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Title:

Measurement of sulfur isotope compositions by tunable laser spectroscopy of SO_2

Abstract:

The following is supplemental information pertaining to the paper. It consists of Table S-1 which lists modeled line parameters of $^{32}SO_2$ and $^{34}SO_2$ for the spectral region investigated. Also included are three figures. Figure S-1 which demonstrates that modeled line parameters agree with experimental results. Figure S-2 which describes the correction needed to W_x to correct for the Beer-Lambert Law. Figure S-3 which shows an Allan-variance plot of W_x and $\delta^{34}S$ for sample E2.

Supplemental Table S-1. Line parameters of $^{32}SO_2$ and $^{34}SO_2$ rovibrational transitions in the spectral window in which measurements were taken.

Iso	$\nu_{\eta\eta'}$ (cm^{-1})	$S_{\eta\eta'}$(296K)† (cm $molec^{-1}$)	E'' (cm^{-1})	vib. trans.	rot. trans.
32	1351.6668	2.2×10^{-20}	176	001-000	$13_{8,5}$-$14_{8,6}$
34	1351.6708	2.4×10^{-20}	123	001-000	$12_{7,6}$-$11_{7,5}$
34	1351.6755	4.0×10^{-20}	61	001-000	$11_{4,7}$-$10_{4,6}$
34	1351.6948	1.6×10^{-20}	183	001-000	$13_{9,4}$-$12_{9,3}$
34^{*}	1351.7136	5.2×10^{-20}	34	001-000	$11_{0,11}$-$10_{0,10}$
32	1351.7416	4.2×10^{-20}	119	001-000	$14_{5,10}$-$15_{5,11}$
34	1351.7657	7.1×10^{-21}	303	001-000	$15_{12,3}$-$14_{12,2}$
32^{*}	1351.7730	5.5×10^{-22}	626	011-010	$7_{7,0}$-$8_{7,1}$
32^{*}	1351.7741	2.7×10^{-21}	575	011-010	$8_{4,5}$-$9_{4,6}$

* Denotes transitions used for isotopic analysis.

† $S_{\eta\eta'}$ not scaled by isotopic abundance.

Supplemental Figure S-1.

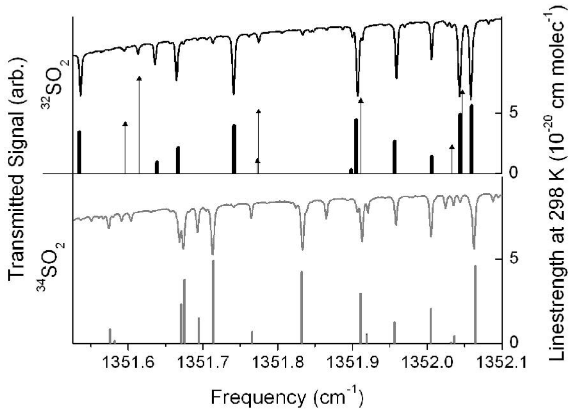

Figure S.1. Experimental spectra of gas samples containing ~95% $^{32}SO_2$ (top half) and ~90% $^{34}SO_2$ (bottom half) compared with modeled linestrengths. In the top half, thick vertical lines are positions and linestrengths for 001-000 of $^{32}SO_2$ from HITRAN and thin lines with arrows are modeled lines for 011-010 of $^{32}SO_2$. In the bottom half, vertical lines are modeled lines for 001-000 of $^{34}SO_2$.

Supplemental Figure S-2.

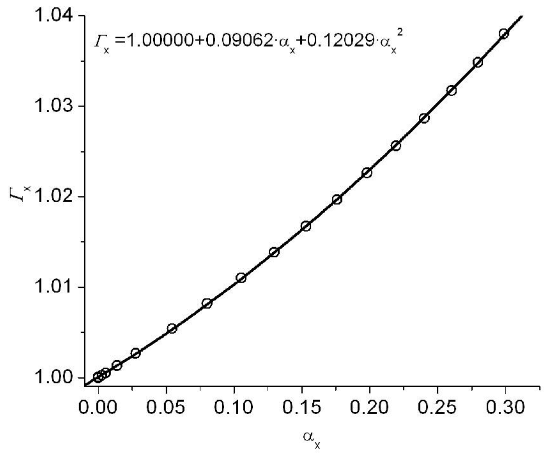

Figure S-2. Correction needed, Γ_x, so that $\Gamma_x = \gamma \cdot \alpha_x / W_x$. Values of α_x and W_x were acquired from numerically modeled spectra using a Voigt profile for direct absorption at 1.0 mbar, 298.0 K, 30.0 MHz HWHM Gaussian laser linewidth, γ_{self}(296 K) = 0.400 cm^{-1} atm^{-1} (only considered self-broadening), n = 0.50, modulation amplitude = 0.0040 cm^{-1}. Mixing-ratio was varied to vary α_x. The value of γ was determined from a linear fit of W_x versus α_x for fractional absorption < 1×10^{-4}.

Supplemental Figure S-3.

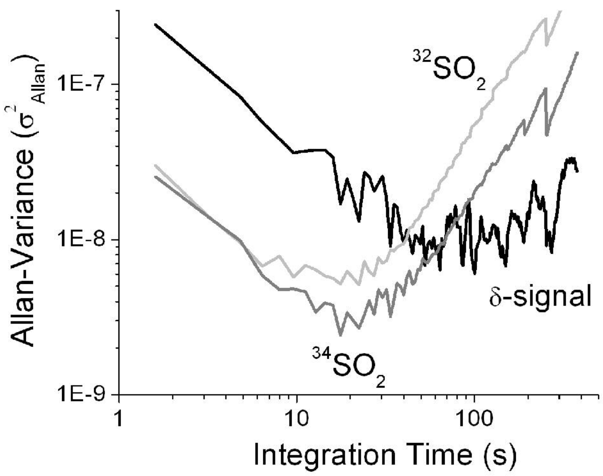

Figure S-3. Allan variance plot of data from sample E2. Dark and light grey lines are for W_{34} and W_{32} signals, respectively, both scaled by 10^{-12}. Black line is $\delta^{34}S$ signal. Sample E2 was chosen because it was typical of other measurements.