.

4. Conclusion

[18] Asymmetry of the oxygen 118 GHz atmospheric line due to the air pressure shift of the center frequency of this transition found in previous laboratory experiments is predicted, and estimations are given for some observation modes. The observability of oxygen line asymmetry by the appropriate instruments is shown. The necessity of considering the pressure shift in atmosphere propagation models such as the well-known MPM is demonstrated. Pressure line shift as a new source of information about the atmosphere already is used for improving the existing methods of recovery of the atmosphere parameters. Also, the new principal possibility of the remote sensing of the temperature of atmosphere using the measurements of shift-to-broadening ratio for the atmospheric line is pointed out. At the moment the 118 GHz oxygen and 183 GHz water lines are the only known microwave lines used for remote sensing exhibiting appreciable air pressure shift of the central frequency. The possible directions of further studies, including studies of shift and broadening temperature dependencies and the search for other atmosphere lines exhibiting air pressure shifts, are discussed.

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