

Submillimeter Microwave Spectrum and Spectroscopic Constants of the OCS Molecule

Isotopic Species $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ and $^{18}\text{O}^{12}\text{C}^{32}\text{S}$

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Microwave spectra of $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ and $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ in their natural isotopic abundances were investigated in the range 280–510 GHz. The effective rotational and centrifugal constants have been determined for all observed vibrational states. An analysis of the rotational spectrum taking account of *l*- and Fermi-resonances has been performed within each isotopic species.

INTRODUCTION

In our first paper devoted to the investigation of the OCS submillimeter spectrum the less abundant isotopic species of the molecule (natural abundance $i_c < 0.05\%$) were considered (1). The present paper describes the results of studies of the microwave spectrum of OCS isotopic species with abundances $0.05\% < i_c < 1\%$. This interval includes two isotopic species $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ and $^{18}\text{O}^{12}\text{C}^{32}\text{S}$. Their spectra were observed at room temperature in the range 280–510 GHz by a submillimeter microwave spectrometer RAD (2). The experimental procedure including correction of the influence of the wings of neighbouring lines on the measured absorption frequencies ν_{meas} is exactly the same as in Ref. (1). The absorption line frequencies obtained after correction and denoted ν_{exp} are given in Table I together with the correction values $\delta = \nu_{\text{meas}} - \nu_{\text{exp}}$.

PROCESSING OF EXPERIMENTAL DATA

Experimental data for the isotopic species $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ obtained in this investigation were processed together with lower frequency data from Ref. (3). Low-frequency data were not used for the isotopic species $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ since we did not take into account the quadrupole splitting observed in the low-frequency region. The processing was performed in two steps.

1. The rotational molecular spectrum for each observed vibrational state was described within the model

$$F(J) = B_{\text{eff}}[J(J+1) - l^2] - D_{\text{eff}}[J(J+1) - l^2]^2. \quad (1)$$

All designations are the same as in Ref. (1). The values obtained for B_{eff} , D_{eff} , and their correlation coefficient R_{BD} as well as the upper limit for the sextic

TABLE I
Experimental Frequencies of Rotational Transitions of the Isotopic Species $^{16}\text{O}^{12}\text{C}_3\text{S}$ and $^{18}\text{O}^{12}\text{C}_3\text{S}$

Time	Lat	Long	Alt	Speed	Heading	Roll	Pitch	Yaw	Roll Rate	Pitch Rate	Yaw Rate	Roll Acc	Pitch Acc	Yaw Acc
00:00	30.00	156.29	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
00:01	30.01	156.28	10.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
00:02	30.02	156.27	10.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
00:03	30.03	156.26	10.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
00:04	30.04	156.25	10.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
00:05	30.05	156.24	10.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
00:06	30.06	156.23	10.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06
00:07	30.07	156.22	10.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07
00:08	30.08	156.21	10.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08
00:09	30.09	156.20	10.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09
00:10	30.10	156.19	10.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
00:11	30.11	156.18	10.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11
00:12	30.12	156.17	10.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12	0.12
00:13	30.13	156.16	10.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13	0.13
00:14	30.14	156.15	10.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14
00:15	30.15	156.14	10.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15
00:16	30.16	156.13	10.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
00:17	30.17	156.12	10.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17
00:18	30.18	156.11	10.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18
00:19	30.19	156.10	10.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19
00:20	30.20	156.09	10.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20
00:21	30.21	156.08	10.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21
00:22	30.22	156.07	10.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22
00:23	30.23	156.06	10.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.23
00:24	30.24	156.05	10.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24
00:25	30.25	156.04	10.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
00:26	30.26	156.03	10.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26	0.26
00:27	30.27	156.02	10.27	0.27	0.27	0.27	0.27	0.27	0.27	0.27	0.27	0.27	0.27	0.27
00:28	30.28	156.01	10.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28
00:29	30.29	156.00	10.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29
00:30	30.30	155.99	10.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30	0.30
00:31	30.31	155.98	10.31	0.31	0.31	0.31	0.31	0.31	0.31	0.31	0.31	0.31	0.31	0.31
00:32	30.32	155.97	10.32	0.32	0.32	0.32	0.32	0.32	0.32	0.32	0.32	0.32	0.32	0.32
00:33	30.33	155.96	10.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
00:34	30.34	155.95	10.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34	0.34
00:35	30.35	155.94	10.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35
00:36	30.36	155.93	10.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36	0.36
00:37	30.37	155.92	10.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37
00:38	30.38	155.91	10.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38	0.38
00:39	30.39	155.90	10.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39
00:40	30.40	155.89	10.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40	0.40
00:41	30.41	155.88	10.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41	0.41
00:42	30.42	155.87	10.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42
00:43	30.43	155.86	10.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43
00:44	30.44	155.85	10.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44
00:45	30.45	155.84	10.45	0.45	0.45	0.45	0.45	0.45	0.45	0.45	0.45	0.45	0.45	0.45
00:46	30.46	155.83	10.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46	0.46
00:47	30.47	155.82	10.47	0.47	0.47	0.47	0.47	0.47	0.47	0.47	0.47	0.47	0.47	0.47
00:48	30.48	155.81	10.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48	0.48
00:49	30.49	155.80	10.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49
00:50	30.50	155.79	10.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50
00:51	30.51	155.78	10.51	0.51	0.51	0.51	0.51	0.51	0.51	0.51	0.51	0.51	0.51	0.51
00:52	30.52	155.77	10.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52	0.52
00:53	30.53	155.76	10.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53
00:54	30.54	155.75	10.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54
00:55	30.55	155.74	10.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55
00:56	30.56	155.73	10.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56
00:57	30.57	155.72	10.57	0.57	0.57	0.57	0.57	0.57	0.57	0.57	0.57	0.57	0.57	0.57
00:58	30.58	155.71	10.58	0.58	0.58	0.58	0.58	0.58	0.58	0.58	0.58	0.58	0.58	0.58
00:59	30.59	155.70	10.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59	0.59
01:00	30.60	155.69	10.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60	0.60
01:01	30.61	155.68	10.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61	0.61
01:02	30.62	155.67	10.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62	0.62
01:03	30.63	155.66	10.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63	0.63
01:04	30.64	155.65	10.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64
01:05	30.65	155.64	10.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65
01:06	30.66	155.63	10.66	0.66	0.66	0.66	0.66	0.66	0.66	0.66	0.66	0.66	0.66	0.66
01:07	30.67	155.62	10.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67	0.67
01:08	30.68	155.61	10.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68	0.68
01:09	30.69	155.60	10.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69	0.69
01:10	30.70	155.59	10.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70	0.70
01:11	30.71	155.58	10.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71
01:12	30.72	155.57	10.72	0.72	0.72	0.72	0.72	0.72	0.72	0.72	0.72	0.72	0.72	0.72
01:13	30.73	155.56	10.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73
01:14	30.74	155.55	10.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74
01:15	30.75	155.54	10.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.75
01:16	30.76	155.53	10.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76
01:17	30.77	155.52	10.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77
01:18	30.78	155.51	10.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78	0.78
01:19	30.79	155.50	10.79	0.79	0.79	0.79	0.79	0.79	0.79	0.79	0.79	0.79	0.79	0.79
01:20	30.80	155.49	10.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80	0.80
01:21	30.81	155.48	10.81	0.81	0.81	0.81	0.81	0.81	0.81	0.81	0.81	0.81	0.81	0.81
01:22	30.82	155.47	10.82	0.82	0.82	0.82	0.82	0.82	0.82	0.82	0.82	0.82	0.82	0.82
01:23	30.83	155.46	10.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83
01:24	30.84	155.45	10.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84	0.84
01:25	30.85	155.44	10.85											

Note. *—Exp. frequency = Meas. frequency - δ correction, a—Ref. (3), b—the present paper.

centrifugal constant H_{eff} , under which the influence of this constant may be neglected, are presented in Table II. The method of obtaining the upper limit for the neglected constant H_{eff} is analogous to that used in Refs. (1, 4). The differences $v_{\text{calc}}^{\text{exp}}$ obtained are given in the first difference column of Table I.

TABLE IV
Spectroscopic Constants of the Isotopic Species $^{18}\text{O}^{12}\text{C}^{32}\text{S}$

$^{18}\text{O}^{12}\text{C}^{32}\text{S}$										
B_0	5	704.857 16(15)	MHz	1						
Δ_1		18.320 9(49)	MHz	0.032	1					
Δ_2		-10.265 7(17)	MHz	0.199	0.215	1				
ν_{22}		-45.35(53)	KHz	0.119	0.228	0.989				
D_0		1.132 965(53)	KHz	0.943	0.030	0.185	0.110			
β_1		-5.1(27)	Hz	-0.003	0.725	-0.147	-0.148	-0.003		
β_2		-17.946(98)	Hz	0.501	0.019	0.466	0.339	0.532	-0.063	
ϵ_{11}		12.134(44351)	GHz	0.026	-0.427	0.193	0.194	0.028	-0.789	0.090
Δ_1	5	532.627(343415)	GHz	-0.026	0.429	-0.191	-0.192	-0.028	0.789	-0.090
q_0		2.826 49(23)	MHz	0.001	0.000	-0.088	-0.088	0.001	0.011	-0.127
q_J		-1.790(84)	Hz	-0.001	0.000	0.072	0.055	-0.001	-0.009	0.104
$K_{(100)}^{122}$	1	505.884(630851)	GHz	0.026	-0.430	0.191	0.192	0.028	-0.789	0.090
λ_J		-3.265 06(576480)	MHz	0.026	-0.431	0.190	0.191	0.028	-0.789	0.090
				Δ_1	1					
				q_0	0.013	1				
				q_J^{122}	-0.011	-0.933	1			
				$K_{(100)}^{122}$	-0.999995	-0.013	0.011	1		
				λ_J	-0.999994	-0.013	0.011	0.999998	1	

in Ref. (2). The spectroscopic constants obtained as a result of processing together with the correlation coefficient matrix are presented in Tables III and IV for the isotopic species $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ and $^{18}\text{O}^{12}\text{C}^{32}\text{S}$, respectively. The designations of constants are the same as in Ref. (5) (taking account of the correction performed in Ref. (1)) with the exception of the constants α_1^* and α_2^* which in the present paper are determined as $\alpha_1^* = \alpha_1 - 2\gamma_{11} - \gamma_{13}$, $\alpha_2^* = \alpha_2 - \gamma_{13}$. The differences $\nu_{\text{exp}} - \nu_{\text{calc}}$ obtained here are presented in the second difference column of Table I.

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