

The broadening coefficients of SO₂

The current air-broadening coefficients of sulfur dioxide in the HITRAN database is a constant, $\gamma_{\text{air}}=0.1025 \text{ cm}^{-1}$ for line positions lower than 3000 cm^{-1} ; $\gamma_{\text{air}}=0.1000 \text{ cm}^{-1}$ for line positions larger than 3000 cm^{-1} (based on a private communication of J.-M. Flaud, see HITRAN2008 paper for details). Recently, different measurements have been made of the air-broadening coefficients of SO₂ from infrared and submillimeter-wave spectra. All the available experimental results have been collected in Table1. A slow decrease of the air-broadening coefficients with increasing ($J''+0.2Ka''$) lower-state quantum number combination can be seen in Fig.1. The vibrational dependence of the broadening parameters is demonstrated to be very small or negligible.

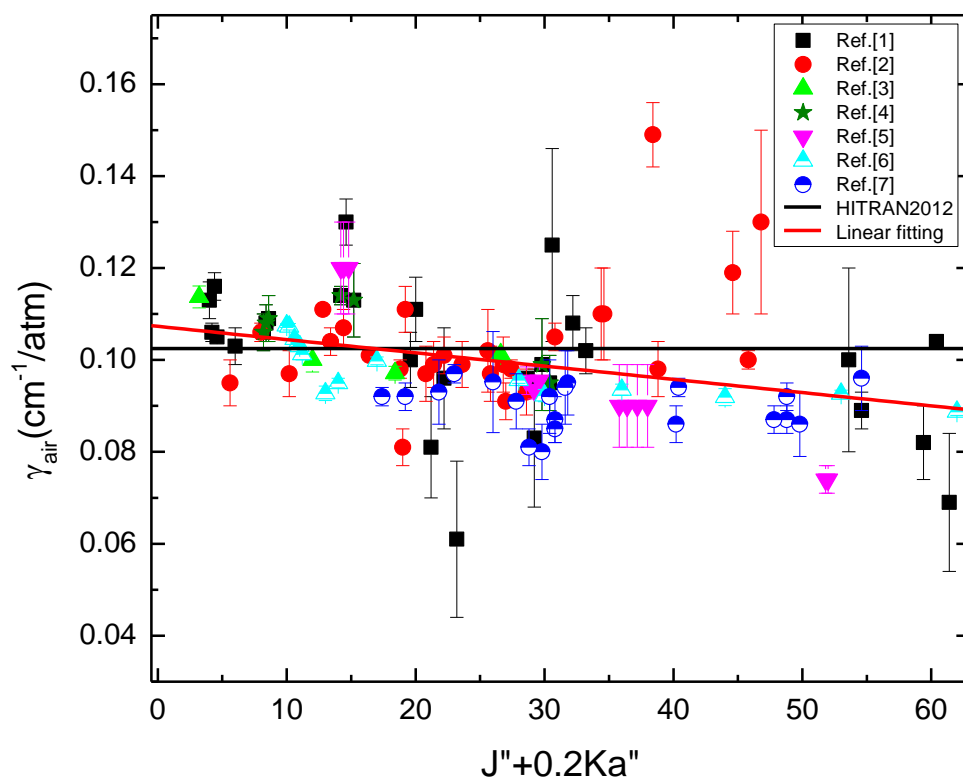


Fig. 1. The air-broadening coefficients plotted as a function of the lower-state rotational quantum number ($J''+0.2Ka''$)

We use a linear extrapolation (see Table2) up to $(J''+0.2Ka'') < 62$, and for the other transitions with $(J''+0.2Ka'') > 62$, the value corresponding to the experimental value with the largest $(J''+0.2Ka'')$ was used.

Table1

SO₂ air-broadening coefficients (in cm⁻¹/atm)

J''	Ka''	γ_{air}	error	Reference
4	1	0.106	0.002	Ref. [1]
8	1	0.106	0.004	
14	1	0.114	0.002	
15	1	0.113	0.008	
32	1	0.108	0.006	
33	1	0.102	0.005	
4	2	0.116	0.003	
8	2	0.108	0.004	
30	2	0.095	0.006	
59	2	0.082	0.008	
60	2	0.104	0.001	
61	2	0.069	0.015	
4	3	0.105	0.001	
8	3	0.109	0.005	
14	3	0.13	0.005	
30	3	0.125	0.021	
5	5	0.103	0.004	
19	5	0.111	0.007	
18	8	0.1	0.006	
28	9	0.099	0.010	
27	11	0.083	0.015	
26	13	0.096	0.003	
52	13	0.089	0.004	
18	16	0.081	0.011	
19	16	0.096	0.011	
20	16	0.061	0.017	
50	18	0.1	0.020	
16	2	0.101	0.001	Ref. [2]
5	3	0.095	0.005	
25	3	0.102	0.009	
28	3	0.093	0.005	
18	6	0.111	0.005	
13	7	0.107	0.004	
22	8	0.099	0.005	
25	12	0.098	0.002	

43	14	0.1	0.002	
44	14	0.13	0.020	
35	17	0.149	0.007	
31	18	0.11	0.010	
22	19	0.097	0.006	
23	19	0.099	0.006	
27	19	0.105	0.003	
23	20	0.091	0.004	
10	1	0.097	0.005	
22	1	0.101	0.004	
21	2	0.099	0.005	
18	4	0.098	0.002	
20	4	0.097	0.006	
37	9	0.098	0.006	
32	12	0.11	0.010	
40	23	0.119	0.009	
12	4	0.111	0.001	
18	5	0.081	0.004	
18	2	0.09712	0.00147	<i>Ref. [3]</i>
12	0	0.10002	0.00265	
3	1	0.11371	0.0024	
26	3	0.10123	0.00147	
14	2	0.12	0.010	
14	4	0.12	0.010	
13	6	0.12	0.010	
28	6	0.0935	0.002	<i>Ref. [4]</i>
28	3	0.0955	0.003	
29	3	0.0955	0.003	
35	4	0.09	0.009	
36	2	0.09	0.009	
37	1	0.09	0.009	
38	0	0.09	0.009	
50	9	0.074	0.003	
51	5	0.074	0.003	
8	1	0.106	0.004	<i>Ref. [5]</i>
8	2	0.108	0.004	
8	3	0.109	0.005	
14	1	0.114	0.002	
15	1	0.113	0.008	
28	9	0.099	0.010	
30	2	0.095	0.006	
11	10	0.09273	0.00157	<i>Ref. [6]</i>

12	10	0.09496	0.00104	
15	10	0.09981	0.00086	
26	10	0.09565	0.00074	
28	10	0.09225	0.00134	
34	10	0.09352	0.00122	
42	10	0.09192	0.00185	
51	10	0.09266	0.00076	
60	10	0.08873	0.00079	
10	0	0.10749	0.00041	
10	1	0.10723	0.00071	
10	3	0.10457	0.0003	
10	4	0.10336	0.00043	
10	5	0.103	0.00117	
10	6	0.10125	0.00124	
25	14	0.091	0.006	Ref. [7]
16	16	0.092	0.003	
28	19	0.095	0.007	
51	18	0.096	0.007	
27	19	0.087	0.005	
38	11	0.086	0.004	
26	19	0.08	0.006	
47	9	0.087	0.003	
29	13	0.094	0.008	
25	19	0.081	0.004	
20	15	0.097	0.002	
39	7	0.094	0.002	
47	14	0.086	0.007	
29	9	0.085	0.003	
15	12	0.092	0.002	
46	14	0.092	0.003	
45	14	0.087	0.003	
24	10	0.0952	0.011	
19	14	0.093	0.007	
28	12	0.092	0.008	

Note: All experiments have been made at room temperature, so the temperature dependence of γ_{air} has been neglected.

Table2

Linear fit:	value	Standard Error
$Y = a + b * X$		

Intercept	0.10731	7.13901E-4
Slope	-2.88311E-4	2.92377E-5

The error code 4 was used for air-broadening coefficients of SO₂, and the ref code is 3 corresponding to this report.

A complete line-by-line database of room temperature self-broadening coefficients for about 1650 SO₂ transitions have been compiled by Tasinato et al.[8]. And these data have been used to update the self-broadening coefficients for the corresponding transitions. The error code has been set to 5 with the estimated accuracy of 5-6%, and the ref code is 2. We also use the average values from Ref.[8] of the same quantum numbers (*J*”, *Ka*”) for all the other transitions with corresponding rotational quantum numbers. The error coder is 4 and ref code is still 2.

- [1] Sumpf B, Schöne M, Kronfeldt H-D. Self- and Air-Broadening in the ν_3 Band of SO₂. *J Mol Spectrosc* 1996;179:137–41. doi:10.1006/jmsp.1996.0191.
- [2] Sumpf B, Fleischmann O, Kronfeldt H-D. Self-, Air-, and Nitrogen-Broadening in the ν_1 Band of SO₂. *J Mol Spectrosc* 1996;176:127–32. doi:10.1006/jmsp.1996.0068.
- [3] Ball CD, Dutta JM, Goyette TM, Helminger P, De Lucia FC. The pressure broadening of SO₂ by N₂, O₂, He, and H₂ between 90 and 500 K. *J Quant Spectrosc Radiat Transf* 1996;56:109–17. doi:10.1016/0022-4073(96)00016-7.
- [4] Kühnemann F, Heiner Y, Sumpf B, Herrmann K. Line broadening in the ν_3 band of SO₂: Studied with diode laser spectroscopy. *J Mol Spectrosc* 1992;152:1–12. doi:10.1016/0022-2852(92)90111-Z.
- [5] Sumpf B, Schöne M, Fleischmann O, Heiner Y, Kronfeldt H-D. Quantum Number and Temperature Dependence of Foreign Gas-Broadening Coefficients in the ν_1 and ν_3 Bands of SO₂: Collisions with H₂, Air, He, Ne, Ar, Kr, and Xe. *J Mol Spectrosc* 1997;183:61–71. doi:10.1006/jmsp.1996.7239.
- [6] Cazzoli G, Puzzarini C. N₂-, O₂-, H₂-, and He-broadening of SO₂ rotational lines in the mm-/submm-wave and THz frequency regions: The *J* and *Ka* dependence. *J Quant Spectrosc Radiat Transf* 2012;113:1051–7. doi:10.1016/j.jqsrt.2012.01.011.
- [7] Tasinato N, Pietropolli Charmet A, Stoppa P, Giorgianni S, Buffa G. N₂-, O₂- and He-collision-induced broadening of sulfur dioxide ro-vibrational lines in the 9.2 μ m atmospheric window. *Spectrochim Acta - Part A Mol Biomol Spectrosc* 2014;118:373–9. doi:10.1016/j.saa.2013.08.071.
- [8] Tasinato N, Charmet AP, Stoppa P, Buffa G, Puzzarini C. A complete listing of sulfur

dioxide self-broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations. *J Quant Spectrosc Radiat Transf* 2013;130:233–48. doi:10.1016/j.jqsrt.2013.03.015.

The new HITRAN ref table for SO₂:

Half-widths (air)

[GlobRef 1075] **3.** This report.

Half-widths (self)

[GlobRef 1074] **2.** N. Tasinato, A.P. Charmet, P. Stoppa, G. Buffa, C. Puzzarini, “ A complete listing of sulfur dioxide self-broadening coefficients for atmospheric applications by coupling infrared and microwave spectroscopy to semiclassical calculations”, *J Quant Spectrosc Radiat Transf*, **130**, 233–248(2013)