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Research Article

Calculation of the Absorption Cross Sections of Some Molecules from GEISA Database at the Wavelengths of Isotopically Different CO_2 Lasers

Asylkhan Rakhymzhan[1] and Alexey Chichinin[1,2]

[1] *Institute of Chemical Kinetics and Combustion, Novosibirsk 630090, Russia*
[2] *Novosibirsk State University, Novosibirsk 630090, Russia*

Correspondence should be addressed to Alexey Chichinin; chichinin@kinetics.nsc.ru

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A calculation of the absorption cross section of some molecules (NH_3, C_2H_4, CO_2, O_3, NO_2, PH_3, HNO_3, SF_6, CH_3OH, HCOOH, OCS, CH_3CN, C_2H_6, SO_2, and H_2O) at the wavelengths transmitted by a CO_2 laser filled with different isotopes ($^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{12}C^{18}O_2$, $^{14}C^{16}O_2$, $^{14}C^{18}O_2$, $^{13}C^{18}O_2$, and $^{12}C^{16}O^{18}O$) is presented. The spectroscopical parameters for the molecules from GEISA database have been used. Hence the selection of the molecules was substantially based on the availability of the parameters in the database. The results of the calculations may be used in designing the differential absorption technique for remote monitoring of these molecules. The pressure and temperature dependence of the cross sections are described by K_T and K_P coefficients; these coefficients were calculated for the largest absorption cross sections for each molecule. The absorption cross sections of CH_3OH and HCOOH at low pressures for all these CO_2 lasers are also presented. These calculations are provided for design of new CO_2-laser-pumped far-infrared lasers.

1. Introduction

In this paper we report molecular absorption cross sections $\sigma(M)$ at CO_2-laser emission frequencies for several selected gases of atmospheric relevance ($M = NH_3$, C_2H_4, CO_2, O_3, NO_2, PH_3, HNO_3, SF_6, CH_3OH, HCOOH, OCS, CH_3CN, C_2H_6, SO_2, and H_2O). This information may be useful mainly in the differential absorption (Light Detection and Ranging) LIDAR technique for remote measurement of the gas species [1–8] and also may be used to monitor the CO_2 content in fuel combustion products [9], remote sensing of gases in human breath [10], or multiphoton dissociation processes or to measure water vapor concentration and wind speed vector in the plume of volcano [11, 12]. Note that the LIDAR technique sometimes is used for remote sensing of some exotic gases, like, for example, chemical warfare [13].

In some cases (CH_3OH and HCOOH) it also may be used in designing optically pumped FIR (far infrared=THz) lasers where CO_2 laser is used as a source of a pump radiation [14]. Also, the absorption of CO_2-laser radiation by a cell with a mixture of some of these gases is used in our lab for quick check and assignment of the CO_2-laser lines.

The focus of the present study is to predict absorption cross section in pure air at wavelengths of seven isotopic CO_2 lasers: $^{12}C^{16}O_2$ (normal), $^{13}C^{16}O_2$, $^{12}C^{18}O_2$, $^{14}C^{16}O_2$, $^{14}C^{18}O_2$, $^{13}C^{18}O_2$, and $^{12}C^{16}O^{18}O$, which we hereafter denote as 26-, 36-, 28-, 46-, 48-, 38-, and 268-lasers.

In the clear atmosphere, absorption at 9–11 μm is due primarily to water vapor and carbon dioxide. Since the fraction of CO_2 in the atmosphere is about 3.8×10^{-4} and $\sigma(CO_2) \sim 10^{-22}$ cm^2, the resonant absorption of 50% of the 26-laser radiation by atmospheric molecules occurs at the distance about 7 km. This distance may be not large enough for typical LIDAR applications, like monitoring of air pollution over the large town or early detection of small forest fires [15, 16]. Also, the fluctuations of the CO_2 concentration in the atmosphere decrease strongly the accuracy of the LIDAR based on the 26-laser. Hence the first advantage of latter six

CO_2 lasers over conventional 26-laser is low attenuation from atmospheric CO_2, which may extend strongly the detection distance and/or the accuracy of the LIDAR. Moreover, these isotopically substituted CO_2 lasers may be used to detect the concentration of CO_2 in the atmosphere or, more simply, to monitor the CO_2 content in fuel combustion products [9].

Another advantage is another set of wavelengths; sometimes it makes it possible to detect molecules, unavailable for conventional 26-laser LIDAR.

It is important to note that the use of CO_2 lasers for LIDAR remote sensing offers some advantages over that of the more current LIDAR experiments being conducted using the fundamental absorption transitions of hydrocarbons near 3 to 4 μm and CW Quantum Cascade Lasers, in that the absorption values near 10 μm are not too high and not too low for remote sensing at ranges of a few hundred meters, and the output power of the CO_2 laser is high offering good detection ranges.

Note that commercially available CO_2 lasers often may be filled with different isotopic gases (e.g., PL3 series from Edinburgh Photonics). Also, CO_2 lasers make up to 10^8 shots without changing of the gas mixture (e.g., InfraLight series of CO_2 lasers); hence there is no large difference, which isotopic modification of CO_2 gas to use.

This work was greatly facilitated by usage of GEISA spectroscopical database [17], and only the molecules from the database were involved in calculations. We have not included several gases (N_2H_4, C_6H_6, C_2Cl_4, C_2HCl_3, C_2H_3Cl, C_2H_5SH, $C_2H_4Cl_2$, CF_2Cl_2, and $CFCl_3$) which may be detected by CO_2 lasers [18], since no information is available on their absorption cross sections in the GEISA and HITRAN databases.

There were a lot of experimental measurements of the absorption coefficients at 26-laser frequencies. The most popular molecules are SF_6 [19–21], C_2H_4 [22–24], and NH_3 [22–26], and the list of references here is very large. A lot of σ(M) for more complicated molecules are also reported in the literature, for example, for acetonitrile, benzene, cyclohexane, 1,2-dichloroethane, ethyl acetate, freon-12, freon-113, furan, isopropanol, methyl chloroform, methyl ethyl ketone, *t*-butanol, vinyl chloride, and iodopropane [27]; seven hydrazine fuel gases [28]; hydrazine, unsymmetrical dimethylhydrazine, and monomethylhydrazine [29]; C_2H_4, $C_2H_3Cl_3$, C_2HCl_3, and Freon-113 [3]; and triacetone triperoxide [8].

However, much less information is available regarding σ(M) of CO_2 lasers other than 26-laser. For example, we know the measurements of $\sigma(H_2O)$ at 26-, 36-, and 46-laser wavelengths [30], $\sigma(ClO_2)$ at 28-laser wavelengths [31], $\sigma(NH_3)$ at a 36-laser [32]. Also, the photoacoustic spectroscopy has been used to determine σ(M) for M = NH_3, CCl_2F_2, $CHClF_2$, $CFCl_3$, and $CClF_3$ at 36-laser wavelengths [33].

To the best of our knowledge, the FIR lasers normally are pumped by 26-lasers or, much rarely, by 36-laser [34–37]; the other CO_2 lasers are used very rarely [38, 39]. Note that while 26-laser has about 100 laser lines, using different isotopic CO_2 lasers gives up to 1000 lines; hence the amount of different FIR-lasers pumped by CO_2 lasers should increase accordingly.

With this in mind, we performed the calculation which hopefully provides the information of the quality comparable with that of the experimental studies. We hope that it will stimulate using isotopically different CO_2 lasers for different applications.

2. Results

Assuming Lorentzian line shapes, we calculated the absorption cross sections σ(M) at all possible CO_2-laser frequencies. Tables 1, 2, and 3 show σ(M) for 26-, 36-, and 28-lasers, respectively, for CO_2-laser lines between P(40) and R(40), excluding the range P(6)–R(6). Atmospheric pressure $P_0 = 1$ bar and temperature $T_0 = 296$ K are assumed everywhere, and the self-broadening is neglected (i.e., [M]≪[air]). The following expressions were used:

$$\sigma(\mathrm{M}) = \sum_i \frac{S_i(T)}{\pi} \frac{\Delta\nu_i(P,T)}{\Delta\nu_i^2(P,T) + \left(\nu - \nu_i - \delta_i P\right)^2},$$
$$S_i(T) = S_{i0}\left(\frac{T_0}{T}\right)^L \exp\left(-\frac{E_i}{kT} + \frac{E_i}{kT_0}\right), \quad (1)$$
$$\Delta\nu_i(P,T) = \Delta\nu_{i0}\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)^{m_i},$$

where the index i labels all transitions in molecule M, $S_i(T)$ is intensity of the ith spectral line, $S_{i0} = S_i(T_0)$, $\Delta\nu_i(P,T)$ is Lorentzian width, $\Delta\nu_{i0} = \Delta\nu_i(P_0,T_0)$, ν_i is the absorption maximum frequency of the ith spectral line, δ_i is the pressure shift of the line transition, E_i is the energy of the lower state for ith transition, $L = 1$ for linear molecules like CO_2 and $L = 3/2$ for nonlinear molecules, P and T are air pressure and temperature, respectively, and k is Boltzmann constant.

The parameters ν_i, S_{i0}, $\Delta\nu_{i0}$, m_i, δ_i, and E_i are taken from GEISA database for each transition of each M molecule. Note that the pressure shifts δ_i are given in the database only for CH_3CN and NO_2 molecules. All of them are rather small ($\approx 10^{-3}$ cm^{-1}/atm), and they change only the third digit in calculated absorption cross sections. We hope that there is the same situation with all other molecules; hence we present the cross sections with three-digit accuracy; the last digit may be wrong due to the pressure shifts. All CO_2-laser frequencies were taken from Freed et al. [40].

In Table 4 we present the "best" laser transitions for each isotopic variation of CO_2 laser and for each molecule M. The pressure and temperature dependence of the cross sections are described by K_T and K_P coefficients as $K_T = d\ln\sigma/d\ln T$, $K_P = d\ln\sigma/d\ln T$, and the coefficients have been calculated from (1) and presented in Table 4 also.

It is not easy task to point out the "best" CO_2-laser line for detection of molecule M. Normally the "best" CO_2-laser line should lie in the ranges R(10)–R(40), P(10)–P(40) and has the largest absorption by M molecules; if the largest σ(M) values occur outside these ranges, we mark it by asterisk shown in the table also. However, if the largest σ(M) values occur at marginal lines of CO_2 laser and are much larger than all other cross sections, we present this marginal line only.

Table 1: Absorption cross sections of $^{12}C^{16}O_2$-lasers radiation (for all the units are 10^{-20}) cm^2, but for H_2O, the units are 10^{-23} cm^2).

Line	$00^\circ1 \rightarrow 10^\circ0, 10.4\,\mu m$[a]										$00^\circ1 \rightarrow 02^\circ0, 9.4\,\mu m$[b]								
	ν, cm^{-1}	CO_2	NH_3	C_2H_4	CH_3OH	O_3	PH_3	HNO_3	SF_6	H_2O	ν, cm^{-1}	CO_2	NH_3	C_2H_4	CH_3OH	HCOOH	O_3	PH_3	H_2O
P(40)	924.97398	0.0019	3.73	2.12	0.006	0.003	0.262	2.91	1.38	3.2576	1027.38217	0.0030	7.67	2.58	15.9	1.01	21.7	0.316	0.0753
P(38)	927.00832	0.0025	16.5	7.86	0.006	0.003	0.075	1.95	1.68	0.0065	1029.44209	0.0038	0.656	3.45	12.8	1.26	32.6	0.446	1.1490
P(36)	929.01744	0.0030	32.9	4.66	0.006	0.004	0.053	1.31	2.10	0.4532	1031.47743	0.0048	2.18	1.68	28.5	1.47	27.1	15.5	0.0072
P(34)	931.00143	0.0039	55.2	5.91	0.007	0.004	0.028	0.892	2.69	0.0023	1033.48800	0.0059	13.5	7.19	103	3.00	13.3	2.08	0.0056
P(32)	932.96042	0.0046	57.6	4.42	0.007	0.004	0.105	0.627	3.57	0.0092	1035.47362	0.0070	0.930	2.36	8.62	1.06	19.8	0.318	0.0027
P(30)	934.89450	0.0054	3.33	6.12	0.007	0.005	0.375	0.476	5.03	0.0041	1037.43411	0.0083	0.234	4.97	6.20	1.10	22.8	1.76	0.0103
P(28)	936.80375	0.0065	1.06	4.95	0.008	0.005	1.34	0.402	8.01	0.0035	1039.36931	0.0096	0.198	0.77	4.30	1.43	32.7	1.80	0.0583
P(26)	938.68826	0.0072	1.02	7.86	0.008	0.006	0.225	0.268	16.1	0.2236	1041.27907	0.0109	0.391	0.81	15.8	1.01	21.5	7.94	0.0163
P(24)	940.54810	0.0079	0.364	8.62	0.009	0.007	0.036	0.204	42.5	0.0205	1043.16324	0.0121	0.915	1.26	15.0	1.64	2.71	5.99	0.0134
P(22)	942.38334	0.0086	0.245	5.38	0.009	0.008	0.037	0.159	119	0.0049	1045.02167	0.0134	1.62	3.04	25.3	3.28	7.20	16.2	0.0122
P(20)	944.19403	0.0094	0.347	7.63	0.010	0.009	5.45	0.131	262	0.0106	1046.85423	0.0138	13.2	1.54	14.8	2.10	16.9	4.44	0.0045
P(18)	945.98023	0.0095	0.395	13.8	0.010	0.010	5.72	0.104	349	0.0150	1048.66081	0.0142	1.06	2.88	29.3	1.64	23.3	6.28	0.0148
P(16)	947.74198	0.0094	2.30	21.4	0.011	0.015	0.134	0.079	862	0.1346	1050.44128	0.0142	0.702	0.69	29.7	1.85	32.8	0.88	0.0202
P(14)	949.47931	0.0092	1.84	133	0.011	0.013	0.030	0.060	412	0.0261	1052.19555	0.0137	1.40	0.47	48.6	2.06	47.4	8.53	0.0030
P(12)	951.19226	0.0085	2.57	17.3	0.012	0.026	0.079	0.046	354	0.0054	1053.92350	0.0128	3.70	0.47	24.8	2.43	44.0	4.62	0.0022
P(10)	952.88085	0.0075	0.675	13.0	0.013	0.022	0.045	0.037	67.9	0.0038	1055.62507	0.0118	1.08	1.28	30.8	3.70	23.0	3.14	0.0040
P(8)	954.54509	0.0063	1.01	5.83	0.014	0.030	4.30	0.032	22.3	0.0431	1057.30016	0.0096	0.208	2.94	26.5	3.14	49.2	2.10	0.0048
P(6)	956.18498	0.0049	2.86	7.96	0.015	0.043	3.78	0.027	12.2	0.0093	1058.94871	0.0073	0.377	1.18	39.0	4.65	34.4	3.42	0.0804
R(6)	966.25036	0.0057	124	7.99	0.030	0.088	0.284	0.011	2.07	0.0159	1069.01409	0.0086	0.541	1.24	11.5	10.6	2.93	1.48	0.0317
R(8)	967.70723	0.0071	102	3.68	0.037	0.128	0.255	0.010	1.76	0.0088	1070.46231	0.0108	7.04	1.33	11.1	13.3	1.76	1.71	0.0978
R(10)	969.13955	0.0083	2.62	5.26	0.059	0.150	0.099	0.010	1.53	0.0068	1071.88377	0.0125	0.972	1.47	9.16	16.6	0.871	9.28	0.0344
R(12)	970.54724	0.0092	1.09	7.58	0.679	0.160	0.127	0.009	1.34	0.3381	1073.27848	0.0139	1.12	0.391	7.25	16.6	0.749	4.55	0.1450
R(14)	971.93026	0.0097	27.6	6.51	1.44	0.215	0.844	0.009	1.18	0.0225	1074.64649	0.0149	2.37	0.257	5.15	23.0	0.616	3.91	0.0539
R(16)	973.28852	0.0099	0.485	3.76	1.60	0.286	0.234	0.009	1.06	0.1583	1075.98782	0.0153	52.1	1.12	4.39	27.0	0.470	2.07	3.2810
R(18)	974.62194	0.0098	0.270	2.39	0.81	0.397	0.834	0.008	0.953	0.0270	1077.30252	0.0152	0.450	2.17	4.28	29.5	0.351	4.00	0.0822
R(20)	975.93044	0.0095	0.193	4.70	3.33	0.429	0.868	0.008	0.864	3.3148	1078.59064	0.0147	0.226	0.520	2.23	33.8	0.408	1.15	0.0213
R(22)	977.21392	0.0089	0.152	12.7	1.78	0.377	0.574	0.008	0.789	0.0128	1079.85226	0.0139	0.225	0.289	2.01	35.1	0.494	1.60	0.0118
R(24)	978.47229	0.0081	0.126	19.3	2.09	0.491	0.846	0.008	0.725	0.0044	1081.08743	0.0134	0.274	0.689	0.718	47.8	0.820	3.53	0.0127
R(26)	979.70542	0.0073	0.109	8.84	3.68	0.520	0.618	0.007	0.669	0.0028	1082.29624	0.0116	0.511	0.276	0.622	35.5	0.446	0.55	0.0829
R(28)	980.91321	0.0063	0.098	10.3	1.32	0.639	3.51	0.007	0.620	0.0054	1083.47878	0.0102	1.90	0.101	0.394	59.4	0.443	0.36	0.0587
R(30)	982.09553	0.0054	0.092	1.47	4.58	0.674	4.60	0.007	0.578	0.0123	1084.63514	0.0089	303	0.671	0.687	57.1	0.359	0.73	0.6919
R(32)	983.25225	0.0046	0.089	3.91	2.91	1.65	8.01	0.007	0.540	0.0046	1085.76544	0.0077	2.35	0.183	0.068	47.1	0.351	5.23	0.0261
R(34)	984.38323	0.0037	0.090	2.39	8.29	0.823	4.43	0.006	0.507	0.0246	1086.86979	0.0062	0.945	0.134	0.053	59.6	0.304	1.35	0.0098
R(36)	985.48831	0.0030	0.097	10.7	3.93	1.05	5.83	0.006	0.478	0.0036	1087.94831	0.0051	0.403	1.39	0.046	54.1	0.533	5.94	0.3016
R(38)	986.56735	0.0024	0.116	14.7	9.68	1.21	2.94	0.006	0.451	0.0104	1089.00112	0.0041	1.73	0.109	0.041	69.9	0.299	0.53	0.0072
R(40)	987.62018	0.0019	0.574	18.8	5.04	1.42	2.12	0.006	0.427	0.1652	1090.02837	0.0036	0.672	0.252	0.038	65.5	0.507	3.16	0.0054

[a] Cross sections for HCOOH are omitted; $\sigma(\text{HCOOH}) < 10^{-21}$ cm^2.
[b] Cross sections for HNO_3 and SF_6 are omitted; $\sigma(HNO_3) < 3 \times 10^{-23}$ cm^2; and $\sigma(SF_6) < 1.1 \times 10^{-21}$ cm^2.

Table 2: Absorption cross sections of $^{13}C^{16}O_2$-lasers radiation (for all the units are 10^{-20} cm^2, but for H_2O, the units are 10^{-23} cm^2).

Line	$00^{\circ}1 \rightarrow 10^{\circ}0, 11\,\mu m$[a]								$00^{\circ}1 \rightarrow 02^{\circ}0, 10\,\mu m$[b]									
	ν, cm^{-1}	CO_2	NH_3	C_2H_4	PH_3	HNO_3	SF_6	H_2O	ν, cm^{-1}	CO_2	NH_3	C_2H_4	CH_3OH	HCOOH	O_3	PH_3	SF_6	H_2O
P(40)	878.43359	0.00003	0.056	3.55	0.823	69.6	0.142	1.6272	980.80503	0.00190	0.099	6.85	1.32	0.051	0.603	1.32	0.625	0.0045
P(38)	880.37051	0.00005	0.055	2.93	0.413	26.7	0.150	0.0211	982.91254	0.00026	0.089	5.95	1.57	0.052	0.736	0.887	0.551	0.0054
P(36)	882.28741	0.00006	0.074	4.07	0.029	33.3	0.159	0.0222	984.99314	0.00015	0.093	4.92	2.11	0.053	0.764	2.58	0.490	0.0044
P(34)	884.18435	0.00005	0.111	2.59	0.026	37.1	0.169	0.1661	987.04662	0.00013	0.139	11.5	2.53	0.085	1.04	2.84	0.440	0.0455
P(32)	886.06142	0.00006	0.327	5.11	0.037	32.9	0.179	0.0348	989.07282	0.00010	0.251	1.61	2.88	0.099	1.82	19.1	0.398	0.0089
P(30)	887.91867	0.00009	58.5	5.77	0.026	38.5	0.190	0.0968	991.07153	0.00008	1.56	3.09	3.49	0.086	1.48	2.31	0.362	0.0085
P(28)	889.75616	0.00008	0.515	6.16	0.228	48.6	0.203	0.0461	993.04260	0.00008	10.1	2.16	4.57	0.110	3.81	7.59	0.331	0.0022
P(26)	891.57394	0.00009	4.53	2.93	0.312	40.8	0.216	0.0541	994.98585	0.00011	0.354	5.15	6.55	0.124	3.16	0.908	0.304	0.0037
P(24)	893.37207	0.00010	0.640	1.91	0.405	35.3	0.231	0.0037	996.90115	0.00008	0.143	22.1	8.66	0.128	5.04	0.736	0.280	0.0016
P(22)	895.15057	0.00013	0.157	3.09	0.389	50.6	0.247	0.0057	998.78832	0.00009	0.100	3.94	14.8	0.282	3.44	0.068	0.260	0.0028
P(20)	896.90948	0.00016	0.087	7.85	0.017	33.7	0.265	0.0036	1000.64726	0.00009	0.095	8.23	23.4	0.204	6.96	3.15	0.242	0.0364
P(18)	898.64883	0.00015	0.072	2.55	0.016	33.4	0.284	0.0017	1002.47781	0.00008	0.185	3.63	27.0	0.281	6.64	0.166	0.226	0.0033
P(16)	900.36865	0.00027	0.406	3.49	0.447	30.2	0.305	0.0018	1004.27987	0.00008	0.197	7.15	27.8	0.253	10.2	2.92	0.212	0.0282
P(14)	902.06895	0.00015	0.109	8.26	0.596	24.1	0.329	0.0037	1006.05332	0.00008	1.14	11.4	28.3	0.291	12.4	0.259	0.199	0.0020
P(12)	903.74974	0.00012	0.134	2.11	0.490	21.3	0.354	0.0039	1007.79807	0.00021	19.3	6.77	26.1	0.386	10.7	0.204	0.188	0.0054
P(10)	905.41104	0.00014	0.253	5.76	0.075	26.4	0.383	0.0183	1009.51402	0.00007	0.699	6.54	18.4	0.392	17.5	0.340	0.177	0.0105
P(8)	907.05284	0.00009	1.17	1.43	1.347	22.1	0.415	0.0379	1011.20110	0.00006	58.0	5.34	23.2	0.423	8.58	2.23	0.168	0.0639
P(6)	908.67515	0.00011	6.65	18.5	0.034	19.4	0.451	0.6599	1012.85922	0.00005	7.21	2.47	19.8	0.597	10.1	0.099	0.159	0.0031
R(6)	918.74396	0.00080	5.33	4.27	0.182	9.07	0.830	0.0581	1022.92804	0.00016	0.425	2.44	10.8	0.648	29.2	0.563	0.120	0.0169
R(8)	920.21948	0.00014	1.01	2.49	0.027	8.22	0.924	0.0159	1024.36774	0.00009	0.315	4.54	18.3	0.693	30.6	9.46	0.115	2.0415
R(10)	921.67529	0.00020	3.94	6.48	0.047	5.97	1.04	0.1895	1025.77827	0.00013	0.688	2.01	12.1	0.804	18.5	1.61	0.111	0.0241
R(12)	923.11133	0.00034	2.35	7.93	3.736	4.15	1.17	0.0353	1027.15966	0.00036	40.1	11.1	14.1	1.01	27.3	1.05	0.107	0.0417
R(14)	924.52755	0.00019	2.12	5.52	4.968	3.16	1.32	0.0856	1028.51193	0.00014	0.657	1.92	10.9	1.29	39.6	0.293	0.103	0.2480
R(16)	925.92391	0.00016	11.1	5.39	1.391	2.50	1.51	0.0223	1029.83513	0.00022	1.22	2.59	11.6	1.32	24.4	4.35	0.100	0.1042
R(18)	927.30032	0.00028	119	2.81	0.166	1.83	1.73	0.0060	1031.12930	0.00029	1.45	2.17	25.2	1.59	23.8	1.31	0.097	0.0084
R(20)	928.65672	0.00028	48.6	3.72	0.033	1.40	2.01	0.0151	1032.39450	0.00021	9.72	3.79	52.2	1.71	34.6	3.37	0.094	0.0245
R(22)	929.99305	0.00017	61.6	7.50	0.159	1.04	2.36	0.0048	1033.63081	0.00118	8.69	2.87	98.2	2.29	16.0	1.48	0.091	0.0048
R(24)	931.30921	0.00031	92.2	6.99	0.026	0.858	2.80	0.0020	1034.83829	0.00032	3.15	0.822	11.3	1.10	41.4	0.571	0.089	0.0033
R(26)	932.60512	0.00033	29.0	3.83	0.064	0.699	3.38	0.0037	1036.01703	0.00023	0.522	1.90	9.385	1.32	22.8	0.586	0.087	0.0031
R(28)	933.88070	0.00035	12.9	4.32	4.787	0.519	4.16	0.0018	1037.16713	0.00063	0.259	4.61	6.56	1.01	18.4	1.12	0.084	0.0056
R(30)	935.13584	0.00054	3.89	2.31	0.778	0.407	5.29	0.0093	1038.28870	0.00019	0.187	2.46	8.77	1.29	23.7	7.02	0.082	0.5229
R(32)	936.37044	0.00028	1.83	4.27	0.305	0.356	7.09	0.0076	1039.38184	0.00934	0.201	0.755	4.29	1.35	32.5	1.70	0.080	0.0622
R(34)	937.58440	0.00029	4.36	7.51	0.100	0.345	10.3	0.0092	1040.44668	0.00036	0.206	1.79	9.24	0.92	28.3	1.31	0.079	0.3301
R(36)	938.77760	0.00287	0.711	8.95	0.122	0.297	16.7	0.0647	1041.48333	0.00122	0.258	1.50	11.7	1.61	21.1	5.00	0.077	0.0152
R(38)	939.94992	0.00021	0.290	8.38	0.020	0.239	30.3	0.0094	1042.49195	0.00045	0.276	1.33	7.18	2.44	3.34	0.876	0.075	0.9977
R(40)	941.10124	0.00023	0.352	9.78	0.020	0.181	58.7	0.3694	1043.47268	0.00068	0.450	1.45	19.0	1.81	2.85	1.22	0.074	0.0074

[a] Cross sections for CH_3OH, HCOOH, and O_3 are omitted; $\sigma(CH_3OH) < 10^{-22}$ cm^2; $\sigma(HCOOH) < 5 \times 10^{-23}$ cm^2, and $\sigma(O_3) < 9 \times 10^{-23}$ cm^2.

[b] Cross sections for HNO_3 are omitted; $\sigma(HNO_3) < 7 \times 10^{-23}$ cm^2.

Table 3: Absorption cross sections of $^{12}C^{18}O_2$-lasers radiation (for all the units are 10^{-20} cm^2, but for H_2O, the units are 10^{-23} cm^2).

Line	$00^{\circ}1 \rightarrow 10^{\circ}0$, 10.5 μm[a]										$00^{\circ}1 \rightarrow 02^{\circ}0$, 9 μm[b]								
	ν, cm^{-1}	CO_2	NH_3	C_2H_4	CH_3OH	O_3	PH_3	HNO_3	SF_6	H_2O	ν, cm^{-1}	CO_2	NH_3	C_2H_4	CH_3OH	HCOOH	O_3	PH_3	H_2O
P(40)	933.98651	0.00023	7.92	3.30	0.007	0.004	1.81	0.553	4.24	0.0019	1052.26317	0.00763	1.41	0.495	45.8	2.24	59.2	4.32	0.0027
P(38)	935.88894	0.00013	14.9	2.92	0.008	0.005	0.217	0.388	6.27	0.0070	1054.01438	0.00542	5.55	0.354	24.1	3.24	39.3	2.96	0.0021
P(36)	937.76432	0.00014	2.43	5.59	0.008	0.006	0.143	0.279	11.0	0.0056	1055.74733	0.00352	0.755	0.775	26.8	3.49	35.0	4.43	0.0047
P(34)	939.61272	0.00022	0.586	8.01	0.008	0.006	0.023	0.224	25.3	0.0054	1057.46193	0.00235	0.194	2.37	33.8	4.15	29.9	2.79	0.0052
P(32)	941.43421	0.00020	0.313	7.15	0.009	0.007	0.021	0.170	70.9	0.0357	1059.15808	0.00168	0.187	1.61	27.5	5.50	26.6	17.3	0.3398
P(30)	943.22886	0.00020	0.291	8.33	0.009	0.009	0.094	0.121	180	0.0044	1060.83568	0.00090	0.178	0.436	28.0	4.57	21.4	0.785	0.0601
P(28)	944.99673	0.00019	0.341	10.0	0.010	0.013	4.10	0.100	319	0.2328	1062.49464	0.00040	0.277	0.547	28.3	6.06	36.7	3.25	0.0111
P(26)	946.73787	0.00039	0.435	16.5	0.010	0.014	0.139	0.075	418	0.1333	1064.13489	0.00024	1.01	0.686	18.2	6.45	9.19	4.82	0.0116
P(24)	948.45233	0.00022	8.59	31.7	0.011	0.014	0.052	0.059	473	0.9095	1065.75632	0.00046	48.1	0.731	21.7	8.65	15.0	0.723	0.1324
P(22)	950.14015	0.00022	0.772	51.2	0.012	0.019	0.021	0.049	476	0.0190	1067.35888	0.00124	1.32	0.523	15.3	12.3	4.85	2.05	0.0094
P(20)	951.80137	0.00023	44.0	14.6	0.013	0.017	0.025	0.040	215	0.0042	1068.94248	0.00500	0.576	1.42	12.4	9.70	3.14	0.949	0.0393
P(18)	953.43603	0.00022	0.402	7.47	0.013	0.025	0.112	0.035	42.0	0.0048	1070.50705	0.00822	11.1	1.42	10.4	13.1	1.71	2.21	0.0788
P(16)	955.04415	0.00022	0.905	11.7	0.014	0.026	0.990	0.030	18.1	0.1436	1072.05253	0.00232	1.15	3.79	10.1	19.7	0.596	2.09	0.0436
P(14)	956.62576	0.00022	0.909	7.80	0.015	0.041	0.246	0.027	10.8	0.0051	1073.57887	0.00101	1.55	0.617	6.17	17.0	0.388	4.11	0.0368
P(12)	958.18087	0.00019	2.76	6.31	0.017	0.040	0.142	0.018	7.31	0.0033	1075.08599	0.00063	9.99	0.250	6.53	21.7	0.890	8.62	0.0940
P(10)	959.70950	0.00015	6.090	7.24	0.018	0.040	0.063	0.016	5.34	0.1043	1076.57386	0.00053	1.62	0.316	3.47	25.7	0.382	1.33	0.6481
P(8)	961.21166	0.00006	10.7	3.56	0.020	0.058	0.087	0.017	4.10	0.0092	1078.04242	0.00056	0.262	0.227	2.65	30.2	0.337	1.21	0.0334
P(6)	962.68734	0.00009	16.0	4.63	0.022	0.077	0.053	0.013	3.27	0.0161	1079.49163	0.00077	0.541	0.973	1.73	37.8	0.352	0.538	0.0132
R(6)	971.63344	0.00066	5.32	2.18	1.60	0.305	0.376	0.009	1.22	0.0693	1088.43774	0.00069	0.500	0.118	0.044	68.5	0.474	0.460	0.0092
R(8)	972.91019	0.00046	0.671	3.69	1.18	0.315	0.889	0.009	1.09	0.0253	1089.74096	0.00046	1.71	0.748	0.039	62.8	0.349	0.461	0.0069
R(10)	974.16030	0.00035	0.315	2.27	1.42	0.257	4.12	0.009	0.98	0.13597	1091.02466	0.00256	0.494	0.345	0.035	64.7	0.341	2.60	0.0203
R(12)	975.38372	0.00029	0.219	10.3	1.86	0.223	0.855	0.008	0.89	0.06139	1092.28884	0.00039	0.682	0.061	0.032	58.1	0.239	1.75	0.0056
R(14)	976.58041	0.00028	0.170	6.73	1.12	0.322	0.935	0.008	0.82	0.04755	1093.53351	0.00028	3.06	0.670	0.029	60.9	0.245	0.184	0.0064
R(16)	977.75031	0.00028	0.139	7.77	3.71	0.344	2.88	0.008	0.76	0.00860	1094.75869	0.00068	1.64	0.654	0.027	49.7	0.546	0.205	0.0159
R(18)	978.89336	0.00031	0.119	18.3	1.15	0.669	1.80	0.007	0.70	0.00365	1095.96438	0.00008	3.93	0.080	0.025	55.0	0.259	1.73	0.0256
R(20)	980.00950	0.00043	0.106	2.27	4.07	0.569	0.884	0.007	0.65	0.00286	1097.15060	0.00006	0.610	0.200	0.024	41.3	0.306	0.702	0.0127
R(22)	981.09866	0.00082	0.097	3.50	1.43	0.766	2.86	0.007	0.61	0.00823	1098.31739	0.00005	0.336	0.538	0.022	38.0	0.284	0.640	0.0109
R(24)	982.16077	0.00287	0.091	1.83	5.35	0.581	2.51	0.007	0.57	0.00986	1099.46477	0.00005	0.219	0.076	0.021	28.0	0.343	0.308	0.0319
R(26)	983.19575	0.00273	0.089	3.92	2.40	1.03	7.74	0.007	0.54	0.00442	1100.59277	0.00006	0.245	0.181	0.020	20.5	0.211	0.424	0.1863
R(28)	984.20351	0.00052	0.090	2.43	5.30	1.04	1.77	0.007	0.51	0.13352	1101.70143	0.00005	0.528	0.367	0.019	15.1	0.338	0.309	0.2239
R(30)	985.18397	0.00020	0.094	2.22	3.01	0.648	1.70	0.006	0.48	0.00385	1102.79079	0.00001	3.34	0.058	0.018	12.9	0.112	0.245	0.0393
R(32)	986.13704	0.00011	0.106	17.3	7.81	2.00	1.62	0.006	0.46	0.00541	1103.86091	0.00001	8.85	0.690	0.017	26.7	0.403	1.41	0.0131
R(34)	987.06260	0.00012	0.140	11.4	2.51	1.08	2.61	0.006	0.44	0.04930	1104.91182	0.00001	0.871	0.113	0.017	228	0.231	0.298	0.0123
R(36)	987.96056	0.00011	0.339	27.6	6.97	1.49	3.63	0.006	0.42	0.02590	1105.94358	0.00001	0.313	0.366	0.016	102	0.177	0.267	0.0115
R(38)	988.83081	0.00020	0.309	3.26	4.97	2.32	10.2	0.006	0.40	0.11022	1106.95625	0.00001	0.248	0.099	0.015	36.9	0.154	1.43	0.0145
R(40)	989.67323	0.00093	0.315	6.78	5.73	1.26	9.46	0.006	0.38	0.00456	1107.94989	0.00000	3.61	0.181	0.015	26.3	0.293	0.682	0.0275

[a] Cross sections for HCOOH are omitted; $\sigma(\text{HCOOH}) < 9 \times 10^{-22}$ cm^2.
[b] Cross sections for HNO_3 and SF_6 are omitted; $\sigma(HNO_3) < 7 \times 10^{-23}$ cm^2 and $\sigma(SF_6) < 6 \times 10^{-22}$ cm^2.

Table 4: For each CO_2 laser and for each molecule M, the laser transitions with the largest absorption by selected molecules are presented. The cross sections σ(M) (in 10^{-20} cm^2 units) and K_T and K_P coefficients are shown.

Laser	M	Transition	ν, cm^{-1}	σ(M)[a]	K_T	K_P
26	NH_3	10R(30)	1084.63514	303	0.38	−0.83
	C_2H_4	11P(14)	949.47931	133	0.16	−0.13
	O_3	10P(14)	1052.19555	47.4	−0.62	0.08
		10P(8)	1057.30016	49.2*	−0.02	−0.12
	NO_2	11P(48)	916.58177	0.143	3.11	−0.36
	PH_3	10P(22)	1045.02167	16.2	−0.19	−0.46
	HNO_3	11P(44)	920.82912	6.89	1.90	−0.02
	SF_6	11P(16)	947.74198	862	−0.02	−0.58
	CH_3OH	10P(34)	1033.48800	103	0.44	−0.05
	HCOOH	10R(28)	1083.47878	59.4	0.37	−0.22
	OCS	10P(32)	1035.47362	1.68	−0.13	−0.14
	CH_3CN	10R(16)	1075.98782	1.82	1.38	−0.30
	SO_2	10R(26)	1082.29624	0.430	2.26	−0.31
	SO_2	10R(40)	1090.02837	0.595*	1.54	0.15
	H_2O	11R(20)	975.93044	0.00331	6.47	−0.85
36	NH_3	11R(18)	927.30032	119	0.57	−0.87
	C_2H_4	10P(24)	996.90115	22.1	−0.14	−0.44
	CO_2	10R(32)	1039.38184	0.009	7.45	−0.93
	O_3	10R(24)	1034.83829	41.4	−0.02	−0.42
	NO_2	11P(38)	880.37051	0.461	1.43	−0.25
	PH_3	10P(32)	989.07282	19.1	0.92	−0.21
	HNO_3	11P(22)	895.15057	50.6	0.36	−0.01
		11P(40)	878.43359	69.6*	0.26	0.05
	SF_6	11R(42)	942.23141	110	0.87	0.14
		11R(44)	943.34030	189*	0.38	0.02
	CH_3OH	10R(22)	1033.63081	98.2	0.45	−0.07
	HCOOH	10R(38)	1042.49195	2.44	1.22	−0.23
	OCS	10R(36)	1041.48333	2.08	−0.14	−0.50
	CH_3CN	10R(10)	1025.77827	2.86	0.23	0.01
	C_2H_6	11P(48)	870.48389	0.493	0.85	0.06
	H_2O	9R(8)	1024.36774	0.00204	6.41	0.65
28	NH_3	11P(20)	951.80137	44.0	−0.89	−0.88
		11P(42)	932.05695	67.9*	−0.37	−0.27
	C_2H_4	11P(22)	950.14015	51.2	0.49	0.04
	CO_2	10P(18)	1070.50705	0.008	5.22	−0.50
		10P(44)	1048.70641	0.010*	6.19	−0.42
	O_3	10P(40)	1052.26317	59.2*	−0.38	−0.38
		10P(36)	1055.74733	35.0	−0.10	0.04
	NO_2	11P(42)	932.05695	0.021*	2.86	−0.54
		11P(34)	939.61272	0.013	3.56	−0.55
	PH_3	10P(32)	1059.15808	17.3	0.58	−0.87
	HNO_3	11P(34)	939.61272	0.224	2.39	0.20
		11P(42)	932.05695	0.756*	2.57	0.03
	SF_6	11P(22)	950.14015	476	−0.33	−0.21
	CH_3OH	10P(40)	1052.26317	45.8	0.42	−0.22
	HCOOH	10R(34)	1104.91182	228	−0.56	−0.26
	OCS	10P(28)	1062.49464	2.06	0.54	−0.58
	CH_3CN	10P(32)	1059.15808	3.74	−0.26	−0.30
	SO_2	10R(36)	1105.94358	1.73	0.80	−0.12
	H_2O	11P(24)	948.45233	0.000910	4.62	0.79

Table 4: Continued.

Laser	M	Transition	ν, cm^{-1}	σ(M)[a]	K_T	K_P
46	NH_3	9P(18)	967.44673	151	−0.95	−0.13
	C_2H_4	9P(36)	949.82361	75.5	0.55	−0.07
	CO_2	9P(38)	947.72257	0.009	6.83	−0.85
	O_3	9R(38)	1007.32003	14.4	1.51	−0.20
	NO_2	10R(18)	880.14964	0.617	1.99	−0.45
	PH_3	9R(12)	992.16155	20.1	−0.75	0.42
	HNO_3	10R(16)	878.74397	116	0.00	−0.16
	SF_6	9P(38)	947.72257	860	−0.01	−0.57
	CH_3OH	9R(36)	1006.33091	31.1	0.96	−0.19
	HCOOH	9R(40)	1008.28028	0.572	0.85	−0.04
	OCS	10R(14)	877.32170	2.41	1.16	−0.59
	CH_3CN	9R(16)	994.82189	0.839	1.88	−0.47
	C_2H_6	10P(4)	862.98995	0.666	0.98	−0.18
	H_2O	11R(16)	878.74397	0.000532	4.97	0.77
38	NH_3	10R(10)	1034.18567	86.9	−0.39	−0.22
	C_2H_4	11R(34)	949.30088	121	0.14	−0.19
	CO_2	10R(32)	1046.81398	0.011	6.41	−0.50
	O_3	10R(14)	1036.67254	33.4	−0.20	−0.28
		10R(8)	1032.91023	38.3*	−0.22	−0.39
		10R(40)	1050.77747	50.5*	−0.62	−0.15
	NO_2	11P(16)	916.81456	0.134	2.86	−0.36
	PH_3	10R(22)	1041.39099	11.3	−0.29	−0.65
		10R(6)	1031.61345	13.9*	−0.57	−0.29
	HNO_3	11P(38)	898.25437	35.3	0.43	−0.07
		11P(40)	896.42949	53.4*	−0.16	−0.03
	SF_6	11R(30)	947.29249	641	−0.06	−0.16
	CH_3OH	10R(10)	1034.18567	66.3	0.16	−0.04
		10R(8)	1032.91023	81.5*	0.79	−0.02
	HCOOH	10R(24)	1042.51764	2.50	1.22	−0.28
		10R(40)	1050.77747	4.01*	1.15	−0.25
	OCS	10R(12)	1035.43977	1.98	0.08	−0.52
	CH_3CN	10R(34)	1047.83586	3.57	−0.10	−0.62
	SO_2	10R(46)	1053.53509	0.024	4.78	0.00
	H_2O	11R(32)	948.30848	0.00577	5.06	−0.34
48	NH_3	9P(20)	967.55794	79.2	−1.48	0.56
	C_2H_4	9P(40)	950.27719	38.0	0.31	0.19
	CO_2	9P(18)	969.16198	0.008	6.48	−0.83
	O_3	9R(32)	1002.18855	11.4	2.01	−0.15
		9R(40)	1006.00000	11.8*	1.68	−0.22
	NO_2	10P(12)	880.59011	0.159	1.00	0.08
	PH_3	9R(14)	992.26858	21.3	−0.08	−0.29
	HNO_3	10P(14)	879.08844	90.0	−0.53	−0.08
	SF_6	9P(40)	950.27719	476	−0.23	−0.23
		9P(42)	948.42788	484*	−0.68	0.20
	CH_3OH	9R(36)	1004.13958	28.9	1.23	−0.25
	HCOOH	9R(34)	1003.17544	0.365	1.63	−0.06
	OCS	10P(30)	866.40889	6.03	−0.43	−0.39
	CH_3CN	10R(28)	907.29104	0.559	−0.06	−0.24
	C_2H_6	10P(36)	861.34626	0.777	0.46	−0.02
	H_2O	11P(24)	871.30294	0.00549	4.02	−0.29

Table 4: Continued.

Laser	M	Transition	ν, cm^{-1}	σ(M)[a]	K_T	K_P
268	NH_3	10P(32)	1046.35094	264	−0.52	−0.64
	C_2H_4	11P(21)	949.43752	149	0.23	−0.30
	CO_2	10R(11)	1081.07931	0.013	7.17	−0.95
	O_3	10P(27)	1050.83825	56.6	−0.54	−0.26
	NO_2	11P(37)	934.69411	0.067	3.71	0.03
	PH_3	11R(36)	988.95058	19.8	1.33	−0.21
		11R(42)	991.76694	38.6*	−1.11	0.02
	HNO_3	11P(50)	921.46702	6.33	2.00	−0.04
	SF_6	11P(23)	947.68595	851	0.00	−0.55
	CH_3OH	10P(46)	1033.08142	95.5	0.73	−0.08
	HCOOH	10R(24)	1089.24975	77.9	−0.33	−0.13
	OCS	10P(16)	1060.23019	2.20	0.14	−0.60
	CH_3CN	10P(24)	1053.46560	2.92	−0.12	−0.55
	SO_2	10R(36)	1095.95040	1.03	1.38	−0.22
	H_2O	9R(16)	1084.33484	0.00439	5.37	0.21

[a]Asterisk marks the cases where the σ(M) is large, but the CO_2 laser line is marginal. The values below 8×10^{-23} cm^2 are omitted.

Table 5: Comparison of our calculation results with the experimental literature data for the strongest transitions in NH_3, C_2H_4, and O_3 molecules at $^{12}C^{16}O_2$ laser frequencies.

M	Laser line	ν, cm^{-1}	σ(M), 10^{-20} cm^2			K_T		K_P	
			[24]	[22]	a	[22]	a	[22]	a
NH_3	9R(16)	1075.98782	51.6	c	52.1	c	0.70	c	−0.29
	11R(8)	967.70723	88.9	92.6	102	−1.07	−0.98	−0.30	−0.33
	11R(14)	971.93026	2.56[b]	30.2	27.6	−0.62	−0.96	−0.59	−0.61
	11P(32)	932.96042	60.9	c	57.6	c	0.03	c	−0.44
	11P(34)	931.00143	50.3	c	55.2	c	−0.87	c	0.60
	9R(30)	1084.63514	c	c	303	c	0.38	c	−0.83
	9P(20)	1046.85423	8.77	12.1	13.2	−1.50	−1.62	0.96	0.92
C_2H_4	11P(14)	949.47931	118.4	145.1	133	−0.54	0.16	0.03	−0.13
	11P(16)	947.74198	c	23.9	21.4	−0.46	−0.55	−0.02	0.01
	11R(24)	978.47229	20.5	20.9	19.3	−0.83	−0.49	−0.06	−0.02
	11P(12)	951.19226	c	19.7	17.3	−0.01	−0.46	0.30	0.42
O_3	9P(14)	1052.19555	51.6	c	47.4	c	−0.62	c	0.08
	9P(12)	1053.92350	49.5	c	44.0	c	−0.38	c	−0.22
	9P(8)	1057.30016	51.6	c	49.2	c	−0.02	c	−0.12

[a]This work.
[b]Probably, misprint.
[c]No data.

3. Discussion

Some of our results are compared with the experimental literature data in Table 5. As one can see from the table, the present results agree favorably with the experimental data of Patty et al. [24] and Persson et al. [22], who have determined σ, K_P, and K_T coefficients for 26-laser absorption by NH_3, O_3, and C_2H_4 molecules.

Note that only in several cases our M molecules are important as "standard" air pollutant (NH_3, C_2H_4, PH_3, and O_3) and in other cases our M molecules may happen in the air only near special industrial objects. As one can see from Tables 1–4, 26-laser is a good choice for all these four gases.

There are several advantages of the other CO_2 lasers: monitoring of HNO_3, NO_2, C_2H_6, and CO_2 molecules requires 46-/48-/36-, 36-, 36-/46-/48-, and 38-/268-lasers, respectively, instead of 26-laser.

We included in Table 4 several molecules with low cross sections (OCS, CH_3CN, C_2H_6, SO_2, and NO_2). Although CO_2 laser is not the best choice to detect these molecules,

Table 6: The largest absorption cross sections (in 10^{-20} cm^2 units) of CH_3OH and HCCOH at low pressure and $T = 296$ K. The Doppler shape of spectral lines is assumed.

M	Laser	Line	ν, cm^{-1}	σ(M)[a]
CH_3OH	26	10P(34)	1033.48800	126
	36	10P(16)	1004.27987	67.2
	28	10P(22)	1067.35888	93.0
	38	10R(8)	1032.91023	200*
	38	10R(40)	1050.77747	193*
	38	10P(36)	998.62350	113
	46	9R(46)	1010.98950	44.7*
	46	9R(28)	1002.08279	19.4
	48	9R(40)	1006.00000	146*
	48	9R(24)	998.01156	107
	268	10P(27)	1050.83825	368
HCOOH	26	10R(18)	1077.30252	186
	26	10R(28)	1083.47878	189
	26	10R(40)	1090.02837	976*
	36	10R(28)	1037.16713	9.59
	28	10P(8)	1078.04242	327
	28	10R(34)	1104.91182	285
	38	10R(44)	1052.63615	19.3
	46	9R(26)	1000.94716	2.64
	48	9R(30)	1001.17880	2.74
	268	10R(19)	1086.22023	118

[a]Asterisk marks the cases where the σ(M) is large, but the CO_2-laser line is marginal.

these data may be useful in special cases, for example, when CO_2 LIDAR is used to monitor the leakage of these gases from industrial areas.

Surely, the data in all our tables are only starting points in discussion about applicability of particular CO_2-laser transitions for remote sensing under atmospheric conditions, because at many wavenumbers, the absorption by H_2O may be much stronger than absorption by the gases of interest. Hence one always should find the tradeoff between the absorption of H_2O and the absorption of these gases.

For example, the "best" line for NH_3 detection by 26-laser in Table 4 is 10R(30) with $\sigma(NH_3) = 303 \times 10^{-20}$ cm^2. However, at this wavelength, the ratio $\sigma(NH_3)/\sigma(H_2O)$ is only 4.4×10^5. If we choose another 26-laser line for NH_3 detection, P(34) (931.0014 cm^{-1}) with $\sigma(NH_3) = 55.2 \times 10^{-20}$ cm^2 and $\sigma(H_2O) = 0.0023 \times 10^{-23}$ cm^2, the ratio will be much higher: $\sigma(NH_3)/\sigma(H_2O) = 2.4 \times 10^7$. Hence, this another 26-laser line is better for NH_3 detection, although the value $\sigma(NH_3)$ is lower.

Therefore, we included H_2O in our calculations; see the results in Tables 1, 2, and 3. Our $\sigma(H_2O)$ data in the tables should help to choose the "best" pairs of CO_2-laser lines (absorbing and nonabsorbing) for remote sensing of the gases of interest. Note that the pair of CO_2-laser wavenumbers may originate from two isotopically different CO_2 lasers; therefore the possibility to use many isotopic variations of CO_2 laser simplifies strongly the choice of such pairs.

4. Application to FIR Lasers

There are several important benchmark molecules which are normally used in CO_2-laser-pumped FIR lasers: CH_3OH, CH_2F_2, HCOOH, $^{15}NH_3$, CD_3OD, CD_3 OH, CD_3Cl, $^{13}CD_3I$, and $^{13}CH_3F$. The absorption of CO_2 radiation by these molecules results in FIR-laser emission. Table 6 lists our σ(M) values for CH_3OH and HCOOH at low pressures, where the shapes of spectral lines of these molecules are given by Doppler effect. As one can see, there are a lot of interesting possibilities to obtain new strong sources of FIR radiation. One of them may be 9R(19) line of 268-laser, which has very large σ(HCOOH) value.

Although there is no direct relation between intensities of CO_2 absorption and FIR emission, it is clear that using 1000 CO_2-laser lines instead of 100–200 should increase strongly the amount of strong FIR-laser transitions.

5. Conclusion

The absorption cross sections and K_T and K_P parameters of some molecules (NH_3, C_2H_4, CO_2, O_3, NO_2, PH_3, HNO_3, SF_6, CH_3OH, HCOOH, OCS, CH_3CN, C_2H_6, SO_2, and H_2O) at CO_2 laser frequencies ($^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{12}C^{18}O_2$, $^{14}C^{16}O_2$, $^{14}C^{18}O_2$, $^{13}C^{18}O_2$, and $^{12}C^{16}O^{18}O$) have been calculated with the use of spectroscopical parameters from GEISA database. The present results are in reasonable agreement

with other experimental measurements for NH_3, O_3, and C_2H_4. The results of the calculations may be used in designing the differential absorption technique for remote monitoring of these molecules.

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