

INFORMATION SYSTEM FOR THE MOLECULAR ABSORPTION OF A CO₂-LASER RADIATION

O.K. Voitsekhovskaya, S.V. Kuznetsov, S.V. Sapozhnikov, N.N. Trifonova, and M.R. Cherkasov

*Institute of Atmospheric Optics,
Siberian Branch of the Academy of Sciences of the USSR, Tomsk
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The development of an information system (IS) supporting investigations of gaseous media using a CO₂-laser with the absolute values of the absorption coefficients of atmospheric and trace gases is reported. In addition to characteristics of the CO₂-lasing transitions, the IS includes the database of the parameters of absorption lines formed using original techniques for calculations. Considerable attention is devoted to the reliability of the stored information, which is compared with other experimental data.

INTRODUCTION

When interpreting data of multiwavelength laser sensing, we must *a priori* know the absolute values of spectral absorption coefficients for each gaseous component for solving the system of equations

$$\{\alpha_{v_i} + \delta\alpha_{v_i}\}_m = \left\{ \sum_{j=1}^N ((k_{v_i j} + dk_{v_i j}) (\rho_j + \delta\rho_j)) \right\}_m,$$

where ρ_j and $k_{v_i j}$ are the concentration and the mass absorption coefficient, $j = 1, \dots, N$, N is the number of gases in air which are taken into account in the calculation, $i = 1, \dots, m$, m is the number of wavelengths at which the measurements are made, α_{v_i} is the measured absorption coefficient, and $\delta\alpha_{v_i}$, $\delta k_{v_i j}$, and $\delta\rho_j$ are the errors.

Conventionally, laboratory measurements of the absorption coefficients (AC) of individual gases are used. The number of investigations, devoted to the determination the spectral characteristics of absorption of the CO₂-laser radiation by individual gases, is quite large, but there are significant discrepancies between the results obtained by various authors. They can be explained by the difficulty of accurate recording the absorbing matter amount and measuring the radiation intensities.

In this paper we make an attempt to exactly calculate the absolute values of the absorption coefficients of atmospheric and trace gases based on the databank of the absorption spectral lines developed at the Institute of Atmospheric Optics of the Siberian Branch of the Academy of Sciences of the USSR. As a result, a subject-oriented information-retrieval system (IRS) "Razbeg" has been developed. This system is intended for scanning the spectral line parameters of atmospheric and trace gases lying within the given tuning interval of the CO₂-lasing wavelengths, and for choosing the optimum wavelength of a CO₂-laser for sensing

a specific impurity. The IRS includes the following databanks (DB):

- a) Characteristics of the lasing lines of the CO₂-laser based on five isotopic modifications of carbon dioxide¹ and
- b) The database of the spectral line parameters of atmospheric and trace gases.

The formation of the first database is easy, and the specification of the retrieval attributes consists in either a quantum identification of the CO₂-laser transition or an indication of the laser radiation wavelength in microns. The formation of the second information component, i.e., the DB of the parameters of spectral lines (PSL), is rather difficult. The latter databank is the ensemble of records of identical length. The record consists of the PSL of a spectral line, viz., position of its center, intensity, half-width, quantum identification, etc. The IRS "Razbeg" includes the base of recommended values of the PSL, whose principles and criteria of formation were previously discussed.^{2,3}

In calculating the position of centers and intensities of the vibrational-rotational (VR) lines and in forming the relevant databanks we used the techniques described in detail in Ref. 2. Table I refers to the starting data sources used in calculations of the above line parameters. Let us only indicate in addition that in the OCS-absorption spectrum five vibrational bands lie within the specified interval, but only the integral intensity of the $2\nu_2$ band is well known.

We have determined the second-order derivative of the dipole moment of the OCS and in the harmonic approximation we have calculated the integral intensities of the rest of the bands $03^10J \leftarrow 01^10$, $04^20 \leftarrow 02^20$, $04^00 \leftarrow 02^00$, and $12^00 \leftarrow 10^00$.

The theoretical approach to the synthesis of the line half-widths was given in Ref. 4. Dry air was regarded as the buffer component, and the line half-widths were determined from the formula

$$\gamma_{\text{air}} = 0,79\gamma_{\text{N}_2} + 0,21\gamma_{\text{O}_2}.$$

TABLE I. Characteristics of vibrational bands of gases.

Molecule	Band center ν_0 (cm^{-1})	Band quantum identification	Integral intensity $S_{V,V}$ ($\text{atm}^{-1} \cdot \text{cm}^{-1}$)	Endpoints of the frequency band		The number of lines	References
				ν_{\min} (cm^{-1})	ν_{\max} (cm^{-1})		
H_2^{16}O	0.0	000 – 000	–	800.7149	1198.5678	216	8
	1594.00	010 – 000	257.3	839.644	1198.5266	120	9
$^{13}\text{C}^{16}\text{O}_2$	913.425	00011 – 10001	$1.917 \cdot 10^{-4}$	864.3066	949.5381	56	26
$^{12}\text{C}^{16}\text{O}_2$	917.647	10011 – 20001	$2.490 \cdot 10^{-5}$	878.7133	945.3592	43	
$^{12}\text{C}^{16}\text{O}_2$	927.156	01111 – 11101	$1.046 \cdot 10^{-3}$	868.9911	963.4634	137	
$^{12}\text{C}^{16}\text{O}_2$	941.698	10012 – 20002	$3.461 \cdot 10^{-5}$	903.4837	973.4982	46	
$^{12}\text{C}^{16}\text{O}_2$	960.959	00011 – 10001	$1.711 \cdot 10^{-2}$	886.3767	1001.3052	75	
$^{12}\text{C}^{16}\text{O}^{17}\text{O}$	963.986	00011 – 10001	$1.120 \cdot 10^{-5}$	937.5717	984.8698	53	
$^{12}\text{C}^{16}\text{O}^{18}\text{O}$	966.269	00011 – 10001	$4.482 \cdot 10^{-5}$	928.7305	992.6507	86	
$^{13}\text{C}^{16}\text{O}_2$	1017.659	00011 – 10002	$1.345 \cdot 10^{-4}$	967.6066	1049.5704	54	
$^{13}\text{C}^{16}\text{O}_2$	1023.701	01111 – 11102	$2.291 \cdot 10^{-5}$	990.4520	1048.5472	72	
$^{12}\text{C}^{16}\text{O}_2$	1043.640	10011 – 20002	$3.984 \cdot 10^{-5}$	1002.7651	1074.6674	47	
$^{12}\text{C}^{16}\text{O}_2$	1063.735	00011 – 10002	$2.428 \cdot 10^{-2}$	988.8178	1084.6356	53	
$^{12}\text{C}^{16}\text{O}_2$	1064.475	10012 – 20003	$8.068 \cdot 10^{-5}$	1016.7574	1084.0220	40	
$^{12}\text{C}^{16}\text{O}_2$	1066.242	11112 – 21103	$7.819 \cdot 10^{-6}$	1044.7623	1084.6693	38	
$^{12}\text{C}^{16}\text{O}^{17}\text{O}$	1067.72	00001 – 10002	$1.594 \cdot 10^{-5}$	1038.5826	1090.9159	64	
$^{12}\text{C}^{16}\text{O}_2$	1071.542	01111 – 11102	$1.912 \cdot 10^{-3}$	1010.1800	1084.5289	102	
$^{12}\text{C}^{16}\text{O}^{18}\text{O}$	1072.687	00011 – 10002	$8.964 \cdot 10^{-5}$	1031.1031	1102.3183	98	
$^{12}\text{C}^{16}\text{O}_2$	1074.250	02211 – 12202	7.79410	1031.4165	1084.529	64	
$^{16}\text{O}_3$	698.3414	020 – 010	1.028	550.9645	884.0983	5209	
	700.9330	010 – 000	15.05	503.2347	210.7256	6889	
	1007.6514	101 – 100	1.491	968.5841	1057.1318	2424	
	1042.0846	001 – 000	216.4	858.9830	1133.877	3044	
	1103.1332	100 – 000	1.305	921.7469	1134.027	1363	
$^{14}\text{N}_2^{16}\text{O}$	938.853	0000 – 1000	0.0514	868.9931	991.1517	147	28
	1055.6244	0001 – 0200	0.007203	982.8614	1092.985	132	29
	1160.298	0310 – 0110	0.6464	1095.1988	1232.730	432	
	1168.133	0200 – 0000	7.003	1098.1939	1248.183	180	
$^{16}\text{O}^{12}\text{C}^{32}\text{S}$	1033.2640	1200 – 1000	0.19883	1003.6856	1075.3379	179	30
	1047.0420	0200 – 0000	10.0	1005.3916	1109.2276	257	31
	1052.9443	0310 – 0110	3.1678	1015.2204	1103.5337	550	
	1057.7857	0400 – 0200	0.4884	1027.5482	1099.6798	177	
	1058.2312	0420 – 0220	0.505	1026.7871	1095.8385	398	32
$^{32}\text{S}^{16}\text{O}_2$	1151.713	100 – 000	89.0424	960.7884	1199.997	6652	33 and 34
H_2^{32}S	1182.577	010 – 000	2.05	895.8660	1199.957	401	35
$\text{H}^{14}\text{N}^{16}\text{O}_3$	879.1082	ν_5		891.0013	951.9149	17482	36
	896.4187	ν_9		891.0007	956.9182	21998	
$^{12}\text{C}^{19}\text{F}_2^{35}\text{Cl}_2$	923.2395	ν_6	292.0	904.8279	941.3651	20776	25
$^{14}\text{NH}_3$	789.537	0200 – 0100	5.85	790.007	1211.9150		27
	950.2778	0100 – 0000	547.8	791.7270	1210.2829		

TABLE II. Calculated data on the coefficients of absorption K_v ($\text{atm}^{-1}\cdot\text{cm}^{-1}$) at $T = 296$ K within the 0001–1000 band of lasing of the CO_2 laser.

Frequency (cm^{-1})	CO_2 -laser line	$K_v(\text{calc.})$			
		N_2O	H_2S	H_2O	O_3
916.5834	P 48	$1.80\cdot 10^{-4}$	$3.12\cdot 10^{-8}$	$9.90\cdot 10^{-7}$	$1.74\cdot 10^{-5}$
918.7197	P 46	$1.40\cdot 10^{-3}$	$6.71\cdot 10^{-8}$	$1.72\cdot 10^{-5}$	$2.36\cdot 10^{-5}$
920.8303	P 44	$4.95\cdot 10^{-4}$	$2.30\cdot 10^{-7}$	$6.62\cdot 10^{-6}$	$4.71\cdot 10^{-5}$
922.9153	P 42	$2.66\cdot 10^{-4}$	$8.24\cdot 10^{-6}$	$1.29\cdot 10^{-5}$	$6.00\cdot 10^{-5}$
924.9749	P 40	$1.21\cdot 10^{-3}$	$4.99\cdot 10^{-7}$	$7.10\cdot 10^{-4}$	$7.97\cdot 10^{-5}$
927.0091	P 38	$9.59\cdot 10^{-4}$	$1.19\cdot 10^{-7}$	$1.59\cdot 10^{-6}$	$4.14\cdot 10^{-5}$
929.0182	P 36	$2.84\cdot 10^{-4}$	$7.20\cdot 10^{-8}$	$9.31\cdot 10^{-5}$	$5.33\cdot 10^{-5}$
931.0022	P 34	$4.71\cdot 10^{-4}$	$1.22\cdot 10^{-7}$	$1.13\cdot 10^{-6}$	$6.26\cdot 10^{-5}$
932.9611	P 32	$2.37\cdot 10^{-3}$	$2.48\cdot 10^{-7}$	$2.48\cdot 10^{-7}$	$9.42\cdot 10^{-5}$
934.8952	P 30	$2.60\cdot 10^{-4}$	$1.65\cdot 10^{-6}$	$1.34\cdot 10^{-7}$	$1.37\cdot 10^{-4}$
936.8045	P 28	$9.97\cdot 10^{-5}$	$1.83\cdot 10^{-6}$	$8.65\cdot 10^{-7}$	$1.85\cdot 10^{-4}$
938.6890	P 26	$2.32\cdot 10^{-5}$	$7.90\cdot 10^{-6}$	$3.53\cdot 10^{-7}$	$1.43\cdot 10^{-4}$
940.5488	P 24	$6.51\cdot 10^{-4}$	$1.82\cdot 10^{-6}$	$2.42\cdot 10^{-6}$	$6.04\cdot 10^{-5}$
942.3841	P 22	$2.69\cdot 10^{-4}$	$3.70\cdot 10^{-7}$	$6.87\cdot 10^{-7}$	$8.73\cdot 10^{-5}$
944.1948	P 20	$2.48\cdot 10^{-4}$	$2.33\cdot 10^{-7}$	$3.63\cdot 10^{-6}$	$7.70\cdot 10^{-5}$
945.9810	P 18	$4.84\cdot 10^{-4}$	$2.32\cdot 10^{-7}$	$2.44\cdot 10^{-6}$	$1.86\cdot 10^{-4}$
947.7427	P 16	$2.32\cdot 10^{-3}$	$3.61\cdot 10^{-7}$	$2.61\cdot 10^{-5}$	$3.78\cdot 10^{-4}$
949.4800	P 14	$1.93\cdot 10^{-3}$	$8.68\cdot 10^{-7}$	$4.97\cdot 10^{-6}$	$2.50\cdot 10^{-4}$
951.1930	P 12	$5.91\cdot 10^{-4}$	$9.15\cdot 10^{-6}$	$1.21\cdot 10^{-6}$	$3.96\cdot 10^{-4}$
952.8816	P 10	$3.99\cdot 10^{-4}$	$5.87\cdot 10^{-6}$	$4.96\cdot 10^{-6}$	$1.40\cdot 10^{-4}$
954.5458	P 8	$4.51\cdot 10^{-4}$	$1.11\cdot 10^{-5}$	$5.54\cdot 10^{-6}$	$2.26\cdot 10^{-4}$
956.1857	P 6	$8.24\cdot 10^{-4}$	$5.61\cdot 10^{-6}$	$3.57\cdot 10^{-6}$	$5.39\cdot 10^{-4}$
957.8012	P 4	$2.52\cdot 10^{-3}$	$7.22\cdot 10^{-7}$	$9.08\cdot 10^{-7}$	$1.11\cdot 10^{-3}$
959.3924	P 2	$2.42\cdot 10^{-3}$	$5.31\cdot 10^{-7}$	$1.95\cdot 10^{-5}$	$1.66\cdot 10^{-3}$
961.7336	R 0	$4.71\cdot 10^{-4}$	$8.51\cdot 10^{-7}$	$4.41\cdot 10^{-6}$	$1.52\cdot 10^{-3}$
963.2638	R 2	$2.56\cdot 10^{-4}$	$2.11\cdot 10^{-6}$	$3.62\cdot 10^{-7}$	$3.55\cdot 10^{-3}$
964.7697	R 4	$1.74\cdot 10^{-4}$	$3.01\cdot 10^{-5}$	$6.02\cdot 10^{-7}$	$2.36\cdot 10^{-3}$
966.2511	R 6	$1.35\cdot 10^{-4}$	$1.31\cdot 10^{-5}$	$5.37\cdot 10^{-6}$	$3.23\cdot 10^{-3}$
967.7079	R 8	$1.13\cdot 10^{-4}$	$7.92\cdot 10^{-5}$	$1.91\cdot 10^{-6}$	$7.15\cdot 10^{-3}$
969.3281	R 10	$4.60\cdot 10^{-4}$	$2.11\cdot 10^{-6}$	$1.00\cdot 10^{-6}$	$4.94\cdot 10^{-3}$
970.5479	R 12	$8.50\cdot 10^{-5}$	$1.02\cdot 10^{-6}$	$7.44\cdot 10^{-5}$	$1.19\cdot 10^{-2}$
971.9310	R 14	$7.10\cdot 10^{-5}$	$6.97\cdot 10^{-7}$	$1.02\cdot 10^{-5}$	$8.07\cdot 10^{-3}$
973.2892	R 16	$5.59\cdot 10^{-5}$	$7.38\cdot 10^{-7}$	$3.74\cdot 10^{-5}$	$9.13\cdot 10^{-3}$
974.6226	R 18	$4.10\cdot 10^{-5}$	$1.90\cdot 10^{-6}$	$5.44\cdot 10^{-6}$	$1.72\cdot 10^{-2}$
975.9311	R 20	$2.80\cdot 10^{-5}$	$8.49\cdot 10^{-6}$	$8.21\cdot 10^{-4}$	$1.17\cdot 10^{-2}$
977.2146	R 22	$1.82\cdot 10^{-5}$	$1.78\cdot 10^{-6}$	$1.74\cdot 10^{-5}$	$1.05\cdot 10^{-2}$
978.4730	R 24	$1.15\cdot 10^{-5}$	$3.75\cdot 10^{-6}$	$1.70\cdot 10^{-6}$	$2.87\cdot 10^{-2}$
979.7061	R 26	$7.38\cdot 10^{-6}$	$6.15\cdot 10^{-5}$	$5.80\cdot 10^{-7}$	$1.44\cdot 10^{-2}$
980.9139	R 28	$5.00\cdot 10^{-6}$	$2.86\cdot 10^{-5}$	$9.76\cdot 10^{-7}$	$1.92\cdot 10^{-2}$
982.0962	R 30	$3.82\cdot 10^{-6}$	$4.13\cdot 10^{-6}$	$1.62\cdot 10^{-5}$	$2.24\cdot 10^{-2}$
983.2530	R 32	$3.52\cdot 10^{-6}$	$3.69\cdot 10^{-6}$	$1.08\cdot 10^{-6}$	$3.06\cdot 10^{-2}$
984.3840	R 34	$4.59\cdot 10^{-6}$	$1.80\cdot 10^{-5}$	$6.71\cdot 10^{-6}$	$3.68\cdot 10^{-2}$
985.4891	R 36	$7.49\cdot 10^{-6}$	$6.42\cdot 10^{-5}$	$3.36\cdot 10^{-7}$	$2.51\cdot 10^{-2}$
986.5682	R 38	$2.08\cdot 10^{-6}$	$7.31\cdot 10^{-6}$	$1.25\cdot 10^{-7}$	$3.64\cdot 10^{-2}$
987.6212	R 40	$5.43\cdot 10^{-7}$	$4.09\cdot 10^{-6}$	$3.12\cdot 10^{-7}$	$7.00\cdot 10^{-2}$
988.6477	R 42	$2.85\cdot 10^{-7}$	$1.75\cdot 10^{-6}$	$9.09\cdot 10^{-7}$	$1.09\cdot 10^{-1}$
989.6478	R 44	$2.92\cdot 10^{-7}$	$1.59\cdot 10^{-6}$	$5.33\cdot 10^{-7}$	$1.97\cdot 10^{-1}$
990.6212	R 46	$7.13\cdot 10^{-7}$	$1.90\cdot 10^{-6}$	$1.10\cdot 10^{-6}$	$1.98\cdot 10^{-1}$
991.5676	R 48	$3.32\cdot 10^{-8}$	$3.06\cdot 10^{-6}$	$1.26\cdot 10^{-7}$	$1.81\cdot 10^{-1}$

TABLE III. Calculated data on the coefficients of absorption due to OCS, H₂S, and H₂O K_v (atm⁻¹·cm⁻¹) at $T = 296$ K within the 0001–0200 lasing band of the CO₂-laser.

Frequency (cm ⁻¹)	CO ₂ -laser line	K_v (calc.)		
		OCS	H ₂ S	H ₂ O
1018.9020	P 48	8.46·10 ⁻³	1.21·10 ⁻⁵	6.57·10 ⁻⁶
1021.0579	P 46	2.18·10 ⁻²	1.20·10 ⁻³	8.40·10 ⁻⁷
1023.1901	P 44	2.06·10 ⁻²	7.53·10 ⁻⁵	5.16·10 ⁻⁷
1025.2984	P 42	7.99·10 ⁻²	2.33·10 ⁻⁵	6.29·10 ⁻⁷
1027.3825	P 40	6.93·10 ⁻²	3.38·10 ⁻⁵	4.38·10 ⁻⁶
1029.4423	P 38	1.07·10 ⁻¹	8.18·10 ⁻⁶	3.67·10 ⁻⁴
1031.4776	P 36	3.09·10 ⁻¹	5.65·10 ⁻⁵	2.30·10 ⁻⁶
1033.5843	P 34	5.09·10 ⁻¹	4.09·10 ⁻⁵	8.55·10 ⁻⁷
1035.4737	P 32	3.93·10 ⁻¹	2.97·10 ⁻⁴	6.63·10 ⁻⁶
1037.4342	P 30	1.93·10 ⁻¹	3.73·10 ⁻⁵	1.42·10 ⁻⁶
1039.3694	P 28	1.85·10 ⁻¹	2.87·10 ⁻⁴	7.45·10 ⁻⁵
1041.2791	P 26	1.55·10 ⁻¹	5.38·10 ⁻⁵	1.06·10 ⁻⁶
1043.1633	P 24	1.52·10 ⁻¹	3.48·10 ⁻³	2.41·10 ⁻⁶
1045.0218	P 22	2.51·10 ⁻¹	2.67·10 ⁻⁴	3.49·10 ⁻⁷
1046.8543	P 20	2.06·10 ⁻²	3.35·10 ⁻⁵	4.19·10 ⁻⁷
1048.6609	P 18	1.87·10 ⁻¹	1.93·10 ⁻⁴	3.39·10 ⁻⁶
1050.4414	P 16	1.39·10 ⁻¹	6.23·10 ⁻⁵	6.99·10 ⁻⁶
1052.1956	P 14	1.20·10 ⁻¹	1.66·10 ⁻⁴	2.23·10 ⁻⁶
1053.9236	P 12	1.37·10 ⁻¹	1.74·10 ⁻³	1.02·10 ⁻⁶
1055.6251	P 10	1.45·10 ⁻¹	3.63·10 ⁻³	1.02·10 ⁻⁴
1058.1953	P 8	1.57·10 ⁻¹	8.64·10 ⁻⁵	3.03·10 ⁻⁶
1058.9488	P 6	4.65·10 ⁻¹	1.07·10 ⁻⁴	5.55·10 ⁻⁶
1060.5707	P 4	2.10·10 ⁻¹	2.02·10 ⁻³	9.38·10 ⁻⁶
1062.1660	P 2	1.43·10 ⁻¹	3.42·10 ⁻⁴	9.45·10 ⁻⁶
1064.5089	R 0	8.22·10 ⁻²	6.35·10 ⁻⁵	6.10·10 ⁻⁶
1066.0374	R 2	1.81·10 ⁻¹	6.56·10 ⁻⁴	8.75·10 ⁻⁴
1067.5391	R 4	1.96·10 ⁻¹	2.50·10 ⁻⁴	8.13·10 ⁻⁶
1069.0141	R 6	6.66·10 ⁻²	4.86·10 ⁻³	2.14·10 ⁻⁶
1070.4623	R 8	4.45·10 ⁻²	1.17·10 ⁻³	1.36·10 ⁻⁶
1071.8838	R 10	3.46·10 ⁻²	1.43·10 ⁻²	3.03·10 ⁻⁶
1073.2785	R 12	2.97·10 ⁻²	8.25·10 ⁻⁴	6.31·10 ⁻⁶
1074.6465	R 14	4.22·10 ⁻²	2.72·10 ⁻³	7.95·10 ⁻⁵
1075.9879	R 16	4.33·10 ⁻²	4.81·10 ⁻⁴	3.64·10 ⁻⁵
1077.3026	R 18	9.03·10 ⁻³	1.32·10 ⁻³	1.27·10 ⁻⁶
1078.5907	R 20	8.48·10 ⁻³	6.85·10 ⁻⁴	4.97·10 ⁻⁷
1079.8523	R 22	9.24·10 ⁻³	1.31·10 ⁻³	4.20·10 ⁻⁷
1081.0875	R 24	4.06·10 ⁻³	5.53·10 ⁻³	5.44·10 ⁻⁶
1082.2983	R 26	3.26·10 ⁻³	1.97·10 ⁻³	6.31·10 ⁻⁷
1083.4788	R 28	4.81·10 ⁻³	9.64·10 ⁻³	2.81·10 ⁻⁷
1084.6352	R 30	1.13·10 ⁻³	5.21·10 ⁻⁴	2.33·10 ⁻⁷
1085.7655	R 32	8.81·10 ⁻⁴	1.40·10 ⁻³	3.10·10 ⁻⁷
1086.8699	R 34	1.38·10 ⁻³	3.03·10 ⁻³	6.25·10 ⁻⁷
1087.9485	R 36	1.86·10 ⁻³	5.35·10 ⁻³	1.11·10 ⁻⁴
1089.0014	R 38	1.36·10 ⁻³	2.57·10 ⁻³	1.60·10 ⁻⁶
1090.0288	R 40	9.65·10 ⁻⁴	2.57·10 ⁻³	4.67·10 ⁻⁶
1091.0308	R 42	6.18·10 ⁻⁴	2.70·10 ⁻²	1.91·10 ⁻⁴
1092.0076	R 44	2.30·10 ⁻⁴	1.88·10 ⁻³	9.95·10 ⁻⁶
1092.9594	R 46	9.21·10 ⁻⁵	8.14·10 ⁻³	2.33·10 ⁻⁶
1093.8863	R 48	7.42·10 ⁻⁵	2.91·10 ⁻³	1.25·10 ⁻⁶

The calculations were performed using those values of the molecular constants, which have been recommended in Refs. 5–7. The comparison with experimental data showed

that on the average the described technique made it possible to obtain the results with an error of not more than +10%, even though the error can be +30% in some cases.

ANALYSIS OF RELIABILITY OF THE INFORMATION SYSTEM COMPONENTS DESCRIBING THE ABSORPTION COEFFICIENTS OF GASES

We estimated the accuracy of calculations of the PSL when constructing physical models and computational algorithms for the PSL. But for gas analysis problem, regardless of the mathematical apparatus employed for interpretation of an experiment, the absolute values of the absorption coefficients (AC) at specific spectral frequencies are needed as the initial data. For this reason, it is important to make the comparison of the experimental AC values with those synthesized based on the available data from the PSL. Tables II and III give the AC values for two fundamental radiation bands of the CO₂ laser, which have been synthesized for the Lorentz line shape with the maximum value of frequency detuning 10 cm⁻¹.

Let us examine the accuracy of the given absorption coefficients and the contributions of the atmospheric gaseous components to the radiation attenuation in the spectral range 9–11 μm.

Water vapor (H₂O). In the spectral range under consideration the absorption due to water vapor is caused by the selective and continuum components. In addition, the selective absorption is caused by weak lines corresponding to the highly excited VR transitions, whose intensities are affected by intramolecular interactions. In the databank of the IRS our accounting for the VR interactions (see in detail in Refs. 8 and 9) has significantly improved the accuracy of the

stored numerical values of the PSL. This is testified by a good agreement of the experimental and synthesized values of the absorption coefficient by the 10P40 lasing line, while the absorption coefficient calculated from the data of Ref. 10 exceeds the experimental values by a factor of two (see Table IV). It is this discrepancy that served as a major premise in Ref. 11 and leads the authors to the erroneous conclusions. The point is that the values, which they took from Ref. 10, were calculated for the rigid-top model, which is not applicable for the H₂O lines. Table IV gives the values of the synthesized total AC due to water vapor in comparison with experimental values, which have been obtained by various authors and represented as a standard format in Ref. 12. The difficulty of correct comparing of these values consists in accounting for the continuum absorption calculated from a number of semi-empirical formulas.^{13,14} The relation obtained in Ref. 13, which takes into account both the linear and quadratic dependences of the AC on the water vapor content, seems to be the most comprehensive. We used a simpler approximation given in Ref. 14. The best agreement of the AC is seen for the 10R16, 10R18, and 10R20 lines, where the discrepancy does not exceed 2–3%. The largest discrepancy is observed for the AC by the 9R14 and 9R30 lines, where our result agrees well with the result of analogous calculation made in Ref. 10 and deviates from the experiment for the 9R14 line by a factor of two and even more for the 9R30 lasing line of the laser. An effect of the absorption due to ammonia is possible for the latter transition, as has been noted in Ref. 12. However, we failed to explain the discrepancy of the experiment and the result of calculation for the 9R14 line.

TABLE IV. Calculated and experimental data on the total absorption coefficients due to H₂O (P = 10 mm Hg).

Frequency (cm ⁻¹)	Lasing line of the CO ₂ laser	Total K _v (calc.) T = 296 K X·10 ⁶	Total K _v (exp.) T = 300 K K _v (exp.) according to Ref. 12					
			X·10 ⁶	X·10 ⁶	X·10 ⁶	X·10 ⁶	Mean X·10 ⁶	Calculation AFGL ¹²
924.9740	10P(40)	10.3			12.4		12.4	20.5 ± 4.1
944.1940	10P(20)	1.01	1.02	1.09	0.69	0.92	0.93 ± 0.15	0.88 ± 0.1
947.7420	10P(16)	1.29	1.09		0.98	1.08	1.05 ± 0.05	1.05 ± 0.11
970.5472	10R(12)	1.86	2.07		2.19	2.07	2.11 ± 0.06	2.03 ± 0.25
971.9303	10R(14)	1.01	1.70	1.80		1.66	1.72 ± 0.06	0.88 ± 0.1
973.2885	10R(16)	1.36	1.60		1.24	1.26	1.37 ± 0.17	1.08 ± 0.12
974.6219	10R(18)	0.94	1.07		0.89	0.88	0.95 ± 0.08	0.79 ± 0.08
975.9304	10R(20)	11.6	12.7	10.7	11.4	9.09	11.3 ± 1.3	10.4 ± 2.1
977.2139	10R(22)	1.09	1.59	1.32	1.20	1.28	1.35 ± 0.15	1.04 ± 0.11
1039.3693	9P(28)	1.71	2.76		3.10		2.93 ± 0.17	1.63 ± 0.18
1055.6251	9P(10)	2.06	2.86	3.40	2.65		2.97 ± 0.32	2.28 ± 0.29
1073.2785	9R(12)	0.77	0.82				0.98 ± 0.16	1.57 ± 0.18
1074.6465	9R(14)	1.73	3.62		3.49		3.56 ± 0.07	1.87 ± 0.21
1075.9878	9R(16)	1.16	0.93		0.84		0.89 ± 0.05	1.00 ± 0.10
1084.6351	9R(30)	0.68			2.78		2.78	0.62 ± 0.06
1085.7654	9R(32)	0.68	0.97		1.13		1.05 ± 0.08	0.75 ± 0.08

Moreover, the author of Ref. 15 has experimentally determined that the value of the selective absorption coefficient (as a difference of the AC measured inside the absorption line and outside of it) equals to 1.1·10⁻⁴cm⁻¹·atm⁻¹. The value of the AC, which has been calculated by us, equals 8.0·10⁻⁵. This results in a discrepancy of 27%, rather than by two times, as follows from Table IV. As a whole, one may assume that based on the PSL of this system the selective absorption coefficients due to H₂O can be calculated with a sufficient accuracy (at the experimental level). For

the 9–μm radiation band, a more rigorous experiment is desirable excluding the effect of foreign gases.

Carbon dioxide (CO₂). In spite of the significant amount of the weak bands, lying in the region under consideration, the accuracy of the calculated PSL is quite high to quantitatively estimate the radiation extinction due to this gas. The spectral line parameters were repeatedly tested, and the reliability of the calculated absorption coefficients was not lower than 90%.

Ammonia (NH₃). The number of measurements of the CO₂-laser radiation extinction due to ammonia is quite large,¹⁵⁻¹⁹ but the spread in the experimental values, as follows from Tables V and VI, is great. An explanation of this fact is given in Ref. 12 when examining the discrepancies between the water-vapor absorption coefficients. These are the differences in the absolute values of the AC due to ethylene, assumed to be the reference in the experiment. A good agreement with experiment for the strong absorption lines of ammonia made it possible to use the given PSL in the 9- μ m band in the gas analysis problem. However, significant discrepancies between the absorption coefficients within the 10P band require an additional improvement of the databanks of the PSL near 10 μ m.

Ozone (O₃). The absorption due to ozone in the spectral range under study was repeatedly investigated,²⁰⁻²⁴ but the spread in the experimental values of the AC amounted to hundreds per cent (9P28). The 9P8 and 9P12 lines, which are the most suitable for ozone sensing, have been measured quite correctly (~20%) and the calculated AC values are adequate to the experimental values (see Table VII).

Dinitrogen oxide (N₂O). The contribution of dinitrogen oxide to the absorption in the range 9-11 μ m is typically ignored. This is explained by the fact that the concentration of N₂O in the real atmosphere is low. However, the absolute values of the AC due to N₂O on the 10P2, 10P14, 10P16, and 10P32 transitions are comparable with the AC due to CO₂, and it is desirable to account for the N₂O effect when the paths are extended.

Sulphur dioxide (SO₂). As follows from Table VIII, the value of the AC due to SO₂ is small and may be significant only on the 9P48-9P10 transitions. The experimental value of the AC by the line 9R26, which absorbs most intensively, reported in Ref. 16, agrees with the theoretical one at a confidence level of 95%. The agreement between the calculated result and the experiment is somewhat worse for the other laser wavelengths, but the single experiment does not give grounds enough to draw final conclusions about the reliability of the PSL of SO₂.

Oxygen sulfide (OCS) and hydrogen sulfide (H₂S). These gases have not yet been experimentally studied with the help of the CO₂ laser because the AC values due to these gases are small in the spectral range under consideration. The AC due to OCS amounts to 0.5 cm⁻¹·atm⁻¹ for the 9P34 lasing line of the laser. It is evident that an employment of the CO₂ laser for gas analysis with respect to these compounds is advisable only for large concentrations of these gases, e.g., in the workshops of chemical and metallurgical plants.

Freon-12 (CF₂Cl₂). The PSL databank incorporates the parameters of the ν_6 -band lines of freon-12, obtained by the authors of Ref. 25. However, the calculated AC values are two times lower than the experimental. In the range 9-11 μ m of the freon-12 spectrum, aside from the

ν_6 band, the $2\nu_2$, $\nu_6 + \nu_4 - \nu_4$, and $\nu_6 + \nu_5 - \nu_5$ overtone and combination bands do absorb. Moreover, one should account the isotopic modifications CF₂³⁷Cl₂ and CF₂³⁵Cl³⁷Cl. In calculating, the half-widths of the freon-12 lines were assumed to be equal to 0.1 cm⁻¹ disregarding the rotational dependence of the half-width. This also leads to an underestimated value of the AC. All above points indicate that there is a need of a spectroscopic study of freon-12 and of the formation of a complete file of the PSL in the region 9-11 μ m, and this requires an additional treatment.

OPERATIONAL MODES OF THE "RAZBEG" PROGRAMMED SYSTEM

The following operational modes, determined by typing the individual letters, are provided for in the "Razbeg" programmed system under description:

S is the choice of the laser line by specifying the line characteristics or the radiation wavelength;

R is the choice of the line parameters from the databank and their scanning;

L is the edition of the laser line characteristics;

C is the choice of a specific (individual) gas, whose analysis is desired;

P is the printed output of the protocol (see Table IX);

M is the choice of the mixture of several gases;

O is the search for the wavelengths which are optimal for the gas analysis and the output of the array of characteristics of the laser lines with enumeration; and,

N is the choice of the laser line needed for the analysis from the found (optimal) lines based on indication of the line number.

The principle for choosing the "optimal" CO₂-laser lines for sensing different atmospheric and pollutant gases is as follows. For the gas, which has been specified from the databank of the PSL, the most intense lines (up to 500 in number) are chosen, for which the following relation is valid:

$$I_i \geq I_{\max} f,$$

where I_i is the intensity of the i th line of the given gas, I_{\max} is the maximum intensity from all of the PSL's of the given gas lying in the considered spectral interval, f is the empirical factor adjusted in such a way that the number of the most intense lines was within the limits 100 - 499 ($0 < f < 1$).

After that each line is compared with the laser lines from the database of laser PSL (CO₂). The lines for which the condition

$$\nu_\lambda - \Delta\nu \leq \nu_g < \nu_\lambda + \Delta\nu$$

is satisfied are chosen as optimal, where ν_λ specifies the position of the laser line center, ν_g specifies the position of the line center of the given gas, and $\Delta\nu$ is the interval of the frequency detuning.

TABLE V. Calculated and experimentally obtained data on the NH_3 absorption coefficients K_v ($\text{atm}^{-1}\cdot\text{cm}^{-1}$) within the 0001–1000 band of lasing of the CO_2 -laser.

Frequency (cm^{-1})	CO_2 -laser line	$K_v(\text{calc.})$ $T = 296 \text{ K}$	$K_v(\text{exp.})$			
			Ref. 16	Ref. 17	Ref. 15	Ref. 18
916.5834	P 48	$1.96\cdot 10^{-1}$				
918.7197	P 46	1.74				
920.8303	P 44	$6.71\cdot 10^{-1}$				
922.9153	P 42	$3.90\cdot 10^{-1}$				
924.9749	P 40	$9.00\cdot 10^{-1}$			1.31	
927.0091	P 38	3.95			3.68	
929.0182	P 36	8.01	7.80		7.45	8.07
931.0022	P 34	$1.36\cdot 10^1$	$1.34\cdot 10^1$	$1.24\cdot 10^1$	$1.33\cdot 10^1$	$1.31\cdot 10^1$
932.9611	P 32	$1.51\cdot 10^1$	$1.58\cdot 10^1$	$1.50\cdot 10^1$	$1.56\cdot 10^1$	$1.54\cdot 10^1$
934.8952	P 30	$8.13\cdot 10^{-1}$	$9.00\cdot 10^{-1}$	$8.60\cdot 10^{-1}$	$8.50\cdot 10^{-1}$	$9.50\cdot 10^{-1}$
936.8045	P 28	$2.44\cdot 10^{-1}$	$3.10\cdot 10^{-1}$	$3.60\cdot 10^{-1}$	$3.70\cdot 10^{-1}$	$3.60\cdot 10^{-1}$
938.6890	P 26	$2.73\cdot 10^{-1}$	$3.50\cdot 10^{-1}$	$3.40\cdot 10^{-1}$	$3.60\cdot 10^{-1}$	$4.50\cdot 10^{-1}$
940.5488	P 24	$7.25\cdot 10^{-2}$	$1.50\cdot 10^{-1}$	$1.30\cdot 10^{-1}$	$1.50\cdot 10^{-1}$	$2.00\cdot 10^{-1}$
942.3841	P 22	$3.22\cdot 10^{-2}$	$1.30\cdot 10^{-1}$	$4.50\cdot 10^{-2}$	$4.00\cdot 10^{-2}$	$1.20\cdot 10^{-1}$
944.1948	P 20	$5.82\cdot 10^{-2}$	$1.40\cdot 10^{-1}$	$1.20\cdot 10^{-1}$	$9.00\cdot 10^{-2}$	$1.90\cdot 10^{-1}$
945.9810	P 18	$9.25\cdot 10^{-2}$	$1.10\cdot 10^{-1}$	$1.40\cdot 10^{-1}$	$8.00\cdot 10^{-2}$	$1.10\cdot 10^{-1}$
947.7427	P 16	$3.41\cdot 10^{-1}$	$5.30\cdot 10^{-1}$	$4.90\cdot 10^{-1}$	$5.80\cdot 10^{-1}$	$5.40\cdot 10^{-1}$
949.4800	P 14	$4.21\cdot 10^{-1}$	$6.10\cdot 10^{-1}$	$8.10\cdot 10^{-1}$	$7.20\cdot 10^{-1}$	$8.70\cdot 10^{-1}$
951.1930	P 12	$4.78\cdot 10^{-1}$	$7.20\cdot 10^{-1}$	$5.70\cdot 10^{-1}$	$5.40\cdot 10^{-1}$	$7.30\cdot 10^{-1}$
952.8816	P 10	$1.38\cdot 10^{-1}$	$2.50\cdot 10^{-1}$	$1.30\cdot 10^{-1}$	$2.20\cdot 10^{-1}$	$7.80\cdot 10^{-1}$
954.5458	P 8	$2.01\cdot 10^{-1}$			3.48	
956.1857	P 6	$5.78\cdot 10^{-1}$			$7.20\cdot 10^{-1}$	
957.8012	P 4	1.86				
959.3924	P 2	2.17				
961.7336	R 0	1.91				
963.2638	R 2	6.89				
964.7697	R 4	1.14			8.20	
966.2511	R 6	$2.78\cdot 10^1$	$3.25\cdot 10^1$		$3.06\cdot 10^1$	$2.90\cdot 10^1$
967.7079	R 8	$2.27\cdot 10^1$	$2.58\cdot 10^1$	$2.19\cdot 10^1$	$2.61\cdot 10^1$	$2.32\cdot 10^1$
969.3281	R 10	$4.51\cdot 10^{-1}$	$3.10\cdot 10^{-1}$	$7.80\cdot 10^{-1}$	$6.30\cdot 10^{-1}$	$5.20\cdot 10^{-1}$
970.5479	R 12	$2.28\cdot 10^{-1}$	$6.00\cdot 10^{-2}$	$4.60\cdot 10^{-1}$	$5.80\cdot 10^{-1}$	$2.30\cdot 10^{-1}$
971.9310	R 14	7.05	7.50	$6.30\cdot 10^{-1}$	7.60	7.03
973.2892	R 16	$9.99\cdot 10^{-2}$	$7.00\cdot 10^{-2}$	$1.00\cdot 10^{-1}$		$1.10\cdot 10^{-1}$
974.6226	R 18	$4.72\cdot 10^{-2}$	$1.60\cdot 10^{-1}$	$2.30\cdot 10^{-1}$		$6.00\cdot 10^{-2}$
975.9311	R 20	$2.63\cdot 10^{-2}$	$1.80\cdot 10^{-1}$	$3.60\cdot 10^{-2}$		$5.00\cdot 10^{-2}$
977.2146	R 22	$1.12\cdot 10^{-2}$	$2.00\cdot 10^{-1}$	$5.70\cdot 10^{-2}$		$4.00\cdot 10^{-2}$
978.4730	R 24	$1.90\cdot 10^{-3}$	$2.70\cdot 10^{-1}$	$2.80\cdot 10^{-2}$		$4.00\cdot 10^{-2}$
979.7061	R 26	$1.37\cdot 10^{-3}$	$1.40\cdot 10^{-1}$	$4.40\cdot 10^{-2}$		$4.00\cdot 10^{-2}$
980.9139	R 28	$1.77\cdot 10^{-3}$	$1.60\cdot 10^{-1}$	$4.40\cdot 10^{-2}$		$4.00\cdot 10^{-2}$
982.0962	R 30	$2.09\cdot 10^{-3}$	$2.60\cdot 10^{-1}$	$2.90\cdot 10^{-2}$		$3.00\cdot 10^{-2}$
983.2530	R 32	$5.56\cdot 10^{-3}$	$2.80\cdot 10^{-1}$	$2.00\cdot 10^{-2}$		$2.00\cdot 10^{-2}$
984.3840	R 34	$7.28\cdot 10^{-3}$	$2.10\cdot 10^{-1}$			
985.4891	R 36	$9.94\cdot 10^{-3}$				
986.5682	R 38	$1.47\cdot 10^{-2}$				
987.6212	R 40	$9.24\cdot 10^{-2}$				
988.6477	R 42	$3.76\cdot 10^{-2}$				
989.6478	R 44	$6.34\cdot 10^{-2}$				
990.6212	R 46	$1.68\cdot 10^{-1}$				
991.5676	R 48	3.30				

TABLE VI. Calculated and experimentally obtained data on the NH_3 absorption coefficients K_v ($\text{atm}^{-1}\cdot\text{cm}^{-1}$) within the 0001–0200 band of lasing of the CO_2 -laser.

Frequency (cm^{-1})	CO_2 -laser line	$K_v(\text{calc.})$ $T = 296 \text{ K}$	$K_v(\text{exp.})$					
			Ref. 16	Ref. 17	Ref. 15	Ref. 18	Ref. 19	
1018.9020	P 48	$1.26\cdot 10^{-2}$						
1021.0579	P 46	$1.36\cdot 10^{-2}$						
1023.1901	P 44	$1.47\cdot 10^{-1}$						
1025.2984	P 42	$8.04\cdot 10^{-2}$						
1027.3825	P 40	1.64						
1029.4423	P 38	$1.40\cdot 10^{-1}$						
1031.4776	P 36	$5.35\cdot 10^{-1}$			$5.80\cdot 10^{-1}$			
1033.5843	P 34	2.33			3.74			
1035.4737	P 32	$2.26\cdot 10^{-1}$	$3.40\cdot 10^{-1}$	$3.10\cdot 10^{-1}$		$2.80\cdot 10^{-1}$	$3.20\cdot 10^{-1}$	
1037.4342	P 30	$5.01\cdot 10^{-2}$	$1.30\cdot 10^{-1}$	$8.20\cdot 10^{-2}$		$8.00\cdot 10^{-2}$	$9.00\cdot 10^{-1}$	
1039.3694	P 28	$3.89\cdot 10^{-2}$	$9.00\cdot 10^{-2}$	$5.60\cdot 10^{-2}$		$8.00\cdot 10^{-2}$	$6.00\cdot 10^{-2}$	
1041.2791	P 26	$3.98\cdot 10^{-2}$	$5.00\cdot 10^{-2}$	$1.00\cdot 10^{-1}$		$1.20\cdot 10^{-1}$	$1.00\cdot 10^{-1}$	
1043.1633	P 24	$2.07\cdot 10^{-1}$	$1.60\cdot 10^{-1}$	$4.30\cdot 10^{-1}$		$4.60\cdot 10^{-1}$	$4.70\cdot 10^{-1}$	
1045.0218	P 22	$3.22\cdot 10^{-1}$	$2.50\cdot 10^{-1}$	$3.50\cdot 10^{-1}$	$4.20\cdot 10^{-1}$	$3.60\cdot 10^{-1}$	$3.80\cdot 10^{-1}$	
1046.8543	P 20	2.73	2.28	2.16	2.38	2.71	2.50	
1048.6609	P 18	$2.25\cdot 10^{-1}$	$1.30\cdot 10^{-1}$	$2.40\cdot 10^{-1}$	$3.20\cdot 10^{-1}$	$2.30\cdot 10^{-1}$	$2.60\cdot 10^{-1}$	
1050.4414	P 16	$1.55\cdot 10^{-1}$	$1.80\cdot 10^{-1}$	$2.00\cdot 10^{-1}$		$1.80\cdot 10^{-1}$	$2.20\cdot 10^{-1}$	
1052.1956	P 14	$3.42\cdot 10^{-1}$	$1.60\cdot 10^{-1}$	$3.10\cdot 10^{-1}$		$3.80\cdot 10^{-1}$	$3.40\cdot 10^{-1}$	
1053.9236	P 12	$9.30\cdot 10^{-1}$	1.03	$9.40\cdot 10^{-1}$		$9.60\cdot 10^{-1}$	1.03	
1055.6251	P 10	$2.61\cdot 10^{-1}$	$6.00\cdot 10^{-2}$	$3.60\cdot 10^{-1}$		$3.80\cdot 10^{-1}$	$3.90\cdot 10^{-1}$	
1058.1953	P 8	$2.98\cdot 10^{-2}$	$3.10\cdot 10^{-1}$					
1058.9488	P 6	$8.11\cdot 10^{-2}$						
1060.5707	P 4	$2.69\cdot 10^{-2}$						
1062.1660	P 2	$4.87\cdot 10^{-2}$						
1064.5089	R 0	$3.89\cdot 10^{-1}$						
1066.0374	R 2	2.02						
1067.5391	R 4	$4.31\cdot 10^{-1}$						
1069.0141	R 6	$1.20\cdot 10^{-1}$			$3.70\cdot 10^{-1}$			
1070.4623	R 8	1.79	3.00		2.76		2.60	
1071.8838	R 10	$1.63\cdot 10^{-1}$	$3.50\cdot 10^{-1}$	$2.40\cdot 10^{-1}$	$3.90\cdot 10^{-1}$	$2.70\cdot 10^{-1}$	$3.70\cdot 10^{-1}$	
1073.2785	R 12	$2.69\cdot 10^{-1}$	$2.50\cdot 10^{-1}$	$3.40\cdot 10^{-1}$	$3.10\cdot 10^{-1}$	$3.20\cdot 10^{-1}$		
1074.6465	R 14	$5.81\cdot 10^{-1}$	$6.70\cdot 10^{-1}$	$6.60\cdot 10^{-1}$	$7.80\cdot 10^{-1}$	$6.90\cdot 10^{-1}$	$7.20\cdot 10^{-1}$	
1075.9879	R 16	$1.47\cdot 10^{+1}$	$1.33\cdot 10^{+1}$	$1.27\cdot 10^{+1}$	$1.35\cdot 10^{+1}$	$1.38\cdot 10^{+1}$	$1.05\cdot 10^{+1}$	
1077.3026	R 18	$9.72\cdot 10^{-2}$	$3.60\cdot 10^{-1}$	$1.30\cdot 10^{-1}$	$2.90\cdot 10^{-1}$	$1.40\cdot 10^{-1}$	$1.40\cdot 10^{-1}$	
1078.5907	R 20	$4.09\cdot 10^{-2}$	$2.10\cdot 10^{-1}$	$2.70\cdot 10^{-2}$		$6.00\cdot 10^{-2}$	$3.00\cdot 10^{-2}$	
1079.8523	R 22	$3.79\cdot 10^{-2}$	$1.00\cdot 10^{-1}$	$6.40\cdot 10^{-2}$		$7.00\cdot 10^{-2}$	$7.80\cdot 10^{-2}$	
1081.0875	R 24	$5.51\cdot 10^{-2}$	$1.20\cdot 10^{-1}$	$6.40\cdot 10^{-2}$		$8.00\cdot 10^{-2}$	$7.00\cdot 10^{-2}$	
1082.2983	R 26	$1.07\cdot 10^{-1}$	$3.70\cdot 10^{-1}$	$1.10\cdot 10^{-1}$		$1.00\cdot 10^{-1}$	$1.20\cdot 10^{-1}$	
1083.4788	R 28	$4.19\cdot 10^{-1}$		$3.80\cdot 10^{-1}$	$5.30\cdot 10^{-1}$	$4.50\cdot 10^{-1}$	$4.20\cdot 10^{-1}$	
1084.6352	R 30	$7.22\cdot 10^{+1}$		$1.20\cdot 10^{+2}$	$7.00\cdot 10^{+1}$	$2.70\cdot 10^{+1}$		
1085.7655	R 32	$5.34\cdot 10^{-1}$			$2.70\cdot 10^{-1}$			
1086.8699	R 34	$2.21\cdot 10^{-1}$						
1087.9485	R 36	$8.72\cdot 10^{-2}$						
1089.0014	R 38	$4.25\cdot 10^{-1}$						
1090.0288	R 40	$1.58\cdot 10^{-1}$						
1091.0308	R 42	$8.88\cdot 10^{-2}$						
1092.0076	R 44	$6.76\cdot 10^{-1}$						
1092.9594	R 46	$9.52\cdot 10^{-2}$						
1093.8863	R 48	$8.28\cdot 10^{-1}$						

TABLE VII. Calculated and experimentally obtained data on the O_3 absorption coefficients K_v ($\text{atm}^{-1}\cdot\text{cm}^{-1}$) within the 0001–0200 band of lasing of the CO_2 -laser.

Frequency (cm^{-1})	CO_2 -laser line	$K_v(\text{calc.})$ $T = 296 \text{ K}$	$K_v(\text{exp.})$					
			Ref. 38	Ref. 17	Ref. 22	Ref. 23	Ref. 24	Ref. 18
1018.9020	P 48	7.66						
1021.0579	P 46	6.39						
1023.1901	P 44	6.48						
1025.2984	P 42	9.72						
1027.3825	P 40	10.4						
1029.4423	P 38	4.17						
1031.4776	P 36	3.78	6.67	6.70	8.00		2.20	
1033.5843	P 34	3.43	2.99	3.00	3.60		3.50	3.60
1035.4737	P 32	4.28	5.98	5.90	6.00		3.70	6.20
1037.4342	P 30	5.07	6.44	6.40	7.80		4.30	6.60
1039.3694	P 28	8.29	9.44	9.40	11.8		2.10	9.00
1041.2791	P 26	5.49	5.98	6.00	6.5	—	1.00	6.00
1043.1633	P 24	0.35	0.69	0.70	1.20	0.71	0.80	0.57
1045.0218	P 22	1.08	1.84	1.80	2.90	1.93	2.30	1.97
1046.8543	P 20	4.52	5.29	5.50	5.20	4.33	2.60	4.70
1048.6609	P 18	2.88	6.45	6.40	8.00	6.11	4.50	5.50
1050.4414	P 16	6.74	8.98	9.00	11.5	8.78	5.00	8.50
1052.1956	P 14	8.76	12.6	12.7	14.6	12.9	5.80	12.8
1053.9236	P 12	12.0	12.2	12.2	14.4	12.4		11.4
1055.6251	P 10	10.2	5.98	6.00	7.40	6.43		5.70
1058.1953	P 8	15.6	12.7	12.7	14.5	14.1		12.3
1058.9488	P 6	5.19						
1060.5707	P 4	10.3						
1062.1660	P 2	7.63						
1064.5089	R 0	5.71						
1066.0374	R 2	3.38						
1067.5391	R 4	2.64						
1069.0141	R 6	1.53						
1070.4623	R 8	1.22						
1071.8838	R 10	$6.67\cdot 10^{-1}$						
1073.2785	R 12	$5.02\cdot 10^{-1}$						
1074.6465	R 14	$2.86\cdot 10^{-1}$						
1075.9879	R 16	$1.15\cdot 10^{-1}$						
1077.3026	R 18	$4.95\cdot 10^{-2}$						
1078.5907	R 20	$5.80\cdot 10^{-2}$						
1079.8523	R 22	$1.80\cdot 10^{-1}$						
1081.0875	R 24	$4.42\cdot 10^{-1}$						
1082.2963	R 26	$9.56\cdot 10^{-2}$						
1083.4788	R 28	$7.42\cdot 10^{-2}$						
1084.6352	R 30	$2.28\cdot 10^{-1}$						
1085.7655	R 32	$1.05\cdot 10^{-1}$						
1086.8699	R 34	$1.85\cdot 10^{-1}$						
1087.9485	R 36	$1.98\cdot 10^{-1}$						
1089.0014	R 38	$2.31\cdot 10^{-1}$						
1090.0288	R 40	$1.18\cdot 10^{-1}$						
1091.0308	R 42	$1.17\cdot 10^{-1}$						
1092.0076	R 44	$1.75\cdot 10^{-1}$						
1092.9594	R 46	$1.44\cdot 10^{-1}$						
1093.8863	R 48	$1.65\cdot 10^{-1}$						

TABLE VIII. Calculated and experimentally obtained data on the SO₂ absorption coefficient K_v (atm⁻¹·cm⁻¹) within the 0001–0200 band of lasing of the CO₂-laser.

Frequency (cm ⁻¹)	CO ₂ -laser line	K_v (calc.)	K_v (exp.) Ref. 16
1018.9020	P 48		
1021.0579	P 46		
1023.1901	P 44		
1025.2984	P 42		
1027.3825	P 40		
1029.4423	P 38		
1031.4776	P 36		
1033.5843	P 34	$4.78 \cdot 10^{-9}$	
1035.4737	P 32	$1.87 \cdot 10^{-8}$	
1037.4342	P 30	$5.60 \cdot 10^{-8}$	
1039.3694	P 28	$1.88 \cdot 10^{-7}$	
1041.2791	P 26	$8.00 \cdot 10^{-7}$	
1043.1633	P 24	$3.25 \cdot 10^{-6}$	
1045.0218	P 22	$6.26 \cdot 10^{-5}$	
1046.8543	P 20	$3.48 \cdot 10^{-5}$	
1048.6609	P 18	$1.53 \cdot 10^{-4}$	
1050.4414	P 16	$3.00 \cdot 10^{-4}$	
1052.1956	P 14	$1.50 \cdot 10^{-3}$	
1053.9236	P 12	$7.99 \cdot 10^{-4}$	
1055.6251	P 10	$6.33 \cdot 10^{-4}$	
1058.1953	P 8	$3.04 \cdot 10^{-3}$	
1058.9488	P 6	$2.59 \cdot 10^{-3}$	
1060.5707	P 4	$5.19 \cdot 10^{-3}$	
1062.1660	P 2	$1.26 \cdot 10^{-2}$	
1064.5089	R 0	$2.97 \cdot 10^{-2}$	
1066.0374	R 2	$3.28 \cdot 10^{-2}$	
1067.5391	R 4	$3.21 \cdot 10^{-2}$	
1069.0141	R 6	$3.11 \cdot 10^{-2}$	
1070.4623	R 8	$3.09 \cdot 10^{-2}$	$3.60 \cdot 10^{-2}$
1071.8838	R 10	$2.53 \cdot 10^{-2}$	$4.40 \cdot 10^{-2}$
1073.2785	R 12	$3.05 \cdot 10^{-2}$	$4.80 \cdot 10^{-2}$
1074.6485	R 14	$3.80 \cdot 10^{-2}$	$5.40 \cdot 10^{-2}$
1075.9879	R 16	$3.88 \cdot 10^{-2}$	$5.60 \cdot 10^{-2}$
1077.3026	R 18	$5.33 \cdot 10^{-2}$	$6.80 \cdot 10^{-2}$
1078.5907	R 20	$5.70 \cdot 10^{-2}$	$8.80 \cdot 10^{-2}$
1079.8523	R 22	$5.53 \cdot 10^{-2}$	$7.20 \cdot 10^{-2}$
1081.0875	R 24	$6.99 \cdot 10^{-2}$	$9.00 \cdot 10^{-2}$
1082.2963	R 26	$1.00 \cdot 10^{-1}$	$1.05 \cdot 10^{-1}$
1083.4788	R 28	$8.82 \cdot 10^{-2}$	$9.20 \cdot 10^{-2}$
1084.6352	R 30	$9.48 \cdot 10^{-2}$	$1.10 \cdot 10^{-1}$
1085.7655	R 32	$8.68 \cdot 10^{-2}$	
1086.8699	R 34	$7.97 \cdot 10^{-2}$	
1087.9485	R 36	$1.05 \cdot 10^{-1}$	
1089.0014	R 38	$1.09 \cdot 10^{-1}$	
1090.0288	R 40	$1.28 \cdot 10^{-1}$	
1091.0308	R 42	$9.73 \cdot 10^{-2}$	
1092.0076	R 44	$1.54 \cdot 10^{-1}$	
1092.9594	R 46	$1.99 \cdot 10^{-1}$	
1093.8863	R 48	$1.22 \cdot 10^{-1}$	

TABLE IX.

ATLAS SYSTEM V-1.0
CO₂-Laser Gas Analysis Subsystem

Session protocol

Wednesday, 22/5/1991 15:15:46

Laser line parameters:

Center: 9.14172 (1093.89);

Quantum identification: 001-020 R(48);

Isotope code: 626

Base line parameters within the interval ± 2 GHz:

Center	Intensity	H/W	Gas
1093.84420	3.976E-06	0.070	20 (OCS)
1093.84620	4.009E-06	0.070	20 (OCS)
1093.86043	3.336E-05	0.080	9 (SO ₂)
1093.87993	9.179E-05	0.080	9 (SO ₂)
1093.89163	4.223E-05	0.080	9 (SO ₂)
1093.95247	3.207E-03	0.080	9 (SO ₂)
1093.95756	1.124E-03	0.080	9 (SO ₂)

Absorption due to H₂O = 1.25E-06

Absorption due to N₂O = 2.796E-08

Absorption due to SO₂ = 1.221E-01

Absorption due to OCS = 7.420E-05

Absorption due to H₂S = 2.915E-03

CONCLUSION

Remote measurements of extinction of the optical radiation passing through the atmosphere contain the information about the atmospheric gaseous composition, i.e., the measured absorption coefficient is the result of overlapping of absorption lines of different gaseous components. Regardless of the mathematical apparatus employed for processing of the remote measurements, the values of the absorption coefficients with prescribed range of variation of the errors must be *a priori* known. Analysis of the experimental values of the AC shows that separate cell measurements of the AC of individual gases do not guarantee the high level of confidence of the obtained data, and the discrepancies of the results of independent experiments may reach several orders of magnitude. In this paper we have shown that developing the principles of databank formation on the basis of the spectral line parameters of the atmospheric and trace gases by means of compilation, systematization, and selection of both experimental and calculated data with analysis of their reliability, one can perform well-posed calculations of the spectral characteristics of absorption due to atmospheric and trace gases for a correct solution of the laser gas analysis problem.

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