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High resolution study of the $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$ “hot” bands and ro-vibrational re-analysis of the $\nu_1 + \nu_2/\nu_2 + \nu_3/3\nu_2$ polyad of the $^{32}\text{SO}_2$ molecule

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ABSTRACT

The weak “hot” absorption bands, $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$, were analysed with high resolution using the Fourier transform interferometer Bruker IFS-120 HR. In order to make possible an analysis of the $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$ bands, as the first step, we re-analysed considerably the stronger “cold” bands, $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$, which are located in the same spectral regions. As the result of analysis we obtained about 2650 and 2050 transitions (1069 and 1001 upper state ro-vibrational energy values) with $J^{max.} = 78$, $K_a^{max.} = 27$ and $J^{max.} = 68$, $K_a^{max.} = 24$ for the bands $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$, respectively, that is considerably higher than in the earlier studies of corresponding bands ($J^{max.} = 33$, $K_a^{max.} = 7$ and $J^{max.} = 50$, $K_a^{max.} = 16$ for the same bands, $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$, respectively). A strong local resonance interaction with the $3\nu_2$ band was taken into account, and the set of parameters that reproduce the initial experimental data with an accuracy close to experimental uncertainties, was obtained. The weak $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$ bands were assigned, and about 870 and 930 transitions (553 and 540 upper state ro-vibrational energy values) with $J^{max.} = 60$ and $K_a^{max.} = 20$ and $J^{max.} = 59$ and $K_a^{max.} = 16$ were assigned to the $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$ bands, respectively. A complete list of assigned transitions is presented, and corresponding spectroscopic parameters are obtained from the fit of assigned transitions (upper energy values).

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1. Introduction

Sulfur dioxide is an important chemical species in many fields such as chemistry, astrophysics, atmospheric optics, laser techniques, etc. (see, e.g., reviews in Refs. [1,2]). Therefore, spectroscopic studies of the sulfur dioxide molecule have been made during many years both in the microwave (see, e.g., review in Ref. [3]),

and submillimeter wave and infrared regions (see, Refs. [4–34]). Recently we fulfilled the analysis of the set of high excited vibrational bands of the SO_2 molecule, Refs. [35–37]. In the present paper we continue our study of the SO_2 high-resolution spectra, and the subject of interest now is the weak bands $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$ (the upper vibrational state, (120) and (021)). We also re-analysed the ro-vibrational structure of the considerably stronger bands, $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$, and more than two times increased the known information about these bands. A strong resonance interaction with the (030) vibrational state is clearly indicated and discussed.

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2. Experimental details

The spectrum of SO₂ in the wavenumber region 1500–2300 cm⁻¹ was measured with the Bruker IFS 120 HR

Fourier transform spectrometer in Oulu, Finland. The interferogram was recorded at room temperature with a sample pressure of 0.83 Torr and an absorption path length of 163 m. A Globar source, a KBr beam splitter, and

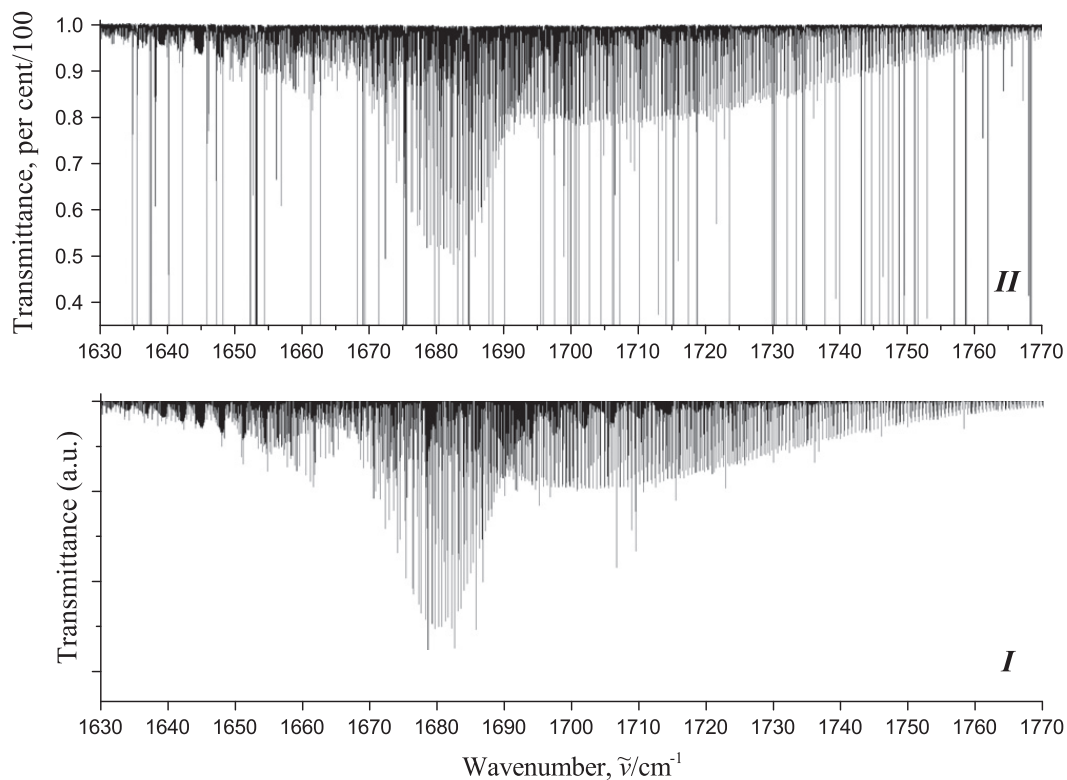


Fig. 1. Survey spectrum of SO₂ in the region of the band $\nu_1 + \nu_2$: *I* and *II* are the simulated and the experimentally recorded spectra, respectively.

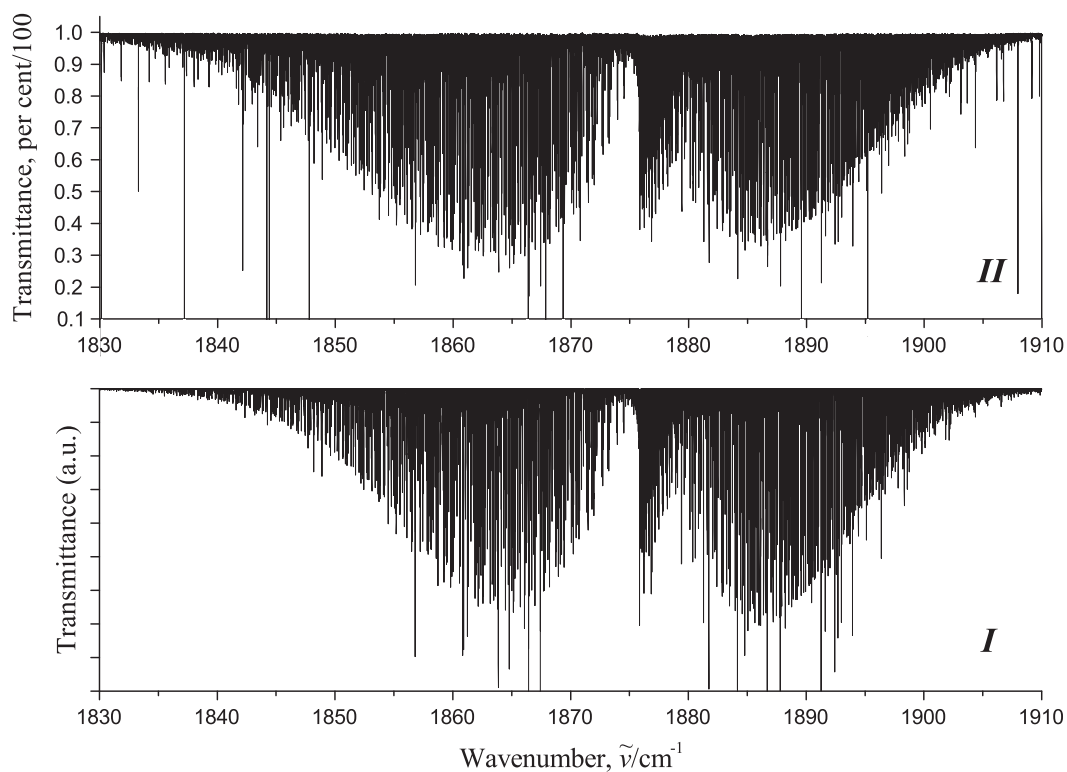


Fig. 2. Survey spectrum of SO₂ in the region of the band $\nu_2 + \nu_3$: *I* and *II* are the simulated and the experimentally recorded spectra, respectively.

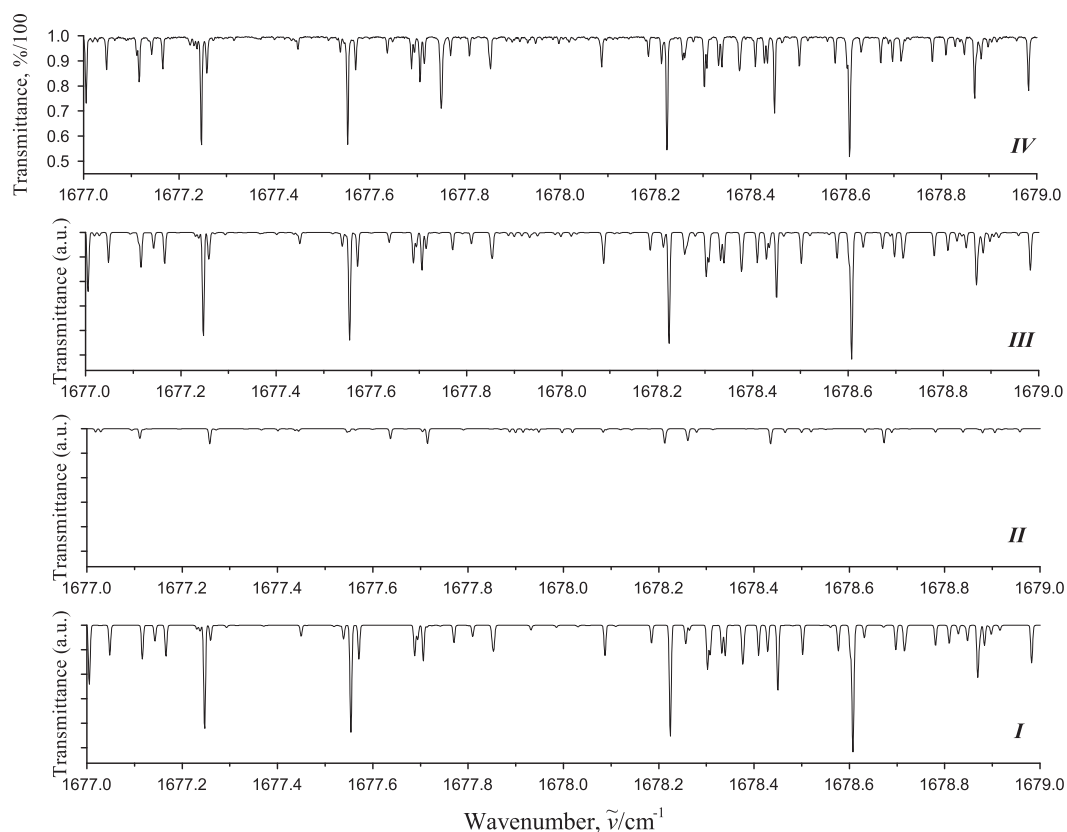


Fig. 3. Small portion of the high resolution spectrum of the SO_2 molecule in the region of the Q-branch of the $\nu_1 + \nu_2$ absorption band: **IV** is the experimentally recorded spectrum, and the three lower traces (**I–III**) present simulated spectra. The traces **I** and **II** show the lines belonging to the “cold” band, $\nu_1 + \nu_2$, and the “hot” band, $\nu_1 + 2\nu_2 - \nu_2$, respectively. The sum of the simulated spectra **I** and **II** is given by trace **III**.

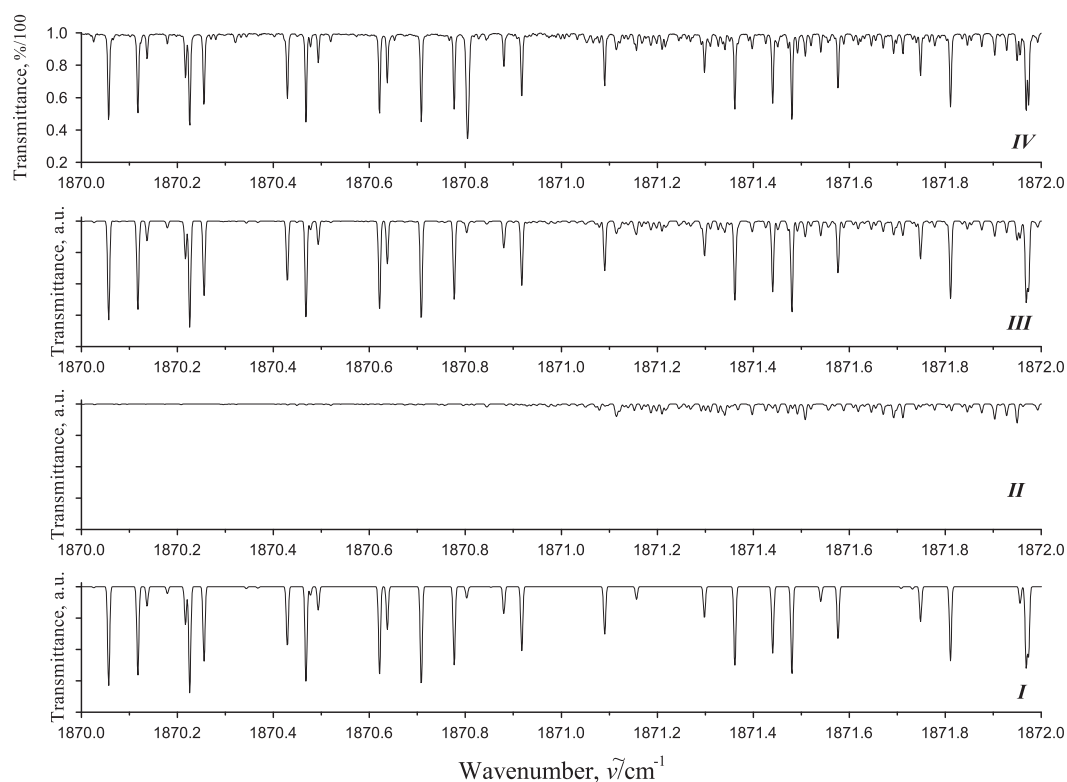


Fig. 4. Small portion of the high-resolution spectrum of the SO_2 molecule in the region of the $\nu_2 + \nu_3$ absorption band: **IV** is the experimentally recorded spectrum, and the three lower traces (**I–III**) present simulated spectra. The traces **I** and **II** show the lines belonging to the “cold” band, $\nu_2 + \nu_3$, and the “hot” band, $2\nu_2 + \nu_3 - \nu_2$, respectively. The sum of the simulated spectra **I** and **II** is given by trace **III**.

Table 1
Experimental ro-vibrational term values for the (1 1 0) vibrational state of the SO₂ molecule (in cm⁻¹).^a

J	K _a			J	K _c			E	Δ	δ	J	K _a			E	Δ	δ					
	K _a	K _c	K _c		K _a	K _c	K _c					K _a	K _c	K _c								
0	0	0	0	11	1	11	11	1708.0886	0	0	15	10	6	1916.6761	1	0	19	4	16	1815.2561	1	-1
1	1	1	1	0	11	10	10	1715.0746	1	-1	15	11	5	1953.0147	2	-2	19	5	15	1830.8555	4	-1
2	2	0	2	4	11	9	9	1724.0317	2	1	15	12	4	1992.7228	2	-1	19	6	14	1849.9779	3	2
2	1	1	1	0	11	8	8	1736.2471	2	1	15	13	3	2035.7762	3	2	19	7	13	1872.5974	3	1
2	2	0	2	1	11	7	7	1751.9521	1	-1	15	14	2	2082.1480	3	3	19	8	12	1898.6833	2	0
3	1	3	1	1	11	6	6	1771.1398	2	0	15	15	1	2131.8107	0	0	19	9	11	1928.2111	0	0
3	2	2	2	1	11	5	5	1793.7925	1	0	16	0	16	1749.9864	2	0	19	10	10	1961.1580	2	2
3	3	1	3	0	11	4	4	1819.8936	1	1	16	1	15	1756.7541	1	1	19	11	9	1997.5005	0	0
4	0	4	0	1	11	3	3	1849.4252	1	1	16	2	14	1761.6108	1	0	19	12	8	2037.2151	1	-1
4	1	3	1	1	11	2	2	1882.3683	1	1	16	3	13	1768.9771	1	-1	19	13	7	2080.2771	1	2
4	2	2	2	1	11	1	1	1918.7016	2	-2	16	4	12	1780.8369	1	0	19	14	6	2126.6591	0	0
4	3	1	3	0	11	0	0	1714.8059	1	0	16	5	11	1796.4696	1	0	19	15	5	2176.3341	2	1
4	4	0	4	0	11	1	1	1719.2286	0	0	16	6	10	1815.6283	1	-1	19	16	4	2229.2726	0	0
5	1	5	1	2	12	2	2	1723.6224	1	1	16	7	9	1838.2680	3	2	19	17	3	2285.4447	2	1
5	2	4	2	1	12	3	3	1731.7435	0	0	16	8	8	1864.3638	1	0	19	18	2	2344.8187	5	3
5	3	3	3	1	12	4	4	1743.8825	1	-1	16	9	7	1893.8955	2	-2	19	19	1	2407.3613	1	-1
5	4	2	4	0	12	5	5	1759.5788	2	-2	16	10	6	1926.8425	2	0	20	0	20	1794.4165	1	-2
5	5	1	5	0	12	6	6	1778.7633	1	0	16	11	5	1963.1826	2	1	20	1	19	1803.9379	2	0
6	0	6	0	1	12	7	7	1801.4147	2	-1	16	12	4	2002.8923	1	0	20	2	18	1810.1746	0	0
6	1	5	1	2	12	8	4	1827.5154	2	-2	16	13	3	2045.9475	2	1	20	3	17	1816.9283	1	0
6	2	4	2	1	12	9	3	1857.0474	3	-3	16	14	2	2092.3217	1	0	20	4	16	1828.1395	0	0
6	3	3	3	1	12	10	2	1889.9917	0	0	16	15	1	2141.9876	1	1	20	5	15	1843.6066	1	-1
6	4	2	4	0	12	11	1	1926.3264	2	-2	16	16	0	2194.9158	2	-1	20	6	14	1862.7063	0	0
6	5	1	5	0	12	12	0	1966.0297	1	2	17	1	17	1760.3996	2	-1	20	7	13	1885.3161	0	-1
6	6	0	6	0	12	13	1	1723.1614	3	2	17	2	16	1769.6862	2	0	20	8	12	1911.3970	1	-2
7	1	7	1	1	13	2	12	1730.8140	4	0	17	3	15	1779.4218	1	0	20	9	11	1940.9226	1	0
7	2	6	2	0	13	3	11	1739.9457	2	-1	17	4	14	1791.6534	1	-1	20	10	10	1973.8688	2	1
7	3	5	3	1	13	4	10	1752.1534	1	1	17	5	13	1807.2902	1	-1	20	11	9	2010.2119	2	0
7	4	4	4	0	13	5	9	1767.8432	2	-2	17	6	12	1826.4392	1	-1	20	12	8	2049.9281	2	0
7	5	3	5	0	13	6	8	1787.0236	1	0	17	7	11	1849.0733	1	-1	20	13	7	2092.9922	3	3
7	6	2	6	1	13	7	7	1809.6731	0	-1	17	8	10	1875.1668	1	0	20	14	6	2139.3767	1	0
7	7	1	7	0	13	8	6	1835.7737	2	2	17	9	9	1904.6979	1	1	20	15	5	2189.0549	2	1
8	0	8	0	1	13	9	5	1865.3058	1	-1	17	10	8	1937.6449	0	0	20	16	4	2241.9970	1	-1
8	1	7	1	1	13	10	4	1898.2508	1	0	17	11	7	1973.9859	1	0	20	17	3	2298.1730	1	0
8	2	6	2	0	13	11	3	1934.5871	1	1	17	12	6	2013.6974	1	0	20	18	2	2357.5509	3	-2
8	3	5	3	0	13	12	2	1974.2915	3	-2	17	13	5	2056.7551	1	4	20	19	1	2420.0984	4	-3
8	4	4	4	1	13	13	1	2017.3407	1	2	17	14	4	2103.1317	2	2	21	0	21	1807.0354	0	-1
8	5	3	5	0	13	14	0	1731.2400	1	-1	17	15	3	2152.8003	2	0	21	1	20	1818.2862	3	-2
8	6	2	6	1	13	15	1	1736.7563	1	1	17	16	2	2205.7321	0	0	21	2	19	1829.0319	2	-1
8	7	1	7	0	13	16	2	1741.2789	2	1	17	17	1	2261.8963	2	-2	21	3	18	1841.4304	1	-1
8	8	0	8	0	13	17	1	1749.0382	2	2	18	0	18	1771.0443	3	2	21	4	17	1856.9894	2	-1
9	1	9	1	1	14	4	10	1761.0739	2	1	18	1	17	1779.1660	1	1	21	5	16	1876.0751	3	2
9	2	8	2	0	14	5	9	1776.7462	1	-1	18	2	15	1791.5964	0	0	21	6	15	1898.6736	1	0
9	3	7	3	0	14	6	8	1795.9208	2	-1	18	3	14	1803.1858	0	0	21	7	14	1924.7486	1	0
9	4	6	4	0	14	7	7	1818.5680	2	0	18	4	13	1818.7542	0	0	21	8	13	1954.2710	1	0
9	5	5	5	1	14	8	6	1844.6673	1	0	18	5	12	1837.8889	1	0	21	9	12	1987.2159	1	0
9	6	4	6	0	14	9	5	1874.1999	2	1	18	6	11	1860.5162	1	-2	21	10	11	2023.5594	0	0
9	7	3	7	0	14	10	4	1757.8016	1	0	18	7	10	1874.1999	2	1	21	11	10	2023.5594	0	0

42	12	30	2490.6200	3	2	45	13	33	2617.6190	3	-1	48	13	35	2707.3076	2	-4	51	16	36	2951.7987	5	4
42	13	29	2533.6615	2	1	45	14	32	2664.0130	4	3	48	14	34	2753.6826	3	1	51	17	35	3008.0924	4	3
42	14	28	2580.0676	1	2	45	15	31	2713.7380	3	-2	48	15	33	2803.3998	1	1	51	18	34	3067.6227	4	-2
42	15	27	2629.7962	2	-2	45	16	30	2766.7604	2	2	48	16	32	2856.4219	2	-1	52	0	52	2484.4745	2	1
42	16	26	2682.8147	1	0	45	17	29	2823.0426	1	-1	48	17	31	2912.7122	2	5	52	1	51	2514.0403	2	3
42	17	25	2739.0874	2	-1	45	18	28	2882.5500	1	0	48	18	30	2972.2323	2	6	52	2	50	2541.4321	1	2
42	18	24	2798.5802	5	-2	45	19	27	2945.2461	-1	-1	48	19	29	3034.9455	3	0	52	3	49	2566.2521	5	4
42	19	23	2861.2584	5	2	45	20	26	3011.0948	-5	-5	48	20	28	3100.8158	2	-2	52	4	48	2587.3407	2	2
42	20	22	2927.0852	3	-2	46	0	46	2309.7763	1	-1	49	1	48	2394.5154	2	-1	52	5	47	2602.8371	6	1
43	1	43	2320.2609	3	2	46	1	45	2335.7363	1	-1	49	2	48	2422.2807	2	0	52	6	46	2615.7745	5	0
43	2	42	2254.4183	3	1	46	2	44	2359.4543	4	3	49	3	47	2447.8689	3	-2	52	7	45	2633.1537	1	0
43	3	41	2276.3756	3	0	46	3	43	2380.2334	1	-1	49	4	46	2471.0530	1	-2	52	8	44	2656.8771	2	-2
43	4	40	2296.0598	2	2	46	4	42	2396.2747	0	2	49	5	45	2492.0066	4	-3	52	9	43	2685.2536	0	-3
43	5	39	2314.3140	2	-1	46	5	41	2408.0592	0	2	49	6	44	2512.1357	7	2	52	10	42	2717.5164	5	0
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44	3	41	2322.7490	0	1	47	4	44	2410.3752	1	1	50	6	44	2548.3369	3	0	53	10	44	2751.3222	2	-2
44	4	40	2337.1150	1	0	47	5	43	2430.3422	2	-1	50	7	43	2566.6359	3	1	53	11	43	2787.1966	2	-2
44	6	38	2362.7835	1	2	47	6	42	2449.9701	1	2	50	8	42	2590.8663	2	-3	53	12	42	2826.6259	2	0
44	7	37	2383.3479	1	0	47	7	41	2471.6235	5	0	50	9	41	2619.4529	3	2	53	13	41	2869.5280	2	-3
44	8	36	2408.5323	1	0	47	8	40	2496.7352	3	-2	50	10	40	2651.8318	2	-2	53	14	40	2915.8528	1	-4
44	9	35	2437.5533	1	-1	47	9	39	2525.5982	3	0	50	11	39	2687.8226	4	-5	53	15	38	3018.5570	1	6
44	10	34	2470.1920	5	1	47	10	38	2558.1244	3	2	50	12	38	2727.3298	4	-5	53	16	36	3134.3877	2	2
44	11	33	2506.3514	3	-4	47	11	37	2594.2089	1	-5	50	13	37	2770.2853	4	2	54	0	54	2547.3454	1	1
44	12	32	2545.9702	2	-2	47	12	36	2633.7793	2	0	50	14	36	2816.6427	5	1	54	2	52	2606.7156	2	-2
44	13	31	2588.9966	1	1	47	13	35	2676.7744	4	-5	50	15	34	2919.3713	5	-1	54	3	51	2632.8166	2	-4
44	14	30	2635.3952	1	3	47	14	34	2723.1565	5	1	50	16	33	2975.6644	2	2	54	6	48	2685.9539	2	0
44	15	29	2685.1222	1	2	47	15	32	2825.8997	2	0	50	17	32	3035.1917	3	1	54	7	47	2702.4402	2	-1
44	16	28	2738.1428	3	-3	47	16	31	2882.1876	2	3	50	18	31	3097.9163	4	0	54	8	46	2725.5282	4	-4
44	17	27	2794.4226	1	-1	47	17	30	2941.7033	-1	-1	50	19	30	3163.8007	3	-1	54	10	44	2785.7740	2	-2
44	18	26	2853.9250	4	-3	47	18	29	3004.4113	-1	-1	51	1	51	2483.9080	7	-3	54	12	42	2861.0015	3	-1
44	19	25	2916.6153	3	-2	48	0	48	2365.6888	1	-1	51	2	50	2482.8744	1	1	54	14	40	2950.1951	3	-3
44	20	24	2982.4570	3	-3	48	1	47	2392.8522	0	1	51	3	49	2509.6737	2	2	54	15	39	2999.8781	3	1
54	16	38	3052.8876	1	56	9	9	47	2824.6406	1	-3	59	1	59	2714.6585	3	-1	65	2	64	2971.8714	2	2
54	18	36	3168.7208	4	2	56	11	45	2892.3370	3	-2	59	2	58	2748.4177	2	-1	65	3	63	3007.0981	2	-2
55	1	55	2579.6503	0	4	56	12	44	2931.6692	1	-1	59	3	57	2780.0443	3	2	65	4	62	3040.0099	0	-6
55	2	54	2611.0146	0	1	56	13	43	2974.5061	3	3	59	4	56	2809.3094	1	0	66	0	66	2973.1932	0	-9
55	3	53	2640.2306	2	-1	56	16	40	3123.4532	1	1	59	5	55	2835.9731	3	0	66	2	65	3046.9605	0	-3

Table 1 (continued)

J	E			Δ	δ	J	K _a			K _c	E	Δ	δ	J	K _a			K _c	E	Δ	δ				
	K _a	K _c	E				K _a	K _c	E						K _a	K _c	E								
1			2	3	4	1			2	3	4	1			2	3	4	1			2	3	4		
55	4	52	2667.0555	7	0	57	1	57	2645.9963	1	-2	59	8	52	2908.0207	1	-7	67	67	3012.4390	1			1	
55	5	51	2691.3303	5	7	57	2	56	2678.5593	4	4	59	11	49	3003.2491	2	-2	67	66	3050.9770	2			2	
55	6	50	2713.6296	3	-1	57	3	55	2708.9810	1	0	60	0	60	2749.8576	3	-1	67	65	3087.4005	3			-2	
55	7	49	2735.9059	3	0	57	4	54	2737.0263	0	0	60	1	59	2784.2149	4	6	68	68	3052.2612	4			1	
55	9	47	2788.7887	4	0	57	5	53	2762.4845	5	-1	60	2	58	2816.4413	2	4	68	67	3128.4167	2			-2	
55	10	46	2820.8662	5	-7	57	7	51	2808.3894	3	-3	61	1	60	2785.6352	0	0	69	69	3092.6600	0			-4	
55	11	45	2856.6493	6	1	57	8	50	2832.9805	2	-6	61	2	60	2820.5907	3	2	69	68	3132.3907	2			0	
55	12	44	2896.0155	2	-5	57	9	49	2861.0599	2	-4	61	3	59	2853.4182	2	-2	69	67	3170.0098	0			0	
55	13	43	2938.8758	2	-3	57	10	48	2892.9878	1	-6	61	4	58	2883.9022	2	-2	70	69	3173.9630	1			1	
55	14	42	2985.1735	3	-2	57	11	47	2928.6660	0	-2	62	0	62	2821.9909	1	-1	71	71	3175.1892	-4			-4	
56	0	56	2612.5338	2	1	57	14	44	3057.0385	1	-1	62	1	61	2857.5439	0	0	71	70	3216.1119	3			3	
56	1	55	2644.4971	0	0	58	0	58	2680.0381	1	-1	62	2	60	2890.9718	2	1	73	73	3260.0245	-8			-8	
56	2	54	2674.3121	4	-1	58	1	57	2713.1988	3	-3	63	1	63	2858.9249	1	-1	75	75	3347.1657	-1			-1	
56	4	52	2725.8195	1	1	58	2	56	2744.2208	2	0	63	2	62	2895.0751	2	-2	76	76	3391.6008	8			8	
56	6	50	2758.8132	4	3	58	9	49	2898.2417	4	-3	64	0	64	2896.4368	1	-1	77	77	3436.6100	2			2	
56	7	49	2774.5262	3	2	58	12	46	3004.8932	1	1	65	1	65	2934.5265	-1	-1	78	78	3482.1953	4			4	
56	8	48	2796.8408	3	-4																				

an MCT detector were used. The instrumental resolution due to the path difference and the aperture broadening was 0.0024 cm⁻¹, whereas the Doppler width in the middle of the measured range is about 0.0028 cm⁻¹. The experimental linewidth of small isolated lines is about 0.0036 cm⁻¹. The spectrum was calibrated using the CO lines, Ref. [38].

3. Description of the spectrum and assignment of transitions

Experimentally recorded spectra in the region of location of the strong bands, ν₁ + ν₂ and ν₂ + ν₃, are shown in the upper parts of Figs. 1 and 2 (Figs. 1(II) and 2(II), respectively). In both cases, all three branches, P, Q, and R, are clearly pronounced. In the first case (Fig. 1), the upper vibrational state is of A₁ symmetry and therefore the observed transitions are of b-type. In this case, one can see a strong Q-branch typical for such type of bands. In the second case (Fig. 2), the upper vibrational state is of B₁ symmetry and therefore the observed transitions are of a-type. Also as an illustration of the quality of the experimentally recorded spectra, Figs. 3(IV) and 4(IV) present small portions of the high-resolution spectra in both regions.

Because the “hot” bands ν₁ + 2ν₂ - ν₂ and 2ν₂ + ν₃ - ν₂, which are the subject of our present interest, are very weak and covered by considerably stronger combinational bands, ν₁ + ν₂ and ν₂ + ν₃, we, first of all, made assignments of transitions belonging to these strong bands. In this case, as in our recent Refs. [35–37], assignments were made by the Ground State Combination Differences method with the ground state rotational energy values calculated with the parameters from Ref. [34]. As a result we assigned more than 2650 and 2050 transitions with J^{max.} = 78, K_a^{max.} = 27 and J^{max.} = 68, K_a^{max.} = 24 for the bands ν₁ + ν₂ and ν₂ + ν₃, respectively. A list of assigned transitions in Appendix A., together with transmittance values and quantum numbers of the upper, (J K_a K_c), and lower, (J' K'_a K'_c), ro-vibrational states (in this case, due to nuclear spin statistics, only transitions with even values, K'_a + K'_c, of the lower quantum numbers are available). It should be mentioned that the bands ν₁ + ν₂ and ν₂ + ν₃ were discussed earlier in the literature (see, Refs. [22,23]). However, because special efforts have been made to record as many “hot” transitions as possible, a considerably greater number of transitions with higher values of quantum numbers J and K_a were recorded and assigned to the bands ν₁ + ν₂ and ν₂ + ν₃: more than 2650 transitions (1069 upper energy values) in our study in comparison with 200 transitions in Ref. [23] for the band ν₁ + ν₂, and more than 2050 transitions (1001 upper energy values) in our study in comparison with 433 upper energy values in Ref. [22] for the band ν₂ + ν₃. Upper ro-vibrational energies of the states (1 1 0) and (0 1 1), obtained on the basis of assigned transitions, are presented in column 2 of Tables 1 and 2 (in cm⁻¹) together with their experimental uncertainties, Δ (in 10⁻⁴ cm⁻¹), see column 3 of Tables 1 and 2.

Table 2 (continued)

J	E				E				E				E				Δ	δ					
	K _a	K _c	J	K _a	K _c	J	K _a	K _c	J	K _a	K _c	J	K _a	K _c	J	K _a			K _c				
1																							
9	0	9	1904.0107	2	2	14	4	11	1970.2472	2	1	18	1	18	1880.7189	0	0	21	3	18	2040.1001	5	-1
9	1	8	1907.1534	0	0	14	5	10	1985.7201	1	-1	18	2	17	1990.4164	2	-2	21	4	17	2050.8965	1	1
9	2	7	1911.5867	0	0	14	6	9	2004.6444	1	1	18	3	16	2000.2700	0	0	21	5	16	2066.0793	2	-1
9	3	6	1919.9775	0	0	14	7	8	2026.9960	1	1	18	4	15	2012.3693	1	-1	21	6	15	2084.9035	0	1
9	4	5	1932.0276	1	0	14	8	7	2052.7559	2	-1	18	5	14	2027.7815	0	0	21	7	14	2107.2064	2	0
9	5	4	1947.5356	1	0	14	9	6	2081.9056	1	1	18	6	13	2046.6667	1	-1	21	8	13	2132.9423	1	0
9	6	3	1966.4762	0	1	14	10	5	2114.4252	2	1	18	7	12	2068.9990	0	0	21	9	12	2162.0826	0	0
9	7	2	1988.8345	0	1	14	11	4	2150.2940	0	0	18	8	11	2094.7501	1	1	21	10	11	2194.6026	3	-1
9	8	1	2014.5954	1	1	14	12	3	2189.4899	1	0	18	9	10	2123.8973	1	1	21	11	10	2230.4793	2	1
9	9	0	2043.7422		0	14	13	2	2231.9890	1	0	18	10	9	2156.4191	1	1	21	12	9	2269.6880	0	0
10	1	10	1910.9189	0	0	14	14	1	2277.7660	0	-1	18	11	8	2192.2930	1	1	21	13	8	2312.2042	1	-1
10	2	9	1917.5491	0	0	15	0	15	1949.8477	0	0	18	12	7	2231.4968	0	0	21	14	7	2358.0021	1	-1
10	3	8	1926.3321	1	-1	15	1	14	1955.9755	0	0	18	13	6	2274.0056	2	-1	21	15	6	2407.0540	1	-2
10	4	7	1938.3919	3	0	15	2	13	1960.5987	1	0	18	14	5	2319.7942	0	-1	21	16	5	2459.3318	2	-2
10	5	6	1953.8963	1	0	15	3	12	1968.0370	0	0	18	15	4	2368.8353	1	-1	21	17	4	2514.8056	2	0
10	6	5	1972.8351	2	-2	15	4	11	1979.8270	1	0	18	16	3	2421.1006	3	-3	21	18	3	2573.4445	1	-1
10	7	4	1995.1932	0	0	15	5	10	1995.2750	1	1	18	17	2	2476.5609	1	-2	21	19	2	2635.2166	1	-1
10	8	3	2020.9544	1	-1	15	6	9	2014.1914	0	0	18	18	1	2535.1849	1	-4	21	20	1	2700.0896	3	3
10	9	2	2050.1019	1	-1	15	7	8	2036.5399	1	1	19	0	19	1991.9955	2	1	21	21	0	2768.0290	2	5
10	10	1	2082.6174	0	0	15	8	7	2062.2985	0	0	19	1	18	2000.8152	0	0	22	1	22	2029.7388	0	-1
11	0	11	1916.9593	0	0	15	9	6	2091.4480	1	0	19	2	17	2006.6064	0	0	22	2	21	2041.4694	1	-1
22	3	20	2052.4544	0	0	24	18	7	2617.4398	1	1	27	9	18	2255.6807	0	0	29	22	7	2969.2861	1	1
22	4	19	2064.7866	0	0	24	19	6	2679.2295	1	1	27	10	17	2288.1834	1	1	29	24	5	3120.3155	2	2
22	5	18	2080.1205	0	0	24	20	5	2744.1207	3	0	27	11	16	2324.0553	1	0	30	1	30	2155.8169	0	-1
22	6	17	2098.9312	0	0	24	21	4	2812.0795	4	-3	27	12	15	2363.2690	1	-1	30	2	29	2172.1096	1	-1
22	7	16	2121.2212	0	0	24	22	3	2883.0720	5	-2	27	13	14	2405.7977	3	1	30	3	28	2186.5555	1	1
22	8	15	2146.9499	1	0	24	23	2	2957.0630	1	3	27	14	13	2451.6132	1	-1	30	4	27	2200.3814	2	1
22	9	14	2176.0865	1	0	24	24	1	3034.0157	1	1	27	15	12	2500.6882	1	0	30	5	26	2215.7856	1	0
22	10	13	2208.6053	1	0	25	0	25	2072.6227	0	-1	27	16	11	2552.9928	1	0	30	6	25	2234.3318	0	1
22	11	12	2244.4820	0	0	25	1	24	2085.5606	2	-2	27	18	9	2667.1697	1	0	30	7	24	2256.4244	1	0
22	12	11	2283.6921	2	-1	25	2	23	2094.8262	0	0	27	19	8	2728.9784	1	-1	30	8	23	2282.0357	1	0
22	13	10	2326.2109	3	-4	25	3	22	2101.7621	2	-1	27	20	7	2793.8904	0	0	30	9	22	2311.1049	4	2
22	14	9	2372.0115	3	-4	25	4	21	2111.4962	1	0	27	21	6	2861.8715	1	1	30	10	21	2343.5881	3	2
22	15	8	2421.0675	1	-2	25	5	20	2126.1973	1	0	27	22	5	2932.8866	1	-4	30	11	20	2379.4504	0	1
22	16	7	2473.3495	1	-2	25	6	19	2144.8743	1	0	27	23	4	3006.9017	4	-2	30	12	19	2418.6618	2	-2
22	17	6	2528.8283	1	1	25	7	18	2167.1084	4	-3	27	24	3	3083.8802	1	0	30	13	18	2461.1938	1	-1
22	18	5	2587.4722	1	-1	25	8	17	2192.8071	1	1	28	1	28	2120.7981	1	-1	30	14	17	2507.0171	2	0
22	19	4	2649.2502	1	0	25	9	16	2221.9269	2	-3	28	2	27	2135.9155	1	0	30	15	16	2556.1027	0	-1
22	20	3	2714.1290	2	2	25	10	15	2254.4386	2	1	28	3	26	2149.3689	0	0	30	16	15	2608.4213	0	-1
22	21	2	2853.0528	3	3	25	11	14	2290.3137	0	1	28	4	25	2162.6649	0	0	30	17	14	2663.9419	2	0
23	0	23	2043.4215	0	-1	25	12	13	2329.5271	3	2	28	5	24	2177.9886	1	0	30	18	13	2722.6332	2	2
23	1	22	2055.0165	1	0	25	13	12	2372.0522	2	2	28	6	23	2196.6100	0	0	30	19	12	2784.4628	6	6
23	2	21	2062.9334	1	0	25	14	11	2417.8621	1	0	28	7	22	2218.7696	1	0	30	20	11	2849.3963	3	0
23	3	20	2069.5744	0	0	25	15	10	2466.9292	1	-1	28	8	21	2244.4222	0	0	30	21	10	2917.4011	1	0
23	4	19	2079.8524	3	-2	25	16	9	2519.2248	1	0	28	9	20	2273.5161	2	2	30	22	9	2988.4421	1	1
23	5	18	2094.8395	0	0	25	17	8	2574.7184	0	0	28	10	19	2306.0130	2	-1	30	23	8	3062.4837	1	1
23	6	17	2113.6026	0	0	25	18	7	2633.3789	3	-3	28	11	18	2341.8824	1	-1	30	24	7	3139.4903	2	2
23	7	16	2135.8763	4	0	25	19	6	2695.1752	3	1	28	12	17	2381.0960	1	1	31	0	31	2174.1968	1	0

23	8	15	2161.5964	0	25	21	4	2828.0394	1	28	13	16	2423.6259	0	31	1	30	2190.9683	0
23	9	14	2190.7285	1	25	23	2	2973.0374	-1	28	14	15	2469.4444	0	31	2	29	2204.6914	1
23	10	13	2223.2453	0	26	1	26	2088.1113	0	28	15	14	2518.5229	1	31	3	28	2214.1669	1
23	11	12	2259.1220	0	26	2	25	2102.0705	0	28	16	13	2570.8320	0	31	4	27	2222.8719	1
23	12	11	2298.3336	2	26	3	24	2114.6082	0	28	17	12	2626.3419	1	31	5	26	2236.0457	1
23	13	10	2340.8543	0	26	4	23	2127.4834	1	28	18	11	2685.0204	1	31	6	25	2254.1938	1
23	14	9	2386.6583	1	26	5	22	2142.7794	0	28	19	10	2746.8361	3	31	7	24	2276.2192	1
23	15	8	2435.7178	2	26	6	21	2161.4729	2	28	20	9	2811.7551	1	31	8	23	2301.8045	1
23	16	7	2488.0044	1	26	7	20	2183.6869	2	28	21	8	2879.7439	2	31	9	22	2330.8589	1
23	17	6	2543.4879	1	26	8	19	2209.3719	1	28	22	7	2950.7677	2	31	10	21	2363.3332	2
23	18	5	2602.1370	7	26	9	18	2238.4848	0	28	23	6	3024.7915	4	31	11	20	2399.1913	1
23	19	4	2663.9211	1	26	10	17	2270.9919	0	28	24	5	3101.7783	-3	31	12	19	2438.4013	2
23	20	3	2728.8059	2	26	11	16	2306.8657	1	29	0	29	2138.0098	0	31	13	18	2480.9333	1
23	21	2	2796.7583	2	26	12	15	2346.0794	1	29	1	28	2153.5293	2	31	14	17	2526.7587	2
23	22	1	2867.7425	0	26	13	14	2388.6062	1	29	2	27	2165.7571	0	31	15	16	2575.8481	0
23	23	0	2941.7261	0	26	14	13	2434.4193	1	29	3	26	2174.1143	0	31	16	15	2628.1711	0
24	1	24	2057.7575	0	26	15	12	2483.4903	1	29	4	25	2182.9847	1	31	17	14	2683.6970	2
24	2	23	2070.5843	0	26	16	11	2535.7903	1	29	5	24	2196.7759	0	31	18	13	2742.3946	1
24	3	22	2082.2960	1	26	17	10	2591.2892	2	29	6	23	2215.1615	1	31	20	11	2869.1725	1
24	4	21	2094.8535	1	26	18	9	2649.9556	-3	29	7	22	2237.2758	1	31	21	10	2937.1858	0
24	5	20	2110.1576	0	26	19	8	2711.7581	2	29	8	21	2262.9084	0	31	22	9	3008.2352	-3
24	6	19	2128.9150	0	26	20	7	2776.6631	1	29	9	20	2291.9907	1	31	23	8	3082.2861	-5
24	7	18	2151.1718	2	26	22	5	2915.6443	2	29	10	19	2324.4812	0	32	1	32	2193.1660	1
24	8	17	2176.8820	1	26	23	4	2989.6509	3	29	11	18	2360.3475	1	32	2	31	2210.6455	0
24	9	16	2206.0087	1	26	24	3	3066.6201	-2	29	12	17	2399.5603	1	32	3	30	2226.1466	0
24	10	15	2238.5231	2	27	0	27	2104.1518	0	29	13	16	2442.0912	1	32	4	29	2240.6129	0
24	11	14	2274.3993	2	27	1	26	2118.3963	0	29	14	15	2487.9122	1	32	5	28	2256.1675	0
24	12	13	2313.6115	3	27	3	24	2136.6260	0	29	15	14	2536.9945	1	32	6	27	2274.6428	1
24	13	12	2356.1347	0	27	4	23	2145.8635	-1	29	16	13	2589.3083	1	32	7	26	2296.6556	0
24	14	11	2401.9419	2	27	5	22	2160.1689	0	29	17	12	2644.8235	0	32	8	25	2322.2152	0
24	15	10	2451.0050	2	27	6	21	2178.7248	0	29	18	11	2703.5084	1	32	9	24	2351.2531	1
24	16	9	2503.2961	0	27	7	20	2200.9072	0	29	19	10	2765.3303	0	32	10	23	2383.7177	0
24	17	8	2558.7846	1	27	8	19	2226.5768	0	29	20	9	2830.2571	1	32	11	22	2419.5705	1
32	12	21	2458.7778	-1	35	8	17	2387.3037	0	38	11	28	2555.2513	0	41	17	24	2916.2620	5
32	13	20	2501.3101	0	35	9	26	2416.2794	0	38	12	27	2594.4308	1	41	18	23	2975.0240	2
32	14	19	2547.1375	0	35	10	25	2448.7062	0	38	13	26	2636.9535	1	42	1	42	2414.8413	0
32	15	18	2596.2300	0	35	11	24	2484.5370	0	38	14	25	2682.7852	1	42	2	41	2438.3081	0
32	16	17	2648.5575	1	35	13	22	2566.2639	0	38	15	24	2731.8935	1	42	3	40	2459.6031	0
32	17	16	2704.0893	3	35	14	21	2612.0951	0	38	16	23	2784.2459	2	42	4	39	2478.6840	1
32	18	15	2762.7933	2	35	15	20	2661.1964	-2	38	17	22	2839.8097	1	42	5	38	2496.4709	0
32	19	14	2824.6363	-2	35	16	19	2713.5370	1	38	18	21	2898.5531	1	42	6	37	2515.1179	1
32	20	13	2889.5861	3	35	17	18	2769.0846	2	39	0	39	2342.2294	2	42	7	36	2536.6180	0
32	21	12	2957.6079	0	35	18	17	2827.8088	4	39	1	38	2363.8828	1	42	8	35	2561.7262	0
32	22	11	3028.6666	3	35	19	16	2889.6736	-2	39	2	37	2383.1372	0	42	9	34	2590.4679	1
33	0	33	2212.7124	2	35	21	14	3022.6962	3	39	3	36	2398.6579	0	42	11	32	2658.4842	2
33	1	32	2230.7189	0	36	1	36	2274.8530	0	39	4	35	2409.5554	1	42	12	31	2697.6269	0
33	2	31	2245.8981	0	36	2	35	2294.7226	1	39	5	34	2420.4307	0	42	13	30	2740.1305	0
33	3	30	2256.7164	0	36	3	34	2312.4695	1	39	6	33	2436.5660	1	42	14	29	2785.9565	1
33	4	29	2265.5142	-3	36	4	33	2328.5305	0	39	7	32	2457.8548	1	42	15	28	2835.0689	5
33	5	28	2278.0118	0	36	5	32	2344.6552	0	39	8	31	2483.1029	0	42	16	27	2887.4347	5
33	6	27	2295.8329	1	36	6	31	2363.0480	0	39	9	30	2511.9608	1	42	17	26	2943.0183	1
33	7	26	2317.7423	2	36	7	30	2384.8655	0	39	10	29	2544.3142	2	43	0	43	2440.2082	2
33	8	25	2343.2685	0	36	8	29	2410.2861	2	39	11	28	2580.1005	0	43	1	42	2464.2693	0
33	9	24	2372.2878	1	36	9	28	2439.2369	0	39	12	27	2619.2725	0	43	2	41	2486.0652	0

45	16	29	2971.5065	2	49	8	41	2767.9260	0	2	53	7	46	2877.1701	1	-1	57	11	46	3136.8470	1	-2
45	17	28	3027.1031	5	49	9	40	2796.2066	0	0	53	8	45	2900.1565	4	3	57	12	45	3175.6422	1	-5
46	1	46	2519.7956	1	0	49	10	2828.2115	1	1	53	9	44	2928.0003	1	-2	57	13	44	3217.9238	1	-2
46	2	45	2545.6587	-1	49	11	38	2863.7735	1	-1	53	10	43	2959.7672	4	1	57	14	43	3263.6184	0	0
46	3	44	2569.3612	0	0	49	13	2945.2393	1	1	53	11	42	2995.1769	1	0	58	1	58	2890.3929	0	3
46	4	43	2590.7192	0	0	49	14	2991.0299	1	1	53	12	41	3034.1066	2	1	58	2	57	2923.4223	1	-1
46	5	42	2610.1518	3	-2	49	15	3040.1326	2	2	53	13	40	3076.4771	0	2	58	3	56	2954.3455	0	-3
46	6	41	2629.4025	1	0	49	16	3092.5075	2	3	53	14	39	3122.2282	1	0	58	4	55	2982.9356	1	2
46	7	40	2650.7847	1	-1	50	1	2634.0445	1	1	53	15	38	3171.3115	0	4	58	5	54	3008.9595	3	0
46	8	39	2675.6228	1	0	50	2	2662.3002	0	0	54	1	54	2757.5798	0	2	58	6	53	3032.6267	2	2
46	9	38	2704.1587	0	0	50	3	2688.4148	0	0	54	3	52	2816.7467	0	-1	58	7	52	3055.3963	-3	-3
46	10	37	2736.3008	2	0	50	4	2712.1523	0	1	54	4	51	2842.9057	0	0	58	8	51	3079.6965	0	0
46	11	36	2771.9509	0	0	50	5	2733.5774	2	2	54	5	50	2866.5615	1	0	58	9	50	3107.3009	1	-2
46	12	35	2811.0380	0	0	50	6	2753.8729	0	0	54	6	49	2888.3498	2	2	58	10	49	3138.7152	1	-6
46	13	34	2853.5091	1	50	7	44	2775.3493	1	1	54	7	48	2910.2581	2	2	58	11	48	3173.8698	-4	-4
46	14	33	2899.3188	-5	50	8	43	2799.9060	0	0	54	8	47	2934.5979	0	0	58	12	47	3212.6258	-8	-8
46	15	32	2948.4293	1	-1	50	9	2828.1756	0	0	54	9	46	2962.5471	-2	-2	58	14	45	3300.5586	2	2
46	17	30	3056.4031	3	5	50	10	2860.1341	3	0	54	10	45	2994.2649	-3	-3	59	0	59	2925.0444	3	0
47	1	47	2547.4868	0	50	11	40	2895.6627	3	0	54	11	44	3029.6311	2	-2	59	1	58	2958.6694	1	-5
47	1	46	2573.9468	1	1	50	12	2934.6706	1	1	54	12	43	3068.5307	-2	-2	59	2	57	2990.1903	2	-3
47	2	45	2598.2145	1	0	50	13	2977.0918	1	1	54	13	42	3110.8814	0	-1	59	3	56	3019.3561	0	0
47	3	44	2619.6951	0	1	50	14	3022.8745	6	6	55	0	55	2789.9137	0	2	59	4	55	3045.6280	2	2
47	4	43	2636.7179	1	1	50	15	3071.9727	0	1	55	1	54	2821.1547	2	2	59	5	54	3067.4544	1	0
47	5	42	2648.9741	0	51	0	51	2664.0581	0	2	55	2	53	2850.2729	1	-2	59	6	53	3083.3678	1	-2
47	6	41	2662.1715	1	0	51	1	2692.9107	0	0	55	3	52	2876.9592	1	0	59	7	52	3098.0987	4	-5
47	7	40	2681.3352	0	51	2	49	2719.6141	1	0	55	4	51	2900.4129	1	4	59	8	51	3118.5184	1	-2
47	8	39	2705.7541	0	51	3	48	2743.7562	0	1	55	5	50	2918.6678	1	2	59	9	50	3145.2232	3	-1
47	9	38	2734.1963	2	2	51	4	2764.1271	0	2	55	6	49	2932.2901	1	-2	59	10	49	3176.4527	3	-3
47	10	37	2766.2949	0	51	5	46	2778.9840	2	-1	55	7	48	2947.9949	2	-1	60	1	60	2960.2757	0	0
47	11	36	2801.9180	1	51	6	45	2791.7212	3	-4	55	8	47	2970.2496	1	-2	60	2	59	2994.4963	1	-1
47	12	35	2840.9875	2	-2	51	7	2809.1409	0	-1	55	9	46	2997.7953	2	-2	60	3	58	3026.6173	0	-2
47	13	34	2883.4479	1	0	51	8	2832.7214	1	-1	55	11	44	3064.7276	2	-2	60	4	57	3056.4209	1	0
47	14	33	2929.2525	1	0	51	9	2860.8062	1	0	55	12	43	3103.5950	0	1	60	5	56	3083.6563	2	1
47	15	32	2978.3610	3	51	10	41	2892.7011	1	-1	55	13	42	3145.9241	1	0	60	6	55	3108.3767	0	4
47	16	31	3030.7350	1	2	51	11	2928.1926	2	-1	55	14	41	3191.6494	1	0	60	7	54	3131.7504	2	0
47	17	30	3086.3391	8	51	12	39	2967.1766	2	1	56	1	56	2822.8272	3	-1	60	8	53	3156.1365	3	-1
48	1	48	2575.7585	2	-2	51	13	3009.5821	5	1	56	2	55	2854.6646	3	-1	60	9	52	3183.5775	0	-6
48	2	47	2602.8186	0	0	51	14	3055.3551	0	1	56	3	54	2884.3886	1	0	60	10	51	3214.8178	0	-5
48	3	46	2627.7273	0	0	51	15	3104.4498	0	5	56	4	53	2911.7625	4	-3	60	11	50	3249.8457	1	-1
48	4	45	2650.2669	1	2	51	16	3156.8236	6	6	56	5	52	2936.5912	1	3	61	0	61	2996.0855	1	2
48	5	44	2670.6590	0	1	52	1	2694.6516	-1	-1	56	6	51	2959.2763	1	2	61	1	60	3030.9008	2	-7
48	6	43	2690.3744	3	-3	52	3	2751.4217	1	0	56	7	50	2981.5579	1	0	61	2	59	3063.6196	1	-2
48	7	42	2711.7695	3	2	52	4	2776.3673	0	1	56	8	49	3005.8477	6	-2	61	3	58	3094.0100	1	0
48	8	41	2736.4647	3	3	52	5	2798.8847	0	1	56	9	48	3033.6247	6	-2	61	4	57	3121.6196	1	1
48	9	40	2764.8746	1	0	52	6	2819.8733	1	1	56	10	47	3065.1982	6	-9	61	5	56	3145.1552	6	6
48	10	39	2796.9315	1	0	52	7	2841.5164	4	2	56	11	46	3100.4661	1	1	61	6	55	3162.6429	0	4
48	11	38	2832.5253	0	-1	52	8	2865.9502	0	-1	56	12	45	3139.2987	1	-1	61	7	54	3177.3563	1	-5
48	12	37	2871.5763	2	1	52	9	2894.0654	0	1	56	13	44	3181.6052	3	3	61	8	53	3196.7587	-2	-2
48	13	36	2914.0245	-2	52	10	43	2925.9110	-1	-1	56	14	43	3227.3154	3	0	61	10	51	3253.8570	2	-5
48	14	35	2959.8226	0	0	52	11	2961.3639	1	-2	57	0	57	2856.3202	1	1	62	1	62	3032.4743	0	3
48	15	34	3008.9282	2	-2	52	12	3000.3217	1	0	57	1	56	2888.7537	1	-2	62	2	61	3067.8849	1	-5
62	3	60	3101.2019	2	-3	63	3	3170.9693	1	1	64	6	59	3266.9881	4	3	66	2	65	3221.6022	1	-10
62	4	59	3132.2173	0	0	63	4	3199.8834	2	2	64	7	58	3291.9014	1	1	66	3	64	3257.3062	1	-4
62	6	57	3186.5035	3	63	5	58	3225.0447	0	0	64	8	57	3316.7447	2	2	66	4	63	3290.7368	3	3

Table 2 (continued)

J	K _a	K _c	E	Δ	δ	J	K _a	K _c	E	Δ	δ	J	K _a	K _c	E	Δ	δ
1			2	3	4	1			2	3	4	1			2	3	4
62	7	56	3210.5943	1	0	63	6	57	3244.2924	-4	-4	65	0	65	3145.1115	1	2
62	8	55	3235.1575	1	1	63	8	55	3277.7826	-5	-5	65	1	64	3182.3063	-3	-3
62	9	54	3262.4567	-4	-4	64	1	64	3106.9875	2	3	65	2	63	3217.4135	1	-3
63	0	63	3069.4416	3	3	64	2	63	3143.5879	3	-2	65	3	62	3250.2339	0	1
63	1	62	3105.4471	0	-5	64	3	62	3178.0990	1	-1	65	5	60	3307.1322	3	-2
63	2	61	3139.3609	2	-3	64	4	61	3210.3229	1	-1	66	1	66	3183.8133	-3	-3
															3321.6418		4
															3349.8138		5
															3223.0939	1	-1
															3261.4768	3	-6
															3331.8034		-3
															3301.9287		-7

^a See footnote to Table 1.

4. Hamiltonian model and determination of spectroscopic parameters of the ν₁+ν₂/ν₂+ν₃/3ν₂ polyad

The Hamiltonian model employed was taken from Refs. [40,41]. However, for the convenience of the reader, we briefly reproduce it here. Because strong local interaction was found between the vibrational states (1 1 0) and (0 3 0), the corresponding Fermi-type interaction operator was taken into account in the Hamiltonian model used for analysis of energy values from Table 1. In this case, in spite of the very small absolute value of the corresponding interaction parameter, an introduction of such parameter into the Hamiltonian model is suitable because, as the analysis showed, differences between some of energy values in the sets of states [J K_a = 13 K_c = J - K_a](1 1 0) and [J K_a = 15 K_c = J - K_a](0 3 0), and [J K_a = 13 K_c = J + 1 - K_a](1 1 0) and [J K_a = 15 K_c = J + 1 - K_a](0 3 0) can decrease up to 0.04 cm⁻¹. At the same time, as the analysis also showed, it is not necessary to introduce into the Hamiltonian model a resonance interaction both between the states (1 1 0) and (0 1 1), and between the states (0 1 1) and (0 3 0). Indeed, as was shown, for example in Ref. [25], an appearance of resonance interaction between the states (1 0 0) and (0 0 1) (that are very similar to the states (1 1 0) and (0 1 1) considered in the present paper) is explained by small (up to 0.63 cm⁻¹) differences between energy values in two sets of ro-vibrational states: [J K_a = 22 K_c = J - K_a](1 0 0) and [J K_a = 19 K_c = J + 1 - K_a](0 0 1), and [J K_a = 22 K_c = J + 1 - K_a](1 0 0) and [J K_a = 19 K_c = J - K_a](0 0 1). At the same time, because of some differences in the rotational and centrifugal distortion parameters of the states (1 1 0) and (0 1 1), on the one hand, and of the states (1 0 0) and (0 0 1), on the other hand, differences between energy values of corresponding ro-vibrational states in the pair (1 1 0)/(0 1 1) are considerably larger than in the pair (1 0 0)/(0 0 1). In particular, for the same sets of upper ro-vibrational states, [J K_a = 22 K_c = J - K_a](1 0 0) and [J K_a = 19 K_c = J + 1 - K_a](0 0 1), and [J K_a = 22 K_c = J + 1 - K_a](1 0 0) and [J K_a = 19 K_c = J - K_a](0 0 1), as in the above discussed pair of vibrational states, (1 0 0) and (0 0 1), the minimum value of difference between corresponding energies is larger than 4.50 cm⁻¹ in our case of the states (1 1 0)/(0 1 1). For that reason, we did not take into account such type of resonance interactions.

Finally, the Hamiltonian model was taken in the present study in the following form:

$$H^{vib.-rot.} = \sum_{v,\tilde{v}=1}^3 |v\rangle \langle \tilde{v}| H^{v\tilde{v}}, \tag{1}$$

where |1⟩ = (1 1 0), |2⟩ = (0 3 0), and |3⟩ = (0 1 1). In this case, the diagonal block operators were taken in the form of traditional Watson operators in A reduction and I' representation, [42]:

$$H^{vv} = E^v + [A^v - \frac{1}{2}(B^v + C^v)]J_z^2 + \frac{1}{2}(B^v + C^v)J^2 + \frac{1}{2}(B^v - C^v)J_{xy}^2 - \Delta_{Kz}^v J_z^4 - \Delta_{JK}^v J_z^2 J^2 - \Delta_J^v J^4 - \delta_K^v [J_z^2 J_{xy}^2]_+ - 2\delta_J^v J^2 J_{xy}^2 + H_{Kz}^v J_z^6 + H_{JK}^v J_z^4 J^2 + H_{JKz}^v J_z^2 J^4 + H_J^v J^6$$

$$\begin{aligned}
 &+ [h_K^v J_z^4 + h_{JK}^v J_z^2 J^2 + h_J^v J^4 J_{xy}^2]_+ + L_{KJ}^v J_z^8 + L_{KKJ}^v J_z^6 J^2 + L_{JKJ}^v J_z^4 J^4 \\
 &+ L_{JJK}^v J_z^2 J^6 + L_J^v J^8 + [I_K^v J_z^6 + I_{KJ}^v J_z^4 J^2 + I_{JK}^v J_z^2 J^4 + I_J^v J^6 J_{xy}^2]_+ \\
 &+ P_{KJ}^v J_z^{10} + P_{KKJ}^v J_z^8 J^2 + P_{KJJ}^v J_z^6 J^4 + P_{JJK}^v J_z^4 J^6 \\
 &+ \dots + S_{KJ}^v J_z^{12} + S_{KKJ}^v J_z^{10} J^2 + \dots, \quad (2)
 \end{aligned}$$

where J_α ($\alpha = x, y, z$) are the components of the angular momentum operator defined in the molecule-fixed coordinate system, $J_{xy}^2 = J_x^2 - J_y^2$, and $[\dots]_+$ denotes anticommutator. In accordance with the above, only the nondiagonal Fermi block was taken different from zero, namely,

$$\begin{aligned}
 H_F^{(1\ 1\ 0)(0\ 3\ 0)} &\equiv H_F^{12} \\
 &= F^{12} + F_K^{12} J_z^2 + F_J^{12} J^2 + \dots + F_{xy}^{12} J_{xy}^2 \\
 &\quad + F_{xyK}^{12} [J_{xy}^2 J_z^2]_+ + F_{xyJ}^{12} J_{xy}^2 J^2 + \dots. \quad (3)
 \end{aligned}$$

To derive numerical values of the parameters of the Hamiltonian, Eqs. (1)–(3), we used ro-vibrational energies of the states (1 1 0) and (0 1 1) that were obtained from assigned transitions of the bands $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ and

are presented in column 2 of Tables 1 and 2. Some transitions unambiguously assigned to the $3\nu_2$ band (see, Table 3) were also used in the fit of parameters of the Hamiltonian (1)–(3).

The initial values of vibrational energies, E , of the states (1 1 0) and (0 1 1), have been taken from Refs. [22,23], respectively; the value of the vibrational energy of the state (0 3 0) was estimated from the parameters of the intramolecular potential energy surface of the SO_2 molecule, Ref. [36], that was obtained on the basis of the method described in Ref. [43]. The initial values of the rotational and centrifugal distortion parameters of the states (1 1 0) and (0 1 1) were estimated from the simple formula

$$P^{(\nu_1 \nu_2 \nu_3)} = P^{(0\ 0\ 0)} + \sum_{\lambda=1}^3 p_\lambda \nu_\lambda, \quad (4)$$

where $P^{(\nu_1 \nu_2 \nu_3)}$ is any rotational or distortion parameter of the state $(\nu_1 \nu_2 \nu_3)$; $P^{(0\ 0\ 0)}$ is a corresponding parameter of the ground vibrational state. The values of parameters

Table 3
List of transitions belonging to the $3\nu_2$ band of the SO_2 molecule.

Upper level			Lower level			Line position (cm^{-1})	Transmittance (%)	Upper energy (cm^{-1})	δ^a (10^{-4}cm^{-1})
J'	K'_a	K'_c	J''	K''_a	K''_c				
1			2			3	4	5	6
28	15	13	27	12	16	1731.6092	99.2	2217.4536	1
			27	14	14	1644.1528	99.6	2217.4530	7
			28	12	16	1713.7085	98.9	2217.4535	1
29	15	15	28	12	16	1732.2181	99.2	2235.9635	2
			30	12	18	1732.8135	95.1	2255.0992	1
30	15	15	30	12	18	1713.6329	98.7	2255.0992	1
			31	15	17	30	12	18	1733.4453

^a The $\delta = (E^{\text{exp.}} - E^{\text{calc.}})$ is the difference between the experimental line position from column 3 and the corresponding value calculated with the parameters from Table 4.

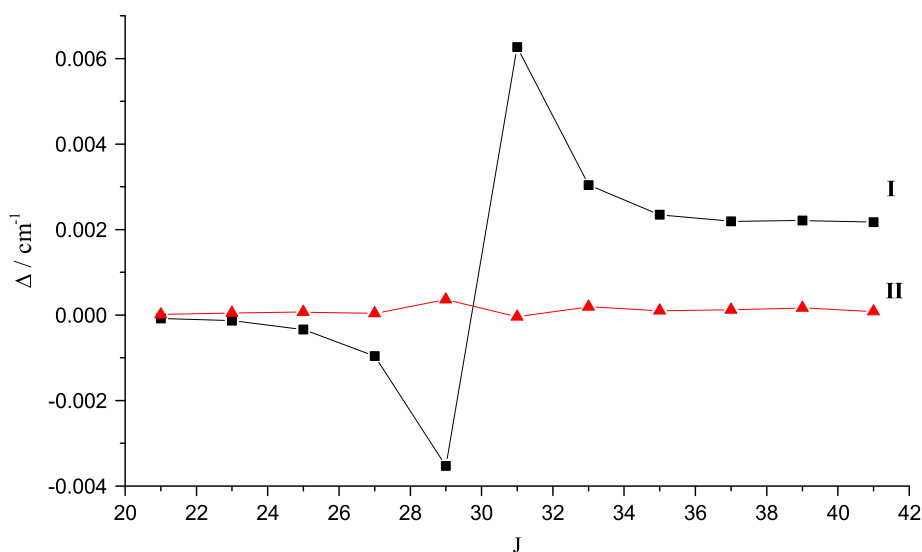


Fig. 5. Plot of dependency of the value of difference $\Delta = (E^{\text{exp.}} - E^{\text{calc.}})$ against the value of the quantum number J for the set of ro-vibrational states $[J K_a = 13 K_c = J + 1 - K_a](1\ 1\ 0)$; the curve I corresponds to the Hamiltonian model of isolated vibrational state; the curve II shows corresponding dependence when the resonance interaction between the states (1 1 0) and (0 3 0) is taken into account.

p_λ ($\lambda = 1, 2, 3$) were estimated on the basis of the values of parameters $P^{(0\ 0\ 0)}$ and $P^{(0\ 1\ 0)}$, Ref. [34], and $P^{(1\ 0\ 0)}$ and $P^{(0\ 0\ 1)}$, Ref. [25]. The initial values of the parameters of the state (0 3 0) have been interpolated in accordance with the formula

$$P^{(0\ 3\ 0)} = P^{(0\ 0\ 0)} + q\nu_3 + r\nu_3^2, \quad (5)$$

and the above-mentioned spectroscopic parameters of the states (0 0 0), (0 1 0), (1 0 0), (0 0 1), as well as, of the state (0 2 0) from Ref. [25], were used to estimate the coefficients q and r .

As was discussed above, the strong local resonance interaction was found between the sets of ro-vibrational states $[J\ K_a = 13\ K_c = J - K_a](1\ 1\ 0)$ and $[J\ K_a = 15\ K_c = J - K_a](0\ 3\ 0)$, and $[J\ K_a = 13\ K_c = J + 1 - K_a](1\ 1\ 0)$ and $[J\ K_a = 15\ K_c = J + 1 - K_a](0\ 3\ 0)$. Table 3 presents some experimental

line centers of the $3\nu_2$ band that are caused by strong Fermi-interaction between ro-vibrational states of the (1 1 0) and (0 3 0) vibrational states. Fig. 5 also illustrates the discussed interaction. Here the curve I shows the value of the difference, ($E^{\text{exp.}} - E^{\text{calc.}}$), for the set of energy values of the states $[J\ K_a = 13\ K_c = J - 12](1\ 1\ 0)$ against the value of the quantum number J when calculated energy values are obtained in the Hamiltonian model of isolated vibrational state. The curve II shows corresponding dependence when the resonance interaction between the states (1 1 0) and (0 3 0) is taken into account. One can see that an addition of the interaction F_{xy} -parameter into the Hamiltonian model improves the situation considerably.

Results of the fit on the base of the method described in Ref. [44] are presented in columns 3, 5, and 7 of Table 4 together with their 1σ statistical confidence intervals.

Table 4

Spectroscopic parameters of the (1 1 0), (0 3 0), and (0 1 1) vibrational states of the SO₂ molecule (in cm⁻¹).

Parameter	(1 1 0) ^a	(1 1 0) ^b	(0 3 0) ^a	(0 3 0) ^b	(0 1 1) ^a	(0 1 1) ^b
1	2	3	4	5	6	7
E	1666.3348	1666.33425172(202)	1551.76	1551.755350(123)	1875.7975	1875.79720415(173)
A	2.06767	2.0679052231(411)	2.15053	2.15053	0.2046	2.045278386(359)
B	0.34259	0.34259395142(631)	0.34437	0.34437	0.3431	0.3430802008(541)
C	0.29159	0.29159987215(513)	0.29192	0.2919251465(375)	0.2919	0.29188667350(495)
$\Delta_K \times 10^4$	0.9705	0.97272142(177)	1.1812	1.1812	0.9444	0.94222360(859)
$\Delta_{JK} \times 10^5$	-0.3936	-0.39294562(210)	-0.4459	-0.4459	-0.4240	-0.42434844(192)
$\Delta_J \times 10^6$	0.2202	0.220507509(991)	0.2212	0.2212	0.2236	0.22371189(713)
$\delta_K \times 10^5$	0.1111	0.11152013(565)	0.1449	0.1449	0.9782	0.0973860(448)
$\delta_J \times 10^7$	0.5687	0.56858427(352)	0.5779	0.5779	0.5777	0.5778873(173)
$H_K \times 10^7$	0.1580	0.16037002(163)	0.2306	0.2306	0.1501	0.14891698(560)
$H_{KJ} \times 10^9$	-0.8234	-0.8253630(206)	-0.9635	-0.9635	-0.7161	-0.699198(115)
$H_{JK} \times 10^{11}$	0.4736	0.4736	0.4064	0.4064	0.1290	0.1290
$H_J \times 10^{12}$	0.3813	0.4105905(453)	0.0370	0.0370	0.3760	0.424046(396)
$h_K \times 10^9$	0.7479	0.697669(139)	1.0650	1.0650	1.0992	1.019660(796)
$h_{JK} \times 10^{12}$	-0.9173	-0.9173	-6.2593	-6.2593	-0.9173	-0.9173
$h_J \times 10^{12}$	0.1788	0.1788	0.2153	0.2153	0.1909	0.1909
$L_K \times 10^{11}$	-0.3873	-0.40709708(325)	-0.4600	-0.4600	-0.3759	-0.3759
$L_{KKJ} \times 10^{12}$	0.1837	0.1837	-0.0609	-0.0609	0.2246	0.2246
$L_{JK} \times 10^{14}$	-0.3727	-0.3727			-0.3727	-0.3727
$L_{JJK} \times 10^{15}$	-0.1517	-0.1517			-0.2207	-0.2207
$L_J \times 10^{17}$	-0.2996	-0.2996			-0.2807	-0.2807
$P_K \times 10^{14}$	0.1081	0.1081			0.1107	0.1107
$P_{KKKJ} \times 10^{16}$	-0.4562	-0.4562			-0.4562	-0.4562
$F_{xy} \times 10^4$	-0.549693(312)					

^a Constrained to the predicted values (see text, for details).

^b Values in parentheses are 1σ statistical confidence intervals (in last digits). Parameters presented without confidence intervals were constrained to predicted values from columns 2, 4, and 6, respectively.

Table 5

Statistical information for the $\nu_1 + \nu_2$, $\nu_2 + \nu_3$, $\nu_1 + 2\nu_2 - \nu_2$, and $2\nu_2 + \nu_3 - \nu_2$ bands of SO₂ molecule.

Band	Center (cm ⁻¹)	J^{max}	K_a^{max}	N_i^{a}	m_1^{b}	m_2^{b}	m_3^{b}
1	2	3	4	5	6	7	8
$\nu_1 + \nu_2$	1666.3337	78	27	1069	79.1	14.5	6.4
$\nu_2 + \nu_3$	1875.7972	68	24	1000	83.7	10.5	5.8
$\nu_1 + 2\nu_2 - \nu_2$	2180.3312	60	20	553	61.4	25.1	13.5
$2\nu_2 + \nu_3 - \nu_2$	2388.9153	59	16	540	82.9	13.4	3.7

^a N_i is the number of obtained upper-state energies.

^b Here $m_i = n_i/N_i \times 100\%$ ($i = 1, 2, 3$); n_1 , n_2 , and n_3 are the numbers of upper-state energies for which the absolute values of differences $\delta = E^{\text{exp}} - E^{\text{calc}}$ satisfy the conditions $\delta \leq 20 \times 10^{-5} \text{ cm}^{-1}$, $20 \times 10^{-5} \text{ cm}^{-1} < \delta \leq 40 \times 10^{-5} \text{ cm}^{-1}$, and $\delta > 40 \times 10^{-5} \text{ cm}^{-1}$.

In columns 2, 4, and 6 one can see the theoretical predictions with the formulas (4) and (5). Parameters in columns 3, 5, and 7 that are presented without confidence intervals have been constrained to the values of corresponding parameters from columns 2, 4, and 6. The $rms = 0.00022 \text{ cm}^{-1}$ indicates the quite satisfactory quality of the fit. As one more confirmation of the correctness of the obtained results, column 4 of Tables 1 and 2 gives values of differences $\delta = (E^{exp.} - E^{calc.})$ in 10^{-4} cm^{-1} . See, in addition, column 6 of Table 3, where the differences between some experimentally recorded and calculated line positions of the $3\nu_2$ band are presented (also in 10^{-4} cm^{-1}). One can see good correlations between the experimental values and ones calculated

with the parameters from Table 4. Statistical information concerning the studied bands, $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$, is presented in Table 5.

5. Analysis of the “hot” bands, $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$

As the next step of our analysis, we constructed simulated spectra of the studied bands, $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ (see, Figs. 1–4). In this case, in construction of the simulated spectra only relative line intensities were calculated. As the analysis showed, the correct spectrum

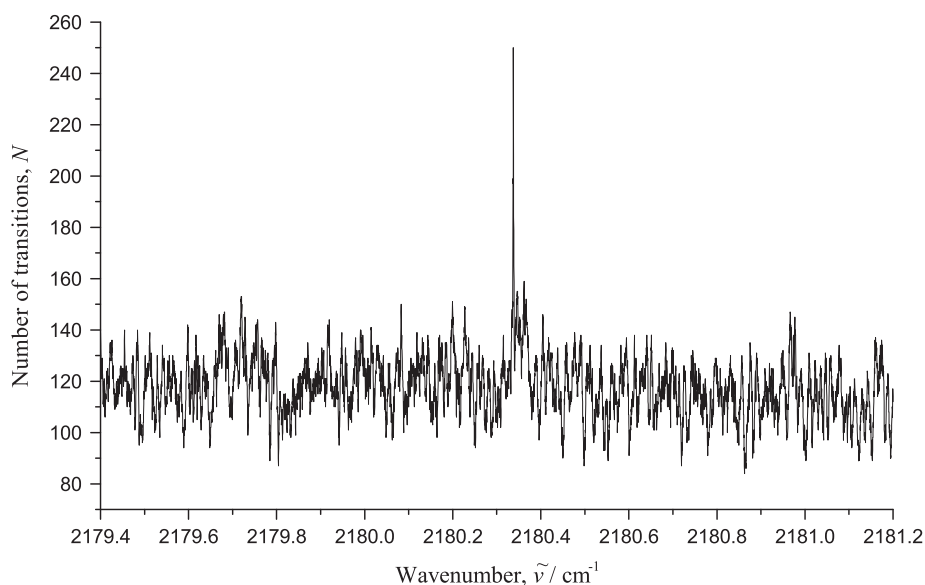


Fig. 6. The number N of observed lines that coincide with calculated lines to within 0.005 cm^{-1} for the $\nu_1 + 2\nu_2 - \nu_2$ “hot” band of SO_2 plotted as a function of the theoretical vibrational energy, E .

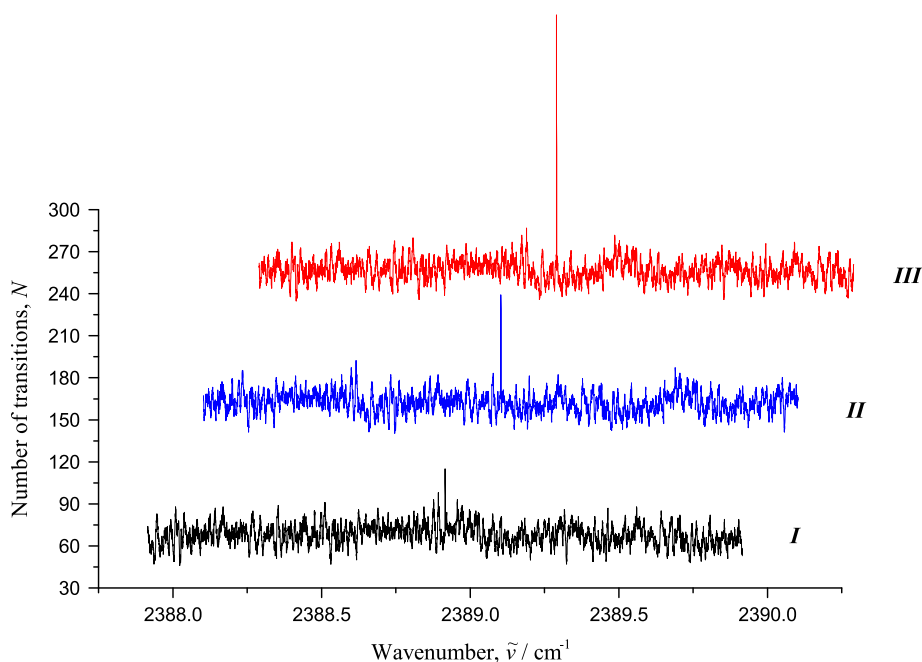


Fig. 7. The number N of observed lines that coincide with calculated lines to within 0.005 cm^{-1} for the $2\nu_2 + \nu_3 - \nu_2$ hot band of SO_2 plotted as a function of the theoretical vibrational energy, E . The plots curves **I–III** correspond to different values of the rotational parameter A (see text).

Table 6
Experimental ro-vibrational term values for the (1 2 0) vibrational state of the SO₂ molecule (in cm⁻¹).^a

J	K _a			K _c			E	Δ	δ	J	K _a			K _c			E	Δ	δ	
	J	K _a	K _c	J	K _a	K _c					J	K _a	K _c	J	K _a	K _c				
1																				
2	0	2	2	2182.2308	2	3	2366.6895	3	-5	16	8	8	2380.9176	-2	19	1	2935.0357	4	4	
2	1	1	2	2184.1020	2	2	2400.3869	4	-2	16	9	7	2411.1306	-2	20	0	2308.2890	4	-2	
3	1	3	3	2185.7702	0	3	2437.5462	5	3	16	10	6	2444.8317	-5	20	1	2317.9488	4	3	
3	2	2	2	2191.3020	3	5	2228.7661	2	2	16	11	5	2481.9975	-4	20	2	2324.2751	1	-1	
3	3	3	1	2200.2571	1	0	2233.2556	3	0	16	12	4	2522.6025	1	20	3	2331.2005	3	0	
4	0	4	4	2186.6522	3	3	2237.7520	3	-2	16	13	3	2566.6190	7	20	4	2342.7034	2	2	
4	1	3	3	2188.7153	-5	2	2246.0781	2	1	16	14	2	2614.0188	1	20	5	2358.5425	3	0	
4	3	1	2	2202.7949	2	4	2258.5069	2	2	16	16	0	2718.8457	3	20	6	2378.0925	7	-3	
4	4	0	2	2215.3203	-5	12	2274.5733	1	1	17	1	17	2274.3225	1	20	7	2401.2322	4	2	
5	1	5	5	2191.2347	3	-5	2294.2076	1	-1	17	2	16	2283.7808	5	20	8	2427.9193	0	0	
5	2	4	4	2197.0017	2	-3	2344.0939	3	-4	17	3	15	2293.7257	2	20	9	2458.1263	3	-1	
5	3	3	3	2205.9678	4	6	2374.3077	3	3	17	4	14	2306.2442	4	-2	10	2491.8277	5	2	
5	4	2	2	2218.4922	-3	3	2408.0056	0	0	17	5	13	2322.2512	1	-1	11	2528.9966	2	-3	
6	0	6	6	2193.5625	2	12	2445.1658	1	-1	17	6	12	2341.8505	3	-2	12	2569.6084	3	1	
6	1	5	5	2195.9557	1	-3	2485.7632	3	1	17	8	10	2391.7133	2	20	13	2613.6341	2	1	
6	2	4	4	2200.8767	1	1	2249.9364	3	2	17	9	9	2421.9259	2	20	14	2661.0449	0	0	
6	3	3	3	2209.7769	4	1	2254.2755	3	0	17	10	8	2455.6275	1	20	15	2711.8106	0	1	
6	4	2	2	2222.2992	3	-1	2266.7717	1	1	17	11	7	2492.7942	2	-1	16	2765.8991	-1	-1	
6	5	1	1	2238.3889	-2	2	2282.8318	1	-1	17	12	6	2533.4007	1	0	17	2823.2778	2	1	
6	6	0	0	2258.0320	2	-2	2302.4623	2	0	17	13	5	2577.4195	1	20	18	2883.9115	-2	-2	
7	1	7	7	2199.1161	1	0	2325.6403	2	-3	17	14	4	2624.8220	2	21	1	2320.8961	3	3	
7	2	6	6	2205.2271	4	2	2352.3467	2	0	17	15	3	2675.5783	7	21	2	2332.3449	3	-1	
7	3	5	5	2214.2204	0	0	2416.2590	2	-3	17	16	2	2729.6553	1	21	3	2343.3052	0	-1	
7	4	4	4	2226.7414	3	-2	2453.4208	2	-1	17	17	1	2787.0219	3	21	4	2355.9878	1	-1	
7	5	3	3	2242.8304	1	1	2494.0202	2	2	18	0	18	2284.9454	0	21	5	2371.9163	3	1	
7	6	2	2	2262.4732	1	1	2538.0293	1	-5	18	1	17	2293.1816	-1	21	6	2391.4525	3	3	
8	0	8	8	2202.9178	1	1	2245.1847	1	0	18	2	16	2298.6957	0	21	7	2414.5802	1	-1	
8	1	7	7	2205.8086	2	2	2250.7800	0	2	18	3	15	2305.8866	2	21	8	2441.2615	1	-1	
8	2	6	6	2210.5106	3	4	2255.3998	2	-1	18	4	14	2317.7682	4	21	9	2471.4656	1	-2	
8	3	5	5	2219.3088	3	-1	2263.3607	4	3	18	5	13	2333.7072	1	0	10	2505.1659	2	0	
8	4	4	4	2231.8200	3	0	2275.6857	2	-1	18	6	12	2353.2929	3	3	11	2542.3355	2	-3	
8	5	3	3	2247.9070	4	1	2291.7288	2	1	18	7	11	2376.4493	2	2	12	2582.9489	1	3	
8	6	2	2	2267.5492	3	-1	2311.3535	1	-1	18	8	10	2403.1452	1	-1	13	2626.9764	2	-2	
8	7	1	1	2317.4376	-2	2	2334.5293	2	0	18	9	9	2433.3568	6	3	14	2674.3906	2	3	
9	1	9	9	2209.4016	4	1	2361.2345	2	0	18	10	8	2467.0579	3	-5	15	2725.1593	-1	-1	
9	2	8	8	2215.9668	5	2	2391.4481	2	0	18	11	7	2504.2267	2	4	16	2779.2518	-2	-2	
9	3	7	7	2225.0212	1	2	2425.1479	2	-2	18	12	6	2544.8343	2	-1	18	2897.2736	1	1	
9	4	6	6	2237.5348	1	0	2462.3111	1	-1	18	13	5	2588.8554	4	0	19	2961.1326	0	0	
9	5	5	5	2253.6193	3	3	2502.9124	3	2	18	14	4	2636.2609	3	21	20	3028.1761	1	5	
9	6	4	4	2273.2607	2	2	2546.9242	2	2	18	15	3	2687.0198	2	22	0	2333.9479	1	-1	
9	7	3	3	2296.4429	1	-1	2254.5499	2	1	18	16	2	2741.1012	4	22	1	21	2345.0313	1	-3
9	8	2	2	2323.1491	-2	2	2263.1332	1	-2	18	17	1	2798.4713	2	22	2	20	2352.4138	2	0
9	9	1	1	2353.3607	0	2	2272.7285	7	-3	18	18	0	2859.0969	6	3	3	19	2359.2436	3	0
10	0	10	10	2214.6674	2	2	2285.2259	1	-1	19	1	19	2296.4400	2	22	4	18	2370.2660	0	-2
10	1	9	9	2218.2520	2	3	2301.2633	1	-3	19	2	18	2306.8576	3	0	5	17	2385.9521	1	1
10	2	8	8	2222.7920	4	-2	2320.8815	5	-2	19	3	17	2317.2562	2	1	6	16	2405.4588	4	3
10	3	7	7	2231.4028	2	-2	2344.0543	1	0	19	4	16	2329.8315	3	22	7	15	2428.5670	0	-1

10	4	6	2243.8875	4	2	15	8	8	2370.7584	2	3	19	5	15	2345.8004	2	0	22	8	14	2455.2413	0
10	5	5	2259.9671	6	-1	15	9	7	2400.9716	2	0	19	6	14	2365.3729	1	0	22	9	13	2485.4417	0
10	6	4	2279.6069	1	-3	15	11	5	2471.8369	1	0	19	7	13	2388.5215	1	-2	22	10	12	2519.1407	4
10	7	3	2302.7894	1	2	15	12	4	2512.4397	0	19	8	8	12	2415.2138	0	-1	22	11	11	2556.3103	-4
10	8	2	2329.4955	3	-3	15	13	3	2556.4538	1	19	9	11	12	2445.4235	1	1	22	12	10	2596.9242	4
10	9	1	2359.7075	3	-1	15	14	2	2603.8510	2	19	10	10	10	2479.1249	2	-1	22	13	9	2640.9547	2
10	10	0	2393.4040	3	2	15	15	1	2654.6008	3	19	11	9	9	2516.2939	2	2	22	14	8	2688.3711	2
11	1	11	2222.0779	3	1	16	0	16	2263.9118	2	19	12	8	8	2556.9037	0	1	22	16	6	2793.2402	2
11	2	10	2229.2080	4	0	16	1	15	2270.7741	2	19	13	7	6	2600.9269	0	-1	22	17	5	2850.6273	-4
11	3	9	2238.3722	4	0	16	2	14	2275.7239	1	0	19	14	7	2648.3349	0	-1	22	18	4	2911.2711	4
11	4	8	2250.8763	3	-1	16	3	13	2283.2842	1	0	19	15	5	2699.0974	1	22	20	2	3042.1837	-3	
11	6	6	2286.5893	3	-1	16	4	12	2295.4349	2	0	19	16	4	2753.1828	7	7	23	1	23	2347.6860	3
11	7	5	2309.7708	1	0	16	5	11	2311.4385	4	3	19	17	3	2810.5562	3	-3	23	2	21	2360.2240	3
11	8	4	2336.4775	5	0	16	6	10	2331.0475	2	2	19	18	2	2871.1862	1	-1	23	3	21	2371.8555	0
23	4	20	2384.7138	1	1	26	13	13	2703.2231	3	-2	30	12	18	2731.6215	1	-1	35	3	33	2594.4773	3
23	5	19	2400.6043	1	1	26	14	12	2750.6507	3	-3	30	13	17	2775.6623	5	-7	35	4	32	2610.4610	1
23	6	18	2420.0928	2	0	26	15	11	2801.4371	2	-6	30	14	16	2823.0995	1	-5	35	5	31	2626.9102	4
23	7	17	2443.1925	3	-3	27	1	27	2408.2551	2	4	31	1	31	2478.1286	3	3	35	6	30	2645.9990	2
23	8	16	2469.8587	0	2	27	2	26	2423.0937	2	4	31	2	30	2495.3629	5	5	35	7	29	2668.6984	1
23	9	15	2500.0542	2	-2	27	3	25	2436.3752	2	0	31	3	29	2510.6386	1	1	35	8	28	2695.1095	6
23	10	14	2533.7511	1	-1	27	4	24	2449.8494	4	4	31	4	28	2525.1478	3	-1	35	9	27	2725.1512	1
23	11	13	2570.9210	0	27	27	5	23	2465.7155	2	0	31	5	27	2541.1571	4	-1	35	10	26	2758.7588	2
23	12	12	2611.5361	1	-1	27	6	22	2485.0773	2	0	31	7	25	2583.2498	1	1	35	11	25	2795.8814	4
23	13	11	2655.5681	1	-3	27	7	21	2508.0923	1	0	31	8	24	2609.7845	4	2	35	12	24	2836.4811	4
23	14	10	2702.9880	0	1	27	8	20	2534.7087	1	1	31	9	23	2639.9036	1	0	36	0	36	2578.5407	-1
23	15	9	2753.7636	1	-4	27	9	19	2564.8766	1	0	31	10	22	2673.5583	6	3	36	1	35	2598.7853	2
23	16	8	2807.8640	3	-6	27	10	18	2598.5593	2	3	31	11	21	2710.7084	4	0	36	2	33	2616.3237	3
23	17	7	2865.2562	4	-8	27	11	17	2635.7238	0	0	31	12	20	2751.3208	3	0	36	3	34	2629.4890	5
23	18	6	2925.9041	4	-2	27	12	16	2676.3406	0	-1	31	13	19	2795.3620	5	-6	36	4	32	2639.1598	2
24	0	24	2361.9250	1	3	27	13	15	2720.3794	4	-2	31	14	18	2842.8014	5	1	36	6	30	2669.1724	1
24	1	23	2374.4060	3	-2	27	14	14	2767.8095	0	-4	31	15	17	2893.6040	3	-5	36	7	29	2691.6837	1
24	2	22	2383.0539	3	-3	27	16	12	2872.7167	1	-6	32	0	32	2497.0466	3	3	36	9	27	2748.0628	6
24	3	21	2390.0119	1	0	28	0	28	2424.8411	1	2	32	1	31	2514.7842	3	3	36	10	26	2781.6543	3
24	4	20	2400.4888	2	2	28	1	27	2440.0083	1	0	32	2	30	2529.4239	0	0	36	11	25	2818.7678	4
24	5	19	2415.9461	3	1	28	2	26	2451.5897	4	2	32	3	29	2539.6024	3	-1	36	12	24	2859.3623	1
24	6	18	2435.3767	1	3	28	3	25	2459.6048	1	-1	32	4	28	2548.6276	3	-4	37	1	37	2600.3664	5
24	7	17	2458.4578	1	1	28	4	24	2469.0554	2	-1	32	5	27	2562.1052	2	-1	37	2	36	2621.2609	1
24	8	16	2485.1134	1	-1	28	5	23	2483.7454	0	0	32	6	26	2580.8424	3	4	37	3	35	2639.9437	4
24	9	15	2515.3044	5	3	28	6	22	2502.9401	2	1	32	7	25	2603.6477	0	0	37	4	34	2656.8160	4
24	10	14	2548.9984	2	1	28	7	21	2525.9192	5	2	32	8	24	2630.1539	2	1	37	5	33	2673.6320	2
24	11	13	2586.1684	3	9	28	8	20	2552.5180	3	-1	32	9	23	2660.2569	4	2	37	6	32	2692.7020	2
24	12	12	2626.7836	3	0	28	9	19	2582.6761	1	0	32	10	22	2693.9012	1	0	37	7	31	2715.2942	1
24	13	11	2670.8175	1	-1	28	10	18	2616.3528	1	-1	32	11	21	2731.0463	2	1	37	8	30	2741.6227	5
24	14	10	2718.2397	1	-3	28	11	17	2653.5155	3	3	32	12	20	2771.6562	2	-1	37	9	29	2771.6134	0
24	15	9	2769.0192	1	-4	28	12	16	2694.1312	5	-4	32	13	19	2815.6974	2	-4	37	11	27	2842.2913	4
24	17	7	2880.5200	4	-8	28	13	15	2738.1712	5	-4	32	14	18	2863.1374	2	-8	37	12	26	2882.8803	1
25	1	25	2376.8058	4	-3	28	14	14	2785.6035	5	-8	33	1	33	2516.5518	2	2	38	0	38	2622.7703	2
25	2	24	2390.4785	3	2	28	15	13	2836.3971	5	-7	33	2	32	2535.0009	2	0	38	2	36	2663.1688	2
25	3	23	2402.8865	4	4	28	16	12	2890.5186	8	-8	33	3	31	2551.3701	2	-2	38	3	35	2677.9690	-1
25	4	22	2416.0039	3	1	29	1	29	2442.0290	1	1	33	4	30	2566.5640	2	3	38	4	34	2688.4310	4
25	5	21	2431.8689	5	-4	29	2	28	2458.0575	2	-2	33	5	29	2582.7483	5	0	38	5	33	2700.0012	3
25	6	20	2451.2993	1	-1	29	3	27	2472.2998	2	-1	33	6	28	2601.8880	2	2	38	6	32	2717.2916	4
25	7	19	2474.3624	1	1	29	4	26	2486.2359	5	-3	33	7	27	2624.6854	3	0	38	7	31	2739.5825	3
25	8	18	2501.0070	3	3	29	5	25	2502.1447	2	-2	33	8	26	2651.1642	2	2	38	8	30	2765.8453	-4

Table 6 (continued)

<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>E</i>	Δ	δ	<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>E</i>	Δ	δ	<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>E</i>	Δ	δ
1			2	3	4	1			2	3	4	1			2	3	4
25	9	17	2531.1908			29	6	24	2521.4312	1	0	33	9	25	2681.2486	2	-2
25	10	16	2564.8817	2	-1	29	8	22	2570.9667	1	-2	33	10	24	2714.8823	2	0
25	11	15	2602.0501	1	0	29	9	21	2601.1134		-2	33	12	22	2792.6279	2	-2
25	12	14	2642.6666	4	-2	29	10	20	2634.7839	4	-1	33	14	20	2884.1101	5	-6
25	13	13	2686.7024		-2	29	11	19	2671.9430		0	34	0	34	2536.6325		0
25	14	12	2734.1274	4	-3	29	12	18	2712.5584	2	-2	34	1	33	2555.6289		0
25	15	11	2784.9105		-4	29	13	17	2756.5989		-5	34	2	32	2571.7443	3	1
26	0	26	2392.2217	4	-3	29	14	16	2804.0336	2	-8	34	3	31	2583.3447	2	2
26	1	25	2406.0644	1	2	29	15	15	2854.8308	5	-4	34	4	30	2592.5405	2	-1
26	2	24	2416.1338	5	-1	30	1	29	2476.2458	3	1	34	5	29	2605.3215	3	1
26	3	23	2423.4797	4	-1	30	2	28	2489.3654	4	-4	34	6	28	2623.6964	4	2
26	4	22	2433.4062	4	-4	30	3	27	2498.3329	5	-3	34	7	27	2646.3742	2	0
26	5	21	2448.5377	3	-2	30	4	26	2507.4604	2	-1	34	8	26	2672.8158	2	0
26	6	20	2467.8702	2	1	30	5	25	2521.5911	5	-3	34	9	25	2702.8801	2	-1
26	7	19	2490.9073	1	1	30	6	24	2540.5939	3	-2	34	10	24	2736.5010	3	-3
26	8	18	2517.5385	1	2	30	7	23	2563.4978	2	1	34	11	23	2773.6328	2	0
26	9	17	2547.7147	4	-2	30	8	22	2590.0555	5	-1	34	12	22	2814.2363	1	1
26	10	16	2581.4020	4	-1	30	9	21	2620.1898	4	4	34	13	21	2858.2754	1	-8
26	11	15	2618.5687	7	-1	30	10	20	2653.8525	4	3	35	1	35	2557.2979	2	1
26	12	14	2659.1857	2	-1	30	11	19	2691.0073	4	-1	35	2	34	2576.9685	3	40
40	3	37	2728.7314	3	-5	41	11	31	2942.7632	5	0	44	3	41	2836.9875		-5
40	4	36	2740.2889		-4	42	2	40	2763.6968		-1	45	1	45	2795.8445		2
40	5	35	2751.5132	1	3	42	3	39	2781.7423		-6	45	3	43	2845.1897	0	0
40	6	34	2768.0797	2	2	42	4	38	2794.6613	3	-4	45	4	42	2866.3443	4	5
40	7	33	2790.0798	2	-3	42	9	33	2898.9847	2	3	45	5	41	2885.7387		-1
40	8	32	2816.2211		-3	42	10	32	2932.4450	2	2	46	1	45	2849.2951	2	-2
40	9	31	2846.1117	2	1	42	12	30	3010.0207	2	3	46	2	44	2873.3997		-2
40	10	30	2879.6240		0	43	1	43	2743.4955		-2	46	3	43	2894.4683		-5
40	11	29	2916.6883	2	-2	43	2	42	2768.0685	2	2	47	1	47	2850.5103		-4
40	12	28	2957.2540	3	6	43	3	41	2790.3863	1	2	47	2	46	2877.5328	1	-1
41	2	40	2716.8127	2	1	43	4	40	2810.3880	1	2	47	3	45	2902.3128		0
41	3	39	2737.9066	3	-1	43	5	39	2828.9732		-2	48	0	48	2878.7124		-3
41	4	38	2756.8014	1	0	43	6	38	2848.3474		1	48	1	47	2906.3454	0	0
41	5	37	2774.6847	2	2	43	8	36	2896.6164	4	-4	48	2	46	2931.7055		5
41	6	36	2793.8808	2	0	43	11	33	2996.8272		-1	48	3	45	2954.1958		0
41	7	35	2816.2491	3	0	44	1	43	2794.5606		-2	49	1	49	2907.4937		-2
41	8	34	2842.3732	2	3	44	2	42	2817.3983		-1	49	2	48	2935.7395		-3
41	10	32	2905.7148	3	3												

^a See footnote to Table 1.

Table 7
Experimental ro-vibrational term values for the (0 2 1) vibrational state of the SO₂ molecule (in cm⁻¹).^a

J	K _a			Δ	δ	J	K _a			Δ	δ	J	K _a			Δ	δ					
	K _c	K _c	K _c				K _c	K _c	K _c				K _c	K _c	K _c			K _c	K _c	K _c	K _c	
1																						
2	1	2	2392.5094	1	0	11	5	6	2474.9918	5	16	5	12	2519.5323	1	0	20	7	14	2608.8189	2	-2
2	2	1	2397.8905	1	0	11	6	5	2494.3686	-1	16	6	11	2538.8819	3	3	20	8	13	2635.1553	2	1
3	0	3	2392.7163		-1	11	7	4	2517.2438	0	16	7	10	2561.7439	0	0	20	9	12	2664.9664	2	0
3	1	2	2394.6452		0	11	8	3	2543.5985	0	16	8	9	2588.0944	2	1	20	10	11	2698.2274	2	-1
3	2	1	2399.7998		-4	11	9	2	2573.4140	1	16	9	8	2617.9109	2	-1	20	11	10	2734.9133	1	-1
3	3	0	2408.6313	2	3	11	10	1	2606.6693	3	-2	16	7	2651.1716	1	0	20	12	9	2774.9987	2	2
4	1	4	2396.7664	2	-1	12	1	12	2437.9128	2	1	16	11	2687.8531	3	2	20	13	8	2818.4560	2	1
4	2	3	2402.3317	1	0	12	2	11	2445.3047	0	16	12	5	2727.9302	2	1	20	14	7	2865.2572	3	1
4	3	2	2411.1716	3	2	12	3	10	2454.4340	2	-1	16	14	2818.1653	3	-2	20	15	6	2915.3722	-4	-4
4	4	1	2423.5309	2	0	12	4	9	2466.7668	-5	16	16	1	2921.6490	4	1	20	16	5	2968.7706	-6	-6
5	0	5	2398.3925	2	-2	12	5	8	2482.6223	3	2	17	0	2482.7907	5	0	21	0	21	2529.5119	0	0
5	1	4	2400.5810	1	0	12	6	7	2501.9965	2	1	17	1	2490.3359	2	2	21	1	20	2539.8816	0	0
5	2	3	2405.5410	1	-1	12	7	6	2524.8704	2	1	17	2	2495.5113	2	-1	21	2	19	2546.7163	1	0
5	3	2	2414.3483	1	0	12	8	5	2551.2249	1	1	17	3	2502.7528	0	0	21	3	18	2553.4698	0	0
5	4	1	2426.7064	0	0	12	9	4	2581.0409	1	0	17	4	2514.6017	2	-2	21	4	17	2564.5494	1	0
5	5	0	2442.5831	1	1	12	10	3	2614.2977	2	-1	17	5	2530.3607	2	-1	21	5	16	2580.0973	1	1
6	1	6	2403.4471	1	-1	12	11	2	2650.9728	0	0	17	6	2549.6987	2	2	21	6	15	2599.3630	3	2
6	2	5	2409.3037	1	0	13	0	13	2445.3140	0	0	17	7	2572.5554	0	-1	21	7	14	2622.1841	2	-2
6	3	4	2418.1609	3	2	13	1	12	2450.3320	1	-3	17	8	2598.9034	2	-2	21	8	13	2648.5145	0	0
6	4	3	2430.5180	3	1	13	2	11	2454.8135	1	0	17	9	2628.7196	1	0	21	9	12	2678.3228	1	0
6	5	2	2446.3939	1	0	13	3	10	2462.8350	0	0	17	10	2661.9808	1	0	21	10	11	2711.5829	6	-2
6	6	1	2465.7765	2	-2	13	5	8	2490.8909	-2	17	11	6	2698.6635	0	1	21	11	10	2748.2693	4	-5
7	0	7	2406.5393	1	1	13	6	7	2510.2613	1	1	17	12	2738.7427	0	0	21	12	9	2788.3566	0	-1
7	1	6	2409.1404	3	4	13	7	6	2533.1335	5	3	17	13	2782.1921	1	-1	21	13	8	2831.8165	2	-1
7	2	5	2413.8765	0	0	13	8	5	2559.4874	-1	17	14	3	2828.9837	3	-1	21	14	7	2878.6211	2	0
7	3	4	2422.6141	0	0	13	9	4	2589.3040	1	-1	17	15	2879.0879	3	-2	21	15	6	2928.7401	-2	-2
7	4	3	2434.9657	3	2	13	10	3	2622.5620	0	18	1	18	2493.7385	3	-3	22	1	22	2942.6885	0	0
7	5	2	2450.8406	1	1	13	11	2	2659.2388	0	18	2	17	2503.6130	4	-2	22	2	21	2954.6244	0	0
7	6	1	2470.2230	0	-2	13	12	1	2699.3097	0	18	3	16	2513.6738	4	-2	22	3	20	2965.8236	0	0
7	7	0	2493.0991	-1	0	13	13	0	2742.7490	0	18	4	15	2526.0537	1	-1	22	4	19	2978.4333	2	0
8	1	8	2412.5408	2	0	14	1	14	2454.1640	1	-1	18	5	2541.8282	1	0	22	5	18	2994.1282	2	0
8	2	7	2418.7976		0	14	2	13	2462.2866	1	1	18	6	2561.1544	2	-2	22	6	17	2613.3802	0	0
8	3	6	2427.6984		-2	14	3	12	2471.6335	1	0	18	7	2584.0049	2	-2	22	7	16	2636.1888	0	0
8	4	5	2440.0500	1	0	14	4	11	2483.9627	6	0	18	8	2610.3498	2	-1	22	8	15	2662.5115	2	0
8	5	4	2455.9232	1	0	14	5	10	2499.7988	3	2	18	9	2640.1649	1	-1	22	9	14	2692.3166	2	-1
8	6	3	2475.3054	1	0	14	6	9	2519.1630	-3	18	10	8	2673.4264	1	0	22	10	13	2725.5759	2	1
8	7	2	2498.1815	0	0	14	7	8	2542.0330	0	18	11	7	2710.1103	1	0	22	11	12	2762.2631	3	3
8	8	1	2524.5351	1	0	14	8	7	2568.3865	0	18	12	7	2750.1917	1	0	22	12	11	2802.3517	4	4
9	0	9	2417.1061	0	0	14	9	6	2598.2033	0	-1	18	14	2840.4384	1	0	22	13	10	2845.8138	3	1
9	1	8	2420.3045	1	6	14	10	5	2631.4623	0	18	15	4	2890.5462	3	-3	22	14	9	2892.6216	3	1
9	2	7	2424.8459	1	1	14	11	4	2668.1409	3	0	19	0	2504.9938	0	0	22	15	8	2942.7446	2	-1
9	3	6	2433.4387	1	-1	14	12	3	2708.2136	4	1	19	1	2513.9416	1	1	23	0	23	2556.3490	1	1
9	4	5	2445.7720	0	0	14	13	2	2751.6558	4	4	19	2	2519.8221	1	-1	23	1	22	2568.1227	2	-2
9	5	4	2461.6423	1	-1	14	14	1	2798.4380	-1	19	3	16	2526.7473	1	0	23	2	21	2576.1392	0	0
9	6	3	2481.0236	0	0	15	0	15	2462.8982	0	19	4	15	2538.2654	4	-4	23	3	20	2582.9259	2	2
9	7	2	2503.8995	-1	0	15	2	13	2473.8300	0	19	5	14	2553.9422	2	2	23	4	19	2593.4825	3	3
9	8	1	2530.2538	3	0	15	3	12	2481.4609	1	0	19	6	2573.2504	1	0	23	5	18	2608.8355	1	-1

Table 7 (continued)

J	K _a			K _c			E			Δ			δ		
	J	K _a	K _c	J	K _a	K _c	J	K _a	K _c	J	K _a	K _c	J	K _a	K _c
9	9	9	0	2560.0676	1	0	15	4	11	2493.5352	0	0	19	7	12
10	1	10	2424.0338	2	-1	15	15	5	10	2509.3459	0	0	19	8	11
10	2	9	2430.8027	1	-1	15	6	6	9	2528.7034	1	0	19	9	10
10	4	7	2452.1314	3	0	15	7	8	8	2551.5694	5	-3	19	10	9
10	6	5	2487.3780	1	1	15	8	7	7	2577.9219	1	-1	19	11	8
10	7	4	2510.2539	4	2	15	9	6	6	2607.7391	1	0	19	12	7
10	8	3	2536.6082	1	1	15	10	5	5	2640.9988	1	0	19	13	6
10	9	2	2566.4229	6	1	15	11	4	4	2677.6786	0	0	19	14	5
10	10	1	2599.6772	1	0	15	12	3	3	2717.7539	2	1	19	15	4
11	0	11	2430.0435	1	-1	15	13	2	2	2761.1984	4	20	2	19	15
11	1	10	2434.0466	0	0	15	14	1	1	2807.9841	5	20	3	18	
11	2	9	2438.4851	2	1	16	2	15	14	2871.7293	0	0	20	4	17
11	3	8	2446.8378	0	-2	16	3	14	13	2491.3830	0	0	20	5	16
11	4	7	2459.1307	0	-2	16	4	13	12	2503.7235	2	1	20	6	15
24	8	17	2692.4222	0	0	28	12	17	16	2899.6883	2	1	33	0	32
24	9	16	2722.2173	0	0	28	13	16	15	2943.1628	0	-1	33	1	32
24	13	12	2875.7175	4	2	28	14	15	14	2989.9895	3	1	33	2	31
24	15	10	2972.6626	2	-3	28	15	14	13	3040.1365	3	-2	33	3	30
24	16	9	3026.0799	2	3	29	0	29	29	2650.7961	0	0	33	4	29
25	0	25	2585.5076	0	0	29	1	28	27	2666.5722	1	-1	33	5	28
25	1	24	2598.6511	0	0	29	2	27	26	2678.9572	1	0	33	6	27
25	2	23	2608.0293	0	0	29	3	26	25	2687.4268	3	3	33	7	26
25	4	21	2625.0996	0	0	29	4	25	24	2696.5299	1	0	33	8	25
25	5	20	2640.1694	0	0	29	5	24	23	2710.6928	1	0	33	9	24
25	6	19	2659.2892	0	0	29	6	23	22	2729.5241	2	0	33	10	23
25	7	18	2682.0426	1	0	29	7	22	21	2752.1582	0	0	33	12	21
25	8	17	2708.3355	3	-2	29	8	21	20	2778.3862	1	1	33	14	19
25	9	16	2738.1243	2	-2	29	9	20	19	2808.1376	1	0	34	1	34
25	10	15	2771.3767	0	0	29	10	19	18	2841.3697	1	1	34	2	33
25	11	14	2808.0626	1	0	29	11	18	17	2878.0476	1	1	34	3	32
25	12	13	2848.1546	2	1	29	12	17	16	2918.1400	3	3	34	4	31
25	13	12	2891.6241	2	2	29	13	16	15	2961.6157	1	-2	34	5	30
25	14	11	2938.4415	1	1	29	14	15	14	3008.4450	3	-2	34	6	29
25	15	10	2988.5766	3	-1	30	1	30	30	2668.5762	1	1	34	7	28
26	1	26	2600.9743	0	0	30	2	29	28	2685.1472	1	1	34	8	27
26	2	25	2615.1731	0	0	30	3	28	27	2699.8414	0	0	34	9	26
26	3	24	2627.9384	1	1	30	4	27	26	2713.9402	1	0	34	10	25
26	4	23	2641.0878	0	0	30	5	26	25	2748.6807	1	-1	34	12	23
26	5	22	2656.7412	2	1	30	6	25	24	2771.2927	0	-1	34	13	22
26	6	21	2675.8756	0	0	30	7	24	23	2797.4990	0	-5	35	0	35
26	7	20	2698.6085	0	0	30	8	23	22	2827.2384	4	3	35	1	34
26	8	19	2724.8883	1	-1	30	9	22	21	2860.4626	3	-2	35	2	33
26	9	18	2754.6699	0	0	30	10	21	20	2897.1371	2	1	35	3	32
26	10	17	2787.9181	0	-1	30	11	20	19	2937.2281	3	-3	35	4	31
26	11	16	2824.6028	1	-2	30	12	19	18	2980.7057	2	2	35	5	30
26	12	15	2864.6956	0	0	30	13	18	17	3131.1380	1	1	35	7	28
26	15	12	3005.1268	3	-1	31	0	31	31	2686.9271	0	0	35	8	27
27	0	27	2616.9896	0	0	31	1	30	29	2703.9789	2	-2	35	9	26

27	1	26	2631.4655	0	31	2	29	2717.8882	1	0	35	10	25	2965.5068	-1	41	4	37	2976.1677	0	-1
27	2	25	2642.3220	0	31	3	28	2727.4732	1	0	35	11	24	3002.1504	3	41	6	35	3002.9783	5	-1
27	3	24	2649.9475	-4	31	4	27	2736.3881	5	3	35	12	23	3042.2287	3	41	7	34	3024.4495	2	3
27	4	23	2659.4386	0	31	5	26	2749.9304		1	36	1	36	2787.4245	0	41	8	33	3050.1563	1	1
27	5	22	2674.1149	0	31	6	25	2768.5269		-1	36	2	35	2807.6346	0	41	9	32	3079.6085	1	2
27	6	21	2693.1144	2	31	7	24	2791.0730	0	0	36	3	34	2825.6755	0	42	1	42	2927.1860	0	0
27	7	20	2715.8163	1	31	8	23	2817.2540	6	0	36	4	33	2842.0189	0	42	2	41	2951.0580	1	1
27	8	19	2742.0807	1	31	9	22	2846.9781	1	0	36	5	32	2858.4807	1	42	3	40	2972.7049	2	0
27	9	18	2771.8535	2	31	10	21	2880.1944	0	1	36	6	31	2877.3041	0	42	4	39	2992.0973	0	-1
27	10	17	2805.0974	0	31	11	20	2916.8642	0	0	36	7	30	2899.6401	1	42	5	38	3010.2128	0	6
27	11	16	2841.7806	0	31	12	19	2956.9541		1	36	8	29	2925.6571	2	42	6	37	3029.2709	1	1
27	12	15	2881.8736	2	31	13	18	3000.4319		1	36	9	28	2955.2784	1	42	7	36	3051.2825	2	-2
27	13	14	2925.3468	3	31	14	17	3047.2664	0	4	36	10	27	2988.4327	1	42	8	35	3076.9877	1	2
27	14	13	2972.1700	3	32	1	32	2705.8673	2	-4	36	11	26	3025.0673	1	42	9	34	3106.4018	1	5
27	15	12	3022.3137	1	32	3	30	2739.4077	5	-4	37	0	37	2809.2656	1	43	0	43	2952.5112	0	0
28	1	28	2633.6115	0	32	4	29	2754.1486	2	1	37	1	36	2830.0586	-5	43	1	42	2976.9876	2	-2
28	2	27	2648.9873	1	32	5	28	2770.0500		3	37	2	35	2848.2742	-1	43	2	41	2999.1377	2	1
28	3	26	2662.6779	3	32	6	27	2788.9624	1	0	37	3	34	2862.3355	1	43	3	40	3018.0070	2	2
28	4	25	2676.2467	0	32	7	26	2811.4942	4	-3	37	5	32	2883.9466	1	43	4	39	3031.8057	5	-5
28	5	24	2691.9249	2	32	8	25	2837.6495	3	-4	37	6	31	2901.2268	2	43	5	38	3042.9312	0	-3
28	6	23	2710.9869	1	32	9	24	2867.3576	0	-1	37	7	30	2923.3088	0	43	6	37	3057.9303	0	-1
28	7	22	2733.6656	0	32	10	23	2900.5640		-2	37	8	29	2949.2676	2	44	1	44	3078.9463	1	0
28	8	21	2759.9131	1	32	11	22	2937.2286		-3	37	9	28	2978.8609	1	44	2	43	2978.4166	2	-1
28	9	20	2789.6761	0	32	12	21	2977.3167	2	-1	37	10	27	3011.9976	1	44	3	43	3003.5090	2	1
28	10	19	2822.9146	0	32	13	20	3020.7948	4	0	37	11	26	3048.6221	3	44	4	42	3026.3788	1	-1
28	11	18	2859.5954	0	32	14	19	3067.6315	3	4	37	12	25	3088.6898	1	44	4	41	3046.9065	0	0
44	5	40	3065.7954	1	46	2	45	3058.2793	1	-3	48	1	48	3087.8379	1	51	1	50	3205.3459	1	1
44	8	37	3132.5991	1	46	4	43	3104.0759	1	0	48	2	47	3115.3679	-3	51	2	49	3232.4960	2	-2
44	9	36	3161.9182	1	46	5	42	3123.8401	1	1	48	3	46	3140.6924	4	51	3	48	3257.0091	2	0
45	0	45	3004.9023	3	46	6	41	3143.4860		0	48	4	45	3163.5926	3	52	1	52	3206.5323	5	2
45	1	44	3030.6011	1	46	8	39	3190.8020		-1	48	5	44	3184.3211	3	53	0	53	3237.6537	0	0
45	2	43	3054.0168	0	47	0	47	3059.6127		0	48	6	43	3204.4245	2	53	1	52	3268.2266	1	-1
45	3	42	3074.3784	-1	47	1	46	3086.5321		-1	49	0	49	3116.6422	2	54	2	53	3300.5353	4	-1
45	4	41	3089.8330	2	47	2	45	3111.2016	0	3	49	1	48	3144.7807	1	54	0	55	3301.6335	4	0
45	5	40	3101.4256	0	47	3	44	3132.9945		2	49	3	46	3226.3276	1	55	1	54	3333.4225	3	3
45	6	39	3115.6481	0	47	4	43	3150.1767	4	0	49	6	43	3239.4845	1	56	1	56	3334.4916	2	2
45	7	38	3136.0826	-1	47	5	42	3162.5820	1	0	50	1	50	3146.0260	0	56	2	55	3366.8877	1	-2
45	8	37	3161.3941	2	47	6	41	3176.1613		-1	50	2	49	3174.7744	-2	57	0	57	3367.9277	1	-1
45	9	36	3190.6433	3	47	7	40	3195.8808		5	50	3	48	3201.3268	3	58	1	58	3401.9424	3	-2
46	1	46	3031.9675	1	47	8	39	3220.9097	1	2	51	0	51	3175.9895	-1	59	0	59	3436.5356	0	0

^a See footnote to Table 1.

Table 8Spectroscopic parameters of the (1 2 0) and (0 2 1) vibrational states of the SO₂ molecule (in cm⁻¹)^a.

Parameter	(1 2 0)	(0 2 1)	(0 2 0) ^b
1	2	3	4
<i>E</i>	2180.33121341(334)	2388.91526214(206)	1035.126371
<i>A</i>	2.1092208990(816)	2.0856995349(690)	2.107649092
<i>B</i>	0.3426644311(134)	0.34314069707(640)	0.3443172408
<i>C</i>	0.29107884147(612)	0.29133813525(682)	0.2924635974
<i>A_K</i> × 10 ³	1.08077235(307)	1.04553061(308)	1.0638447
<i>A_{JK}</i> × 10 ⁵	−0.40994143(329)	−0.44419076(426)	−0.4257225
<i>A_J</i> × 10 ⁶	0.22038905(184)	0.22401456(170)	0.2212268
<i>δ_K</i> × 10 ⁵	0.1315874(112)	0.11694327(502)	0.1236181
<i>δ_J</i> × 10 ⁷	0.57310324(404)	0.58163875(200)	0.5742303
<i>H_K</i> × 10 ⁷	0.19537880(210)	0.18304606(435)	0.188955
<i>H_{KJ}</i> × 10 ⁹	−0.86163	−0.7981250(652)	−0.86163
<i>H_{JK}</i> × 10 ¹¹	0.554	0.554	0.554
<i>H_J</i> × 10 ¹²	0.26162	0.390039(299)	0.26162
<i>h_K</i> × 10 ⁹	0.927	0.927	0.927
<i>h_{JK}</i> × 10 ¹²	−2.78	−2.78	−2.78
<i>h_J</i> × 10 ¹²	0.194	0.194	0.194
<i>L_K</i> × 10 ¹¹	−0.437	−0.437	−0.437
<i>L_{KKJ}</i> × 10 ¹²	0.158	0.158	0.158

^a Values in parentheses are 1σ statistical confidence intervals (in last digits). Parameters presented without confidence intervals were fixed to the values from column 4.

^b From Ref. [25].

for the $\nu_2 + \nu_3$ band can be simulated with only one main effective dipole moment parameter. At the same time, for simulation of the spectrum in the region of the $\nu_1 + \nu_2$ band, it is necessary to use, at least, three parameters, whose relative values were estimated as follows (notations from Ref. [45] are used): $\varphi_x = 1$, $\{i\varphi_y, j_z\} = 0.002$, and $\{\varphi_z, i_j y\} = -0.0012$. After that the experimental spectrum was filtered by taking the lines belonging to the “cold” bands. Weak lines remained in the experimental spectrum belong, as we believed, to the “hot” bands, $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$.¹ Assignments of these remaining lines were made on the basis of the procedure discussed in Refs. [46,47,37], namely:

- (1) We estimated the values of the vibrational energies $E_{(1\ 2\ 0)}$ and $E_{(0\ 2\ 1)}$ with the parameters of the SO₂ potential function from Ref. [36].
- (2) We used formula 4 to estimate the initial values of rotational parameters and distortion coefficients of the states (1 2 0) and (0 2 1). In this case, (a) for estimations we used, as the initial data, parameters of the ground vibrational state, Ref. [34], of the states (1 0 0)/(0 0 1), and (0 2 0), Ref. [25]; (b) as the analysis showed, the Hamiltonian model of isolated vibrational state can be used for description of our experimental “hot” transitions both in the (0 2 1), and (1 2 0) vibrational states.
- (3) We then calculated transitions of the “hot” bands $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$, compared calculated transitions with the experimental line positions in

the filtered spectrum, and determined a number, *N*, of transitions for which the value $(\nu^{exp.} - \nu^{calc.}) \leq 0.005 \text{ cm}^{-1}$.

- (4) We then varied the vibrational energies, *E*, and values of the rotational parameters, *A*, *B*, and *C*, of the states (1 2 0) and (0 2 1) with the step of 0.005, 0.0005, 0.0005, and 0.0005 cm⁻¹, respectively. For each value of the vibrational energy and of the *A*, *B*, and *C* parameters we obtained the corresponding number *N* of experimental transition wavenumbers that coincided with the calculated ones to 0.005 cm⁻¹ or better, and in that way we determined a particular value of the vibrational energy, *E*, and the rotational parameters, *A*, *B*, and *C* for which *N* has a distinct maximum. As an illustration, see Fig. 6 where the value *N* is plotted against the vibrational term value, *E* (the situation, shown in Fig. 6, corresponds to the optimal values of the parameters *A*, *B* and *C*) for the $\nu_1 + 2\nu_2 - \nu_2$ “hot” band. Fig. 7 presents analogous plots of dependency of the value *N* against the vibrational term value, *E*, for the $2\nu_2 + \nu_3 - \nu_2$ hot band. In this case, plots are obtained with the use of optimal values of the parameters *B* and *C*, and plots curves I–III correspond to different values of the rotational parameter *A*. In that way, transitions were assigned with the value of quantum number $J \leq 15$. After that the parameters of the Hamiltonian were fitted, and we were able to assign without problem transitions with $J \leq 20$. Then we again fitted parameters and assigned transitions with higher *J*-values.

¹ Of course, some from weak lines in the recorded spectrum can belong to the ³⁴SO₂ species. However, we consider in the present study only the ³²SO₂ molecule.

As the result of the use of the above procedure we were able to assign 872 and 928 transitions (553 and 540 upper state ro-vibrational energy values) with $J_a^{max.} = 60$, $K_a^{max.} = 20$ and $J_b^{max.} = 59$, $K_b^{max.} = 16$ to the $\nu_1 + 2\nu_2 - \nu_2$ and

$2\nu_2 + \nu_3 - \nu_2$ bands, respectively (corresponding statistical information is presented in Table 5). The list of the assigned transitions is presented in Appendix A, and upper energy values of the states (1 2 0) and (0 2 1) obtained on that basis are given in Tables 6 and 7. Columns 3 and 5 of Table 8 present the results of the fit of parameters of the Hamiltonian, Eq. (2), with the energy terms from Tables 6 and 7. Columns 2 and 4 of that Table 8 show the initial predicted values (see above) of the rotational and distortion parameters. One can see good correlation of both sets of data.

6. Conclusion

We re-analysed the high resolution ro-vibrational structures of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ vibrational bands and, as a result, assigned about 2.5 times more transitions than was made before. Some transitions belonging to the $3\nu_2$ band and caused by the strong Fermi interaction between the (1 1 0) and (0 3 0) states were also assigned. Then the experimental spectrum was filtered by taking the lines belonging to the “cold” bands, $\nu_1 + \nu_2$, $\nu_2 + \nu_3$, and $3\nu_2$, and transitions belonging to the weak “hot” bands, $\nu_1 + 2\nu_2 - \nu_2$ and $2\nu_2 + \nu_3 - \nu_2$, were assigned. We determined parameters of the Hamiltonian that reproduce the initial “experimental” ro-vibrational energies of the states (1 1 0), (0 1 1), (0 3 0), (1 2 0), and (0 2 1) with the “rms” deviation of 0.00022 cm^{-1} that is close to uncertainties in experimental line positions.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jqsrt.2010.09.013.

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