The air-broadening coefficients of HO_2

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The current air-broadening coefficient of the hydroperoxyl radical in the HITRAN database[1] is a constant, γ_{air}=0.107±0.009 cm^{-1}/atm (based on the measurement in Ref.[2]). Different measurements have more recently been made of the air-broadening coefficients of HO_2 from infrared and submillimeter-wave spectra[2–7]. All the available experimental results have been collected in Table 1. A decrease of the air-broadening coefficients with increasing ($N''+0.2K_a''$) quantum number can be seen in Fig.1. It does not seem that there is a strong vibrational dependence, which is not typical for non-linear molecules. In Ref.[4], the measurements were averaged for every N'' value and linear dependence was suggested as a function of N''.

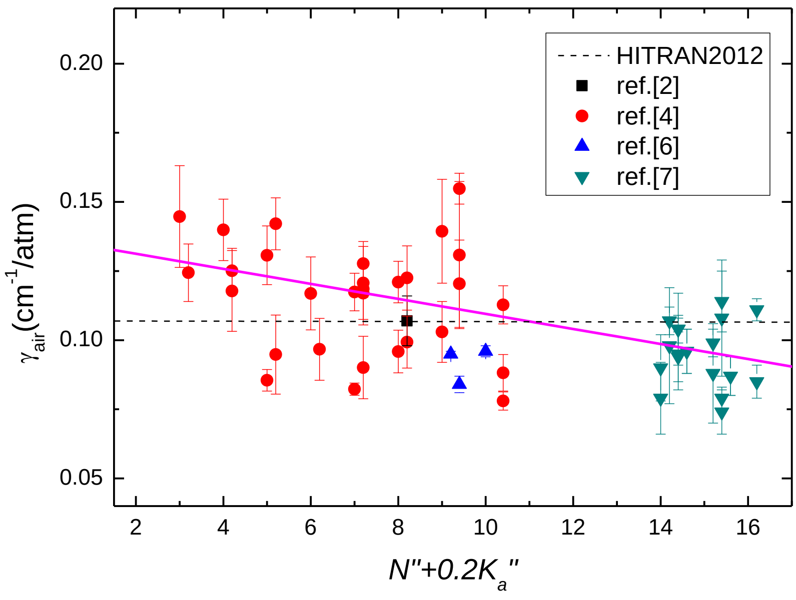

Fig. 1. The air-broadening coefficients plotted as a function of the lower state rotational quantum number ($N''+0.2K_a''$)

Here the index ($N''+0.2K_a''$) instead of N'' was chosen as it better demonstrates the K_a-dependence. A linear fit was carried out, and the corresponding coefficients are given in Table 2.

The following approach was chosen. We used experimental values for all the transitions with corresponding rotational quantum numbers (in all the bands). For everything else we used the linear extrapolation (from Table 2) up to (*N″+0.2K_a″*) < 17. For all transitions with (*N″+0.2K_a″*) > 17, the value corresponding to the experimental value with the largest (*N″+0.2Ka″*) was used.

Table 1

HO_2 (N_2-, O_2-) air-broadening coefficients (in cm^{-1}/atm)

Ref	Wavenumber (cm^{-1})	Transitions ($N\ K_a\ K_c$)	Hyperfine J'-J''	γ_{N2}	γ_{O2}	γ_{air}
[2]	1411.18	$9_{1,9}$- $8_{1,8}$	8.5-7.5			0.107(9)
		$9_{1,9}$- $8_{1,8}$	9.5-8.5			0.107(9)
[3]	83.3178	$13_{2,12}$-$12_{1,11}$	13.5-12.5	0.160(15)	0.068(5)	0.142(13)
[4]	6631.0019	$6_{0,6}$-$6_{1,5}$				0.0967(112)
	6631.0884	$7_{0,7}$-$7_{1,6}$				0.0901(113)
	6631.1887	$5_{0,5}$-$5_{1,4}$				0.0948(143)
	6631.3129	$4_{0,4}$-$4_{1,3}$				0.1251(81)
	6631.3701	$3_{0,3}$-$3_{1,2}$				0.1244(104)
	6631.4543	$8_{0,8}$-$9_{0,9}$				0.1394(188)
	6631.4772	*				0.0964(248)
	6631.6137	$5_{0,5}$-$5_{1,4}$				0.1421(94)
	6631.8267	$4_{0,4}$-$4_{1,3}$				0.1178(146)
	6666.5915	$8_{1,8}$-$7_{1,7}$				0.1185(30)
	6666.6411	$8_{1,8}$-$7_{1,7}$				0.1277(80)
	6666.8618	$10_{2,9}$-$9_{2,8}$				0.1548(56)
	6666.9080	$10_{2,9}$-$9_{2,8}$				0.1204(158)
	6667.0197	*				0.1287(190)
	6667.0640	$10_{2,8}$-$9_{2,7}$				0.1308(266)
	6667.2771	$8_{1,7}$-$7_{1,6}$				0.1170(115)
	6667.3226	$8_{1,7}$-$7_{1,6}$				0.1207(132)
	6669.0059	$11_{2,9}$-$10_{2,8}$				0.0882(66)
	6669.0766	$11_{2,10}$-$10_{2,9}$				0.1128(69)
	6669.1142	$4_{1,3}$-$4_{0,4}$				0.1399(111)
	6669.1383	$11_{2,9}$-$10_{2,8}$				0.0780(33)
	6669.2982	$5_{1,4}$-$5_{0,5}$				0.1307(106)
	6669.4163	$9_{1,8}$-$8_{1,7}$				0.1225(116)
	6669.4464	$9_{1,8}$-$8_{1,7}$				0.0993(94)
	6669.4916	$6_{1,5}$-$6_{0,6}$				0.1169(132)
	6669.5197	$3_{1,2}$-$3_{0,3}$				0.1447(184)
	6669.6789	$5_{1,4}$-$5_{0,5}$				0.0855(39)
	6669.7049	$7_{1,6}$-$7_{0,7}$				0.0823(22)
	6669.9261	$8_{1,7}$-$8_{0,8}$				0.1210(75)
	6670.0064	$7_{1,6}$-$7_{0,7}$				0.1174(68)
	6670.0951	*				0.0938(98)
	6670.1514	$9_{1,8}$-$9_{0,9}$				0.1030(110)

	6670.2049	$8_{1,7}$-$8_{0,8}$				0.0959(77)
	6670.2696	*				0.1404(44)
[5]	1064.909	$13_{0,13}$-$14_{0,14}$	12.5–13.5	0.118(11)		
	1064.913	$13_{0,13}$-$14_{0,14}$	13.5–14.5	0.099(9)		
	1065.203	$13_{1,13}$-$14_{1,14}$	13.5–14.5	0.095(5)		
	1065.221	$13_{1,13}$-$14_{1,14}$	12.5–13.5	0.090(5)		
[6]	8.865	$4_{1,3}$-$3_{1,2}$	4.5 -3.5	0.103(2)		
	20.869	$10_{1,9}$-$10_{0,10}$	10.5-10.5	0.104(1)	0.065(1)	0.0955(17)
	21.403	$10_{1, 10}$-$9_{1,9}$	9.5 -8.5	0.103(1)	0.064(1)	0.0948(15)
	21.671	$10_{2,9}$-$9_{2,8}$	9.5 -8.5	0.088(2)	0.066(3)	0.0836(25)
[7]	1060.172	$15_{1,15}$-$16_{1,16}$	15.5–16.5	0.120(4)	0.075(4)	0.111(4)
	1060.186	$15_{1,15}$-$16_{1,16}$	14.5–15.5	0.091(7)	0.062(2)	0.085(6)
	1062.089	$14_{3,11}$-$15_{3,12}$	13.5–14.5	0.092(7)	0.066(7)	0.087(7)
	1062.090	$14_{3,12}$-$15_{3,13}$	13.5–14.5	0.092(7)	0.066(7)	0.087(7)
	1062.102	$14_{2,12}$-$15_{2,13}$	14.5–15.5	0.124(13)	0.077(5)	0.114(11)
	1062.165	$14_{2,12}$-$15_{2,13}$	13.5–14.5	0.086(5)	0.052(3)	0.079(4)
	1062.171	$14_{2,13}$-$15_{2,14}$	14.5–15.5	0.079(10)	0.057(1)	0.074(8)
	1062.236	$14_{2,13}$-$15_{2,14}$	13.5–14.5	0.116(26)	0.077(4)	0.108(21)
	1062.700	$14_{1,14}$-$15_{1,15}$	14.5–15.5	0.093(21)	0.072(4)	0.088(18)
	1062.716	$14_{1,14}$-$15_{1,15}$	13.5–14.5	0.107(5)	0.066(5)	0.099(5)
	1064.630	$13_{3,10}$-$14_{3,11}$	12.5–13.5	0.103(9)	0.071(3)	0.096(8)
	1064.631	$13_{3,11}$-$14_{3,12}$	12.5–13.5	0.103(9)	0.071(3)	0.096(8)
	1064.639	$13_{2,11}$-$14_{2,12}$	13.5–14.5	0.113(5)	0.071(6)	0.104(5)
	1064.696	$13_{2,12}$-$14_{2,13}$	13.5–14.5	0.099(10)	0.073(4)	0.094(9)
	1064.710	$13_{2,11}$-$14_{2,12}$	12.5–13.5	0.111(12)	0.080(18)	0.104(13)
	1064.768	$13_{2,12}$-$14_{2,13}$	12.5–13.5	0.101(15)	0.074(4)	0.095(13)
	1064.909	$13_{0,13}$-$14_{0,14}$	12.5–13.5	0.083(15)	0.063(7)	0.079(13)
	1064.913	$13_{0,13}$-$14_{0,14}$	13.5–14.5	0.097(14)	0.064(5)	0.090(12)
	1065.203	$13_{1,13}$-$14_{1,14}$	13.5–14.5	0.118(5)	0.068(6)	0.107(5)
	1065.221	$13_{1,13}$-$14_{1,14}$	12.5–13.5	0.105(26)	0.070(2)	0.098(21)

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

*Lines without assignment.

Table2

Linear fit: Y= a+b*X	value	Standard Error
Intercept	0.1367	0.005
Slope	-0.0027	5E-4

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[3] Chance K, Denatale P, Bellini M, Inguscio M, Dilonardo G, Fusina L. Pressure Broadening of the 2.4978-THz Rotational Lines of HO_2 by N_2 and O_2. J Mol Spectrosc 1994;163:67–70. doi:10.1006/jmsp.1994.1007.

[4] Ibrahim N, Thiebaud J, Orphal J, Fittschen C. Air-broadening coefficients of the HO_2 radical in the $2\nu_1$ band measured using cw-CRDS. J Mol Spectrosc 2007;242:64–9. doi:10.1016/j.jms.2007.02.007.

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[7] Minamida M, Tonokura K. Air broadening coefficients for the ν_3 band of hydroperoxyl radicals. J Quant Spectrosc Radiat Transf 2014;148:65–9. doi:10.1016/j.jqsrt.2014.06.020.

Details of the γ_{air} in HITRAN

Values for HO_2 γ_{air}

- ✓ We use the experimental results for the measured transitions in the specific bands.

Wavenumber(cm^{-1})	γ_{air}	Error Code	Ref. Code
1411.182082	0.107	5	1
1411.182506	0.107	5	1
20.869791	0.0955	6	4
21.402922	0.0948	7	4
21.671709	0.0836	6	4
1060.171729	0.111	6	5
1060.185559	0.085	5	5
1062.089333	0.087	5	5
1062.090479	0.087	5	5
1062.101994	0.114	4	5

1062.164996	0.079	5	5
1062.171305	0.074	4	5
1062.235623	0.108	4	5
1062.700079	0.088	3	5
1062.715515	0.099	5	5
1064.630080	0.096	5	5
1064.630900	0.096	5	5
1064.638797	0.104	5	5
1064.695843	0.094	4	5
1064.709590	0.104	4	5
1064.767798	0.095	4	5
1064.709590	0.079	4	5
1064.767798	0.090	4	5
1065.203385	0.107	5	5
1065.220768	0.098	3	5

- ✓ We also use weighted average experimental values for all the transitions with corresponding rotational quantum numbers (in all the bands).

Transitions ($N' K_a' K_c'$- $N'' K_a'' K_c''$)	γ_{air}_exp	γ_{air}_weighted mean	Error Code	Ref. Code
3 0 3 - 3 1 2	0.1244(104)	0.1244	5	3
3 1 2 - 3 0 3	0.1447(184)	0.1447	4	3
4 0 4 - 4 1 3	0.1251(81)	0.1204	5	3
	0.1178(146)			
4 1 3 - 4 0 4	0.1399(111)	0.1399	5	3
5 0 5 - 5 1 4	0.1421(94)	0.1136	4	3
	0.0948(143)			
5 1 4 - 5 0 5	0.1307(106)	0.1185	5	3
	0.0855(39)			
6 0 6 - 6 1 5	0.0967(112)	0.0967	4	3
6 1 5 - 6 0 6	0.1169(132)	0.1169	4	3
7 0 7 - 7 1 6	0.0901(113)	0.0901	4	3
7 1 6 - 7 0 7	0.0823(22)	0.1088	6	3
	0.1174(68)			
8 0 8 - 9 0 9	0.1394(188)	0.1394	4	3
8 1 7 - 7 1 6	0.1170(115)	0.1190	4	3
	0.1207(132)			
8 1 7 - 8 0 8	0.1210(75)	0.1083	5	3
	0.0959(77)			
8 1 8 - 7 1 7	0.1185(30)	0.1252	6	3
	0.1277(80)			
9 1 8 - 8 1 7	0.1225(116)	0.1121	5	3
	0.0993(94)			

9 1 8 - 9 0 9	0.1030(110)	0.1030	4	3
9 1 9 - 8 1 8	0.107(9)	0.1070	5	1
10 1 9 - 10 0 10	0.0955(17)	0.0955	6	4
10 1 10 - 9 1 9	0.0948(15)	0.0948	7	4
10 2 8 - 9 2 7	0.1308(266)	0.1308	3	3
10 2 9 - 9 2 8*	0.0836(25)	0.0836	6	4
	0.1548(56)			3
	0.1204(158)			3
11 2 9 - 10 2 8	0.0882(66) 0.0780(33)	0.0848	5	3
11 2 10 - 10 2 9	0.1128(69)	0.1128	5	3
13 0 13 - 14 0 14	0.079(13) 0.090(12)	0.0843	4	5
13 1 13 - 14 1 14	0.107(5) 0.098(21)	0.0997	4	5
13 2 11 - 14 2 12	0.104(5) 0.104(13)	0.1040	5	5
13 2 12 - 14 2 13	0.094(9) 0.095(13)	0.0946	4	5
13 3 10 - 14 3 11	0.096(8)	0.0960	5	5
13 3 11 - 14 3 12	0.096(8)	0.0960	5	5
14 1 14 - 15 1 15	0.088(18) 0.099(5)	0.0904	4	5
14 2 12 - 15 2 13	0.114(11) 0.079(4)	0.1047	5	5
14 2 13 - 15 2 14	0.074(8) 0.108(21)	0.0986	4	5
14 3 11 - 15 3 12	0.087(7)	0.0870	5	5
14 3 12 - 15 3 13	0.087(7)	0.0870	5	5
15 1 15 - 16 1 16	0.111(4) 0.085(6)	0.0954	5	5

*For transition [10 2 9 - 9 2 8], we have three measurements in two different bands. And we choose the best experimental result γ_{air} =0.0836 instead of the average value.

✓ For the rest of these transitions, we use the linear extrapolation (from Table2) up to (*N"+0.2Ka"*) < 17. And for (*N"+0.2Ka"*) > 17, γ_{air} (16.2) = 0.0930 will be used.
The error code calculated to be 4, and the ref. number will be 6 represent this report.

Ref table for HO_2 γ_{air}

For old HO_2 γ_{air} ref:

Half-widths (air)

1. D.D. Nelson and M.S. Zahniser "Air broadening measurements for the ν_2 vibrational band of the hydroperoxyl radical," *J.Mol.Spectrosc.* **166,** 273-279 (1994).

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Add new references(3-6):

[3] Ibrahim N, Thiebaud J, Orphal J, Fittschen C. Air-broadening coefficients of the HO_2 radical in the $2\nu_1$ band measured using cw-CRDS. J Mol Spectrosc 2007;242:64–9. doi:10.1016/j.jms.2007.02.007.

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[5] Minamida M, Tonokura K. Air broadening coefficients for the ν_3 band of hydroperoxyl radicals. J Quant Spectrosc Radiat Transf 2014;148:65–9. doi:10.1016/j.jqsrt.2014.06.020.

[6] This report for linear fit of HO_2 γ_{air}

NB. The file provided in this report is in the traditional .par format but this data can also be retrieved on www.hitran.org. The universal reference numbers on www.hitran.org do not correspond to the ones here as they are not tied to the .par format. However the mapping between these reference indices is provided when retrieving data from www.hitran.org.