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Vibration–Rotation Emission Spectrum of MgF

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The high-resolution infrared emission spectrum of MgF was recorded with a Fourier transform spectrometer. More than 800 rovibrational lines from the $v = 1 \rightarrow 0$ to $v = 7 \rightarrow 6$ bands were assigned. The Dunham coefficients for the $X^2\Sigma^+$ electronic ground state were obtained.

I. INTRODUCTION

The electronic and microwave spectra of alkaline earth monohalides have been studied extensively (*1–4*). However, little is known about the infrared spectra of these molecules. During our systematic investigation of the infrared spectra of the alkaline earth monofluorides, the high-resolution vibration–rotation emission spectrum of MgF was recorded first.

The rotational analysis of the electronic spectrum of MgF was performed by Barrow and Beale (*5*). The structure and bonding of MgF was determined from its millimeter-wave spectrum (*6, 7*). MgF, like all the other alkaline earth monohalides, is found to

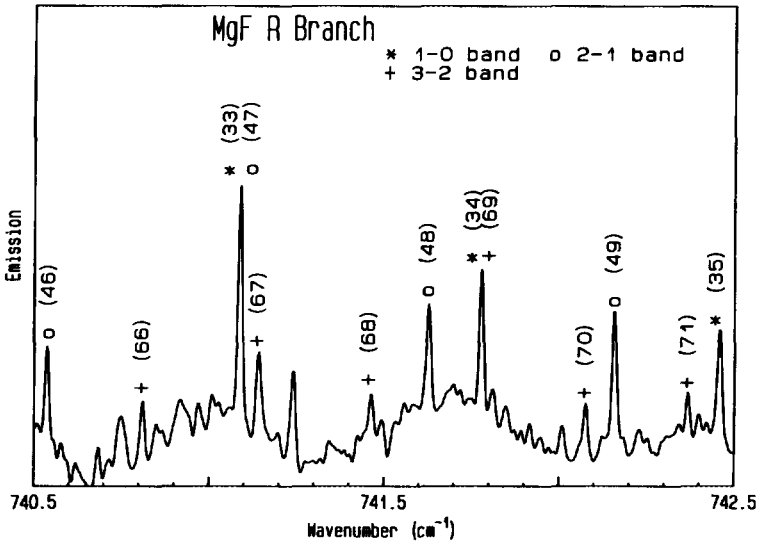

FIG. 1. A portion of the MgF emission spectrum.

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TABLE I

Observed Transitions of MgF in cm^{-1}

N'	N"	Observed	O-C[a]	N'	N"	Observed	O-C	N'	N"	Observed	O-C
						v=1→0 band					
1	0	712.7026	46	3	2	714.7223	36	4	3	715.7179	30
5	4	716.7029	12	6	5	717.6842	53	7	6	718.6459	-07
8	7	719.6108	60	10	9	721.4958	33	11	10	722.4207	-11
12	11	723.3424	07	13	12	724.2495	-22	14	13	725.1544	22
15	14	726.0457	28	16	15	726.9259	21	17	16	727.7993	43
18	17	728.6567	03	19	18	729.5063	-16	20	19	730.3527	30
21	20	731.1817	02	22	21	732.0040	05	23	22	732.8165	10
24	23	733.6155	-21	28	27	736.7284	22	29	28	737.4789	07
30	29	738.2241	38	31	30	738.9509	-11	32	31	739.6747	09
33	32	740.3840	-13	34	33	741.0868	00	35	34	741.7769	-11
36	35	742.4573	-16	37	36	743.1296	-01	38	37	743.7908	05
39	38	744.4395	-08	40	39	745.0798	-04	41	40	745.7113	15
42	41	746.3297	07	43	42	746.9378	00	44	43	747.5358	-02
45	44	748.1246	05	46	45	748.7014	-01	47	46	749.2690	04
48	47	749.8256	05	49	48	750.3702	-09	50	49	750.9050	-15
51	50	751.4311	-03	52	51	751.9432	-26	53	52	752.4497	01
54	53	752.9425	-01	55	54	753.4257	05	56	55	753.8949	-19
57	56	754.3573	-06	58	57	754.8075	-08	59	58	755.2471	-08
60	59	755.6767	-01	61	60	756.0950	01	62	61	756.5015	-07
63	62	756.8982	-05	64	63	757.2852	08	66	65	758.0228	-01
67	66	758.3750	-09	68	67	758.7170	-09	69	68	759.0467	-24
70	69	759.3680	-12	71	70	759.6790	06	72	71	759.9746	-18
74	73	760.5415	18	75	74	760.8018	-28	76	75	761.0588	03
78	77	761.5330	01	69	70	618.2423	-57	68	69	619.8563	-47
67	68	621.4657	-09	66	67	623.0656	07	65	66	624.6556	-00
64	65	626.2347	-42	63	64	627.8149	02	61	62	630.9421	-13
60	61	632.4965	-01	59	60	634.0425	04	58	59	635.5804	06
57	58	637.1074	-24	56	57	638.6309	-11	55	56	640.1463	-03
54	55	641.6522	-12	53	54	643.1530	06	52	53	644.6418	-16
51	52	646.1270	02	50	51	647.6011	-09	49	50	649.0756	61
48	49	650.5295	07	47	48	651.9811	08	46	47	653.4209	-26
45	46	654.8588	-01	44	45	656.2855	-06	43	44	657.7061	09
42	43	659.1151	-10	41	42	660.5196	06	40	41	661.9142	07
39	40	663.3006	07	38	39	664.6794	14	35	36	668.7682	59
34	35	670.1072	03	33	34	671.4430	-02	32	33	672.7713	02
31	32	674.0902	-03	30	31	675.4015	01	29	30	676.7024	-13
28	29	677.9954	-21	27	28	679.2832	04	26	27	680.5613	18
25	26	681.8270	-04	24	25	683.0865	-02	23	24	684.3373	-01
22	23	685.5797	04	21	22	686.8130	05	20	21	688.0374	05
19	20	689.2553	28	18	19	690.4591	-01	17	18	691.6579	08
16	17	692.8467	06	15	16	694.0278	16	14	15	695.2007	33
13	14	696.3608	13	12	13	697.5118	-09	11	12	698.6572	03
10	11	699.7912	-07	9	10	700.9190	09	8	9	702.0337	-12
6	7	704.2397	-17	5	6	705.3277	-32	4	5	706.4121	09
						v=2→1 band					
10	9	713.0293	-03	11	10	713.9497	-08	12	11	714.8637	19
13	12	715.7743	09	14	13	716.6564	09	15	14	717.5373	-05
16	15	718.4098	-07	17	16	719.2744	07	18	17	720.1265	-04
19	18	720.9705	01	20	19	721.8001	-40	21	20	722.6277	-04
22	21	723.4419	-04	23	22	724.2495	28	24	23	725.0420	09
25	24	725.8263	06	26	25	726.5979	-24	27	26	727.3658	07
29	28	728.8639	-05	30	29	729.5991	-01	31	30	730.3230	-09
32	31	731.0388	01	33	32	731.7431	-01	34	33	732.4420	43
35	34	733.1253	32	36	35	733.7960	-02	40	39	736.3800	-11
41	40	737.0106	-37	42	41	737.6263	-08	43	42	738.2241	-55

be highly ionic (*8*). When compared with the other heavier alkaline earth monofluorides, MgF has a greater degree of covalent bonding, as determined by the hyperfine structure.

Ionic molecules are suitable candidates for testing simple semiclassical bond models (*9–13*). Because MgF is a mainly ionic molecule, a Rittner-type model was developed by Torring *et al.* (*10, 11*). However, as Bauschlicher *et al.* (*12*) pointed out, when more accurate polarizabilities are used, the model by Torring *et al.* fails completely. Refined *ab initio* calculations (*9, 13*) were also carried out.

TABLE I—*Continued*

N'	N"	Observed	O-C	N'	N"	Observed	O-C	N'	N"	Observed	O-C
44	43	738.8216	-02	45	44	739.4042	05	46	45	739.9759	07
47	46	740.5352	-09	48	47	741.0868	-00	49	48	741.6258	-12
50	49	742.1565	-02	51	50	742.6761	00	52	51	743.1784	-63
53	52	743.6834	03	54	53	744.1681	-26	55	54	744.6475	-02
56	55	745.1138	-04	57	56	745.5709	07	58	57	746.0132	-21
59	58	746.4497	-02	60	59	746.8740	01	61	60	747.2869	-01
62	61	747.6894	-01	63	62	748.0810	-02	64	63	748.4605	-17
65	64	748.8324	00	66	65	749.1920	02	67	66	749.5397	-06
68	67	749.8784	03	69	68	750.2047	-01	70	69	750.5192	-15
71	70	750.8246	-11	73	72	751.4031	01	74	73	751.6751	-01
86	87	582.4256	-05	85	86	584.1451	05	84	85	585.8577	14
83	84	587.5607	-03	81	82	590.9512	09	80	81	592.6359	13
78	79	595.9842	20	76	77	599.3013	-05	74	75	602.5949	15
73	74	604.2305	21	71	72	607.4739	-30	70	71	609.0866	-37
69	70	610.6957	-08	68	69	612.2955	-00	67	68	613.8855	-16
66	67	615.4714	-00	65	66	617.0485	02	64	65	618.6167	-11
63	64	620.1779	-18	62	63	621.7339	-04	61	62	623.2843	29
60	61	624.8187	-21	59	60	626.3526	-02	58	59	627.8804	31
57	58	629.3953	14	56	57	630.9012	-17	55	56	632.4041	-01
54	55	633.8974	-05	53	54	635.3806	-31	52	53	636.8634	14
51	52	638.3308	-14	50	51	639.7984	37	49	50	641.2498	05
48	49	642.6964	04	47	48	644.1345	-01	46	47	645.5656	01
45	46	646.9916	33	44	45	648.4023	-06	43	44	649.8102	05
42	43	651.2084	00	41	42	652.5985	-03	40	41	653.9819	06
39	40	655.3558	03	38	39	656.7206	-08	37	38	658.0817	24
36	37	659.4294	06	35	36	660.7694	-06	34	35	662.1042	12
33	34	663.4268	-07	32	33	664.7446	08	31	32	666.0500	-15
30	31	667.3553	43	29	30	668.6434	15	28	29	669.9243	-00
27	28	671.1986	03	26	27	672.4611	-25	25	26	673.7208	03
24	25	674.9684	-03	23	24	676.2091	07	22	23	677.4371	-22
21	22	678.6617	00	20	21	679.8762	10	19	20	681.0814	14
18	19	682.2787	26	17	18	683.4637	03	16	17	684.6432	14
15	16	685.8097	-17	14	15	686.9751	29	13	14	688.1223	-16
11	12	690.4015	06	10	11	691.5261	02	9	10	692.6432	13
8	9	693.7509	20								
						v=3-2 band					
9	8	703.7440	10	10	9	704.6612	-34	11	10	705.5770	-00
13	12	707.3732	01	14	13	708.2588	20	15	14	709.1319	09
16	15	709.9959	03	17	16	710.8500	-04	18	17	711.6953	-04
19	18	712.5288	-25	20	19	713.3598	26	21	20	714.1746	12
22	21	714.9804	06	23	22	715.7750	-14	24	23	716.5630	-03
25	24	717.3407	03	26	25	718.1071	-04	27	26	718.8641	-07
29	28	720.3493	-05	30	29	721.0757	-17	32	31	722.5031	03
33	32	723.1999	-05	34	33	723.8880	-01	35	34	724.5661	04
36	35	725.2330	-01	37	36	725.8899	-06	38	37	726.5378	-00
39	38	727.1751	01	41	40	728.4186	-00	42	41	729.0256	03
43	42	729.6219	02	44	43	730.2064	-13	45	44	730.7829	-05
46	45	731.3490	00	47	46	731.9036	-05	49	48	732.9828	-06
50	49	733.5066	-08	56	55	736.4311	-15	57	56	736.8854	20
58	57	737.3209	-26	59	58	737.7535	03	60	59	738.1718	-03
61	60	738.5792	-13	62	61	738.9788	05	63	62	739.3654	00
64	63	739.7414	-03	65	64	740.1084	10	66	65	740.4605	-18
67	66	740.8082	17	68	67	741.1392	-06	69	68	741.4620	-05
71	70	742.0744	-09	72	71	742.3723	68	73	72	742.6449	01
74	73	742.9141	09	76	75	743.4173	02	77	76	743.6540	14
78	77	743.8801	28	80	79	744.2954	19	83	82	744.8335	-14
85	84	745.1423	17	86	85	745.2772	04	83	84	580.3048	-02

II. EXPERIMENTAL DETAILS

The experimental arrangement was similar to that described in a previous paper (*14*). A sample of 30 g of MgF_2 was contained in a carbon boat placed in the center of a carbon liner that was housed inside of a mullite ($3Al_2O_3 \cdot 2SiO_2$) tube. The central 50-cm portion of the mullite tube, which is 1.2 m long and has an outside diameter of 5 cm, was heated by a CM Rapid Temp furnace. The ends of the mullite tube were water-cooled and sealed with KRS-5 windows. The tube was heated to 1550°C at a rate of 200°C per hour. The sample cell was pressurized with 10 Torr of argon gas to prevent condensation of salt vapors on the cell windows.

TABLE I—*Continued*

N'	N"	Observed	O-C	N'	N"	Observed	O-C	N'	N"	Observed	O-C
82	83	581.9866	-15	81	82	583.6636	-07	80	81	585.3334	-03
79	80	586.9965	01	78	79	588.6512	-08	76	77	591.9467	41
73	74	596.8184	-73	72	73	598.4451	57	70	71	601.6475	23
69	70	603.2371	-02	68	69	604.8280	58	67	68	606.3992	-06
66	67	607.9700	-02	65	66	609.5353	19	64	65	611.0925	34
63	64	612.6353	-21	62	63	614.1796	12	61	62	615.7147	02
60	61	617.2396	16	59	60	618.7557	-07	58	59	620.2722	47
57	58	621.7707	-02	56	57	623.2645	-23	55	56	624.7555	04
53	54	627.7097	12	52	53	629.1748	11	51	52	630.6317	06
50	51	632.0787	-20	48	49	634.9564	-02	47	48	636.3824	-03
46	47	637.8004	-06	45	46	639.2114	00	44	45	640.6109	-27
43	44	642.0066	-15	42	43	643.3952	06	41	42	644.7726	-02
40	41	646.1438	06	39	40	647.5100	48	38	39	648.8579	-13
37	38	650.2049	-02	36	37	651.5366	-62	35	36	652.8721	-01
34	35	654.1940	04	33	34	655.5066	01	32	33	656.8113	01
31	32	658.1057	-17	30	31	659.3963	09	29	30	660.6757	07
28	29	661.9459	-02	27	28	663.2084	-04	26	27	664.4631	-00
25	26	665.7091	03	24	25	666.9444	-15	23	24	668.1746	-00
22	23	669.3928	-19	21	22	670.6038	-23	20	21	671.8067	-22
19	20	673.0040	08	18	19	674.1835	-51	17	18	675.3607	-46
16	17	676.5346	12	15	16	677.6955	30	14	15	678.8418	-11
13	14	679.9873	28	12	13	681.1157	-15	11	12	682.2387	-23
10	11	683.3586	26	9	10	684.4626	06				
						v=4-3 band					
1	0	687.8405	-09	3	2	689.8041	-33	5	4	691.7315	-50
6	5	692.6919	46	7	6	693.6262	-22	8	7	694.5615	09
9	8	695.4835	03	10	9	696.3967	02	12	11	698.1961	13
13	12	699.0799	02	14	13	699.9536	-15	15	14	700.8189	-22
17	16	702.5245	-00	18	17	703.3592	-26	19	18	704.1907	11
20	19	705.0075	-01	21	20	705.8162	01	22	21	706.6131	-17
23	22	707.4032	-07	24	23	708.1855	21	25	24	708.9527	-02
26	25	709.7101	-26	27	26	710.4635	07	28	27	711.2015	-14
29	28	711.9333	-00	30	29	712.6554	15	32	31	714.0651	-01
33	32	714.7561	00	34	33	715.4374	04	35	34	716.1079	02
36	35	716.7694	07	37	36	717.4201	07	38	37	718.0586	-16
39	38	718.6904	-05	40	39	719.3096	-19	41	40	719.9221	00
42	41	720.5237	12	43	42	721.1116	-10	44	43	721.6910	-17
45	44	722.2622	-02	46	45	722.8227	06	48	47	723.9127	21
49	48	724.4392	-02	50	49	724.9579	00	52	51	725.9642	03
53	52	726.4537	25	55	54	727.3939	-09	56	55	727.8524	14
58	57	728.7325	06	59	58	729.1565	-00	60	59	729.5734	26
61	60	729.9757	13	63	62	730.7492	-07	64	63	731.1225	07
65	64	731.4777	-52	66	65	731.8349	13	78	79	581.4105	-17
77	78	583.0458	-06	76	77	584.6652	-85	74	75	587.9073	-01
73	74	589.5139	-00	72	73	591.1156	22	69	70	595.8755	64
68	69	597.4375	-25	67	68	598.9951	-87	66	67	600.5595	-09
65	66	602.1080	-18	63	64	605.1870	03	62	63	606.7151	10
61	62	608.2356	15	60	61	609.7425	-42	59	60	611.2513	-06
58	59	612.7505	08	57	58	614.2386	-13	55	56	617.1978	-00
54	55	618.6663	09	53	54	620.1262	09	52	53	621.5770	-06
51	52	623.0270	47	50	51	624.4591	-01	49	50	625.8877	-07
47	48	628.7233	-01	46	47	630.1306	12	45	46	631.5291	18
44	45	632.9176	03	43	44	634.3028	33	42	43	635.6739	02
41	42	637.0419	19	40	41	638.3983	01	39	40	639.7546	62
38	39	641.0924	20	37	38	642.4270	25	36	37	643.7588	84
35	36	645.0693	11	34	35	646.3776	-01	33	34	647.6784	-07
32	33	648.9716	-06	31	32	650.2585	13	29	30	652.8032	11

The infrared radiation emitted from the furnace was introduced through the emission port into a Bruker IFS 120 HR Fourier transform spectrometer. The infrared emission spectrum was recorded with a liquid-helium-cooled Si:B photodetector and a KBr beamsplitter.

The best spectrum was recorded at 1550°C, with 50 scans coadded in about 50 min at a resolution of 0.01 cm^{-1} in the spectral range from 350 to 1000 cm^{-1}. A portion of the infrared emission spectrum of MgF is shown in Fig. 1. Rotational lines are well resolved; however, the spin–rotation splitting in the $X\,^2\Sigma^+$ state was not observed.

TABLE I—*Continued*

N'	N"	Observed	O-C	N'	N"	Observed	O-C	N'	N"	Observed	O-C
28	29	654.0628	09	27	28	655.3139	04	26	27	656.5584	18
25	26	657.7887	-25	24	25	659.0191	15	23	24	660.2364	10
22	23	661.4429	-16	21	22	662.6464	11	20	21	663.8390	16
19	20	665.0220	10	18	19	666.2010	51	15	16	669.6684	-01
14	15	670.8065	-22	13	14	671.9408	07	12	13	673.0607	-20
9	10	676.3753	-21	7	8	678.5425	-03	5	6	680.6787	61
3	4	682.7635	-26	0	1	685.8359	-28				
						v=5-4 band					
6	5	684.5469	-19	8	7	686.4060	10	9	8	687.3247	56
10	9	688.2270	30	11	10	689.1191	-03	12	11	690.0047	-08
14	13	691.7521	25	15	14	692.5991	-83	16	15	693.4565	06
17	16	694.2950	01	18	17	695.1237	-05	20	19	696.7554	09
22	21	698.3504	38	23	22	699.1287	06	24	23	699.8971	-28
25	24	700.6558	-64	26	25	701.4077	-70	27	26	702.1573	-02
28	27	702.8904	-02	29	28	703.6145	06	31	30	705.0304	-06
32	31	705.7224	-26	34	33	707.0828	-03	35	34	707.7454	-19
36	35	708.4024	07	37	36	709.0447	-12	38	37	709.6797	-06
39	38	710.3020	-27	40	39	710.9177	-12	41	40	711.5213	-20
42	41	712.1158	-17	44	43	713.2740	-18	45	44	713.8369	-28
46	45	714.3935	-00	47	46	714.9372	00	48	47	715.4706	00
49	48	715.9917	-20	50	49	716.5057	-10	51	50	717.0092	-02
52	51	717.5011	-07	53	52	717.9843	03	54	53	718.4544	-13
55	54	718.9212	39	56	55	719.3628	-55	57	56	719.8055	-35
58	57	720.2386	-07	59	58	720.6593	01	62	61	721.8552	-08
63	62	722.2343	03	64	63	722.6038	24	65	64	722.9607	24
66	65	723.3058	13	67	66	723.6429	26	68	67	723.9747	93
74	75	580.6992	-04	73	74	582.2912	-06	72	73	583.8757	-14
71	72	585.4540	-14	70	71	587.0270	03	69	70	588.5903	-05
68	69	590.1419	-61	65	66	594.7785	19	64	65	596.3041	-09
63	64	597.8273	10	62	63	599.3357	-44	61	62	600.8510	41
60	61	602.3491	29	59	60	603.8377	-04	58	59	605.3245	18
57	58	606.8049	50	56	57	608.2759	64	54	55	611.1925	61
52	53	614.0758	28	51	52	615.5048	-00	50	51	616.9300	08
49	50	618.3441	-17	48	49	619.7556	08	47	48	621.1586	26
46	47	622.5475	-18	45	46	623.9342	-07	44	45	625.3150	22
43	44	626.6897	69	42	43	628.0455	06	40	41	630.7429	-23
39	40	632.0845	09	38	39	633.4107	-31	37	38	634.7366	05
36	37	636.0536	32	35	36	637.3569	04	34	35	638.6540	-04
33	34	639.9460	16	32	33	641.2268	07	31	32	642.4995	-01
29	30	645.0229	09	28	29	646.2708	01	27	28	647.5050	-61
26	27	648.7424	-09	25	26	649.9680	09	24	25	651.1825	00
23	24	652.3905	11	22	23	653.5869	-09	21	22	654.7801	21
20	21	655.9607	12	19	20	657.1328	04	18	19	658.2963	-05
16	17	660.6013	13	15	16	661.7370	-15	14	15	662.8697	12
12	13	665.1027	03								
						v=6-5					
16	15	685.3322	29	17	16	686.1582	-21	20	19	688.5968	-00
21	20	689.3934	33	22	21	690.1711	-26	23	22	690.9468	-10
26	25	693.2079	-47	27	26	693.9499	16	28	27	694.6795	52
29	28	695.3912	07	30	29	696.0962	-08	31	30	696.7919	-20
32	31	697.4822	12	33	32	698.1597	14	34	33	698.8234	-23
35	34	699.4799	-35	36	35	700.1296	-16	37	36	700.7682	-08
39	38	702.0157	04	40	39	702.6217	-16	42	41	703.8093	-04
43	42	704.3895	15	44	43	704.9568	07	45	44	705.5132	-09
46	45	706.0618	-04	49	48	707.6474	17	51	50	708.6497	-08

III. RESULTS

Rotational spectral lines were measured by using the program PC-DECOMP written by J.W. Brault. Centers of lines were determined by fitting line profiles to Voigt line-shape functions. Rotational lines of HF, which were present in our spectrum as an impurity, were used to calibrate MgF line positions (*15*). The assignment of the MgF spectrum was facilitated by an interactive color Loomis–Wood program. The accuracy of most calibrated line positions is 0.001 cm^{-1}. More than 800 spectral lines of bands from $v = 1 \rightarrow 0$ to $v = 7 \rightarrow 6$ were assigned. The observed MgF line positions are listed in Table I.

TABLE I—*Continued*

N'	N"	Observed	O-C	N'	N"	Observed	O-C	N'	N"	Observed	O-C
68	69	582.9438	-12	67	68	584.4828	14	66	67	586.0107	01
65	66	587.5316	-10	64	65	589.0442	-33	63	64	590.5587	33
60	61	595.0274	-79	58	59	597.9884	29	57	58	599.4413	-83
56	57	600.8968	-95	54	55	603.7967	-07	53	54	605.2286	-31
52	53	606.6566	-19	51	52	608.0792	13	50	51	609.4920	24
49	50	610.8917	-19	47	48	613.6761	-28	45	46	616.4296	-38
44	45	617.8011	19	43	44	619.1599	29	42	43	620.5138	67
41	42	621.8485	-07	40	41	623.1854	18	39	40	624.5086	-13
37	38	627.1400	08	36	37	628.4462	45	35	36	629.7359	-03
34	35	631.0244	16	32	33	633.5717	00	31	32	634.8361	22
30	31	636.0897	17	28	29	638.5722	07	26	27	641.0236	14
25	26	642.2374	23	24	25	643.4387	-07	22	23	645.8311	75
20	21	648.1741	01	19	20	649.3363	-02	16	17	652.7732	01
15	16	653.9010	-04	14	15	655.0115	-97	13	14	656.1248	-76
11	12	658.3297	09	9	10	660.4880	-24	8	9	661.5592	10
3	4	666.7640	-02								
						v=7→6 band					
11	10	673.0389	-20	14	13	675.6197	-26	15	14	676.4693	50
16	15	677.2982	13	17	16	678.1131	-69	18	17	678.9294	-46
20	19	680.5342	05	22	21	682.0955	-00	23	22	682.8607	-15
29	28	687.2610	-12	30	29	687.9619	-00	32	31	689.3374	50
34	33	690.6639	01	35	34	691.3152	02	37	36	692.5890	11
39	38	693.8198	-17	42	41	695.6026	46	44	43	696.7349	23
46	45	697.8246	-25	48	47	698.8829	10	50	49	699.8971	08
51	52	600.7378	-23	50	51	602.1395	01	49	50	603.5309	-01
48	49	604.9164	12	47	48	606.2948	31	46	47	607.6653	47
45	46	609.0162	-54	43	44	611.7246	35	42	43	613.0583	-08
41	42	614.3975	79	39	40	617.0263	-04	37	38	619.6345	20
36	37	620.9274	39	30	31	628.5048	30	24	25	635.7871	-08
23	24	636.9773	39	22	23	638.1512	05	21	22	639.3189	-06
20	21	640.4796	-04	19	20	641.6313	-09	17	18	643.9050	-61
13	14	648.3625	-47	12	13	649.4670	71	7	8	654.7945	12
5	6	656.8656	-00	2	3	659.9051	-32				

a) observed minus calculated in units of 10^{-4} cm^{-1}.

Since spin–rotation splitting was not resolved in the spectrum, the ground state of MgF was treated as if it were a $^1\Sigma^+$ state. Dunham Y_{ij} constants for MgF were obtained by fitting the observed frequencies and available microwave data to the energy expression

$$E(v, N) = \sum_{i,j} Y_{ij}\left(v + \frac{1}{2}\right)^i [N(N+1)]^j.$$

TABLE II

Dunham Coefficients of MgF in cm^{-1}

Y_{ij}	Value
Y_{01}	0.519272510(42)
$10^6\,Y_{02}$	-1.08079(16)
$10^{13}Y_{03}$	1.78(20)
Y_{10}	720.14042(30)
$10^3\,Y_{11}$	-4.717446(43)
$10^9\,Y_{12}$	-3.229(14)
Y_{20}	-4.26018(16)
$10^5\,Y_{21}$	1.7529(10)
$10^{11}Y_{22}$	2.69(27)
$10^2\,Y_{30}$	1.6509(32)
$10^5\,Y_{40}$	-4.19(21)

Pure rotational transitions (*8*) were corrected for the effect of the fine structure and hyperfine structure and included in the final fit. The Dunham coefficients are listed in Table II. The R_e value calculated from Y_{01} is 1.749937(1) Å.

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