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The Infrared Emission Spectrum of Gaseous AlF

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The high-resolution infrared emission spectrum of aluminum monofluoride has been observed with a Fourier transform infrared spectrometer. More than 500 rovibrational lines from bands with $v = 1 \rightarrow 0$ to $v = 5 \rightarrow 4$ were assigned. The infrared data have been combined with previous microwave and millimeter-wave transition frequencies from the literature to yield improved Dunham coefficients for the $X\,^1\Sigma^+$ electronic ground state of AlF. © 1992 Academic Press, Inc.

INTRODUCTION

At high temperatures aluminum monofluoride is easily produced in the gas phase by heating AlF_3 or a mixture of AlF_3 and Al. There is chemical evidence that AlF is the stable constituent of aluminum–fluorine systems at high temperatures (*1*).

AlF has been the subject of numerous spectroscopic studies. The electronic spectra of AlF were recorded both in emission (*2–7*) as well as in absorption (*7–13*). An excellent overview of the electronic spectra was given by Barrow *et al.* (*13*). The microwave spectrum has been intensively studied (*14–18*). A compilation of the data can be found in Huber and Herzberg's book (*19*).

AlF has also been observed to give stimulated infrared emission (laser action) in an exploding wire experiment (*20*). Visible chemiluminescence has been observed from the reaction of Al vapor with various fluorine containing molecules (*21–23*). Dyke *et al.* have reported the photoelectron spectrum (*24*). Recently, Dearden *et al.* (*25*) observed Rydberg states of AlF by using resonance-enhanced multiphoton ionization (REMPI) spectroscopy. In addition there are several excellent ab initio calculations of the molecular properties of the ground and excited states of AlF (*26–28*).

In the infrared region a matrix isolation spectrum (*29*) and a diode laser spectrum (*30*) have been studied in detail. In this work we present the Fourier transform emission spectrum of AlF. The spectrum was "accidentally" found during an attempt to measure the infrared spectrum of MgF_2.

EXPERIMENTAL DETAILS

The high-resolution infrared emission spectrum of AlF was observed with the McMath Fourier transform spectrometer of the National Solar Observatory at Kitt Peak. The unapodized resolution was 0.0055 cm^{-1} with liquid helium cooled As:Si detectors and a KCl beamsplitter. The spectral bandpass was limited to 500–1400 cm^{-1} by an InSb filter for the upper limit and by the detector response and the transmission of the KCl beamsplitter for the lower limit.

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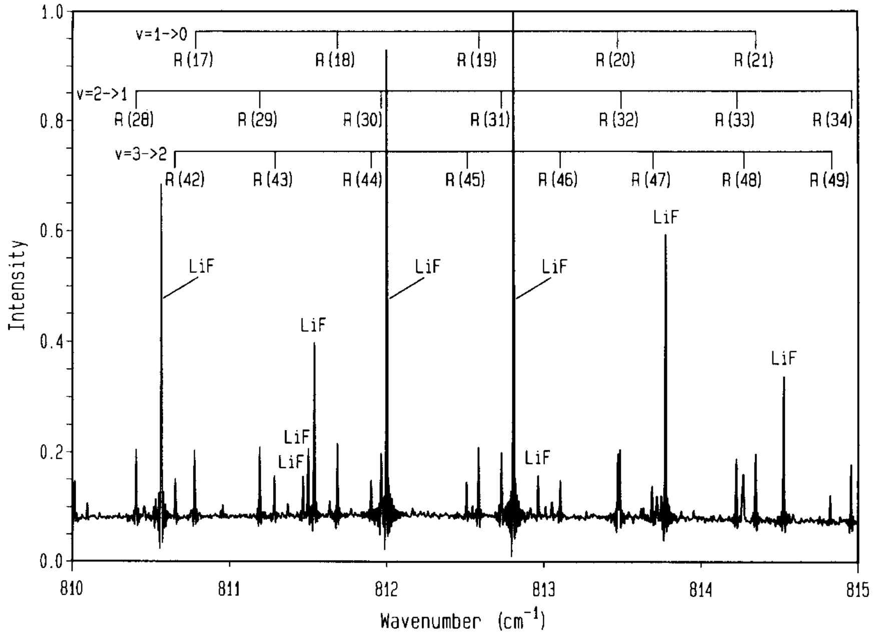

FIG. 1. A portion of the high resolution infrared emission spectrum of AlF and LiF (810–815 cm^{-1}).

Solid MgF_2 was heated to about 1500 K in an alumina tube furnace. The apparatus used was described in detail in the observation of the SiS emission spectrum (*31*). Deposition of solid material onto the KBr windows was avoided by pressurizing the system with 5 Torr of argon. The temperature of the furnace, as measured by a chromel–alumel thermocouple placed between the heating elements and the ceramic tube, was increased at a steady rate of about 5 K/min. A series of spectra were taken as the furnace heated up and then cooled down. Initially a globar was placed behind the tube furnace and its image was focused on the 8-mm aperture of the Fourier transform spectrometer. No absorption spectra were observed, but when the globar was shut off (at a temperature of about 1300 K) a strong emission feature was monitored. At higher temperatures the line intensities increased. The maximum temperature which is accessible with our current oven system is about 1500 K and it was at this temperature that the best emission spectrum was obtained. The emission signal decreased rapidly as the furnace cooled and disappeared at about 1200 K.

RESULTS

The emission features were observed in the region where the infrared spectrum of MgF_2 was expected. However, the high-resolution spectrum showed a pattern typical of a diatomic molecule. After some thought and a literature search, we found that the emission spectrum belonged to LiF (*32*). At higher temperatures MgF_2 could react with water, which is always present in our system, and form HF. Pure rotational lines of HF were observed in the spectrum (*33, 34*). The HF reacted with Li impurities and formed LiF (*33*). After assigning the LiF spectrum, several hundred emission lines with weaker intensities remained (Fig. 1). A literature search showed that these lines belong to AlF (*30*). The explanation for this observation is, presumably, the reaction of HF with the alumina tube at high temperature.

TABLE I

Observed Line Positions of AlF

J'	J''	v'	v''	observed /cm^{-1}	obs.-calc. /10^{-5}cm^{-1}	uncertainty /10^{-5}cm^{-1}	J'	J''	v'	v''	observed /cm^{-1}	obs.-calc. /10^{-5}cm^{-1}	uncertainty /10^{-5}cm^{-1}
78	79	1	0	677.43482	−18	50	16	15	1	0	808.92433	−8	50
77	78	1	0	679.22596	36	50	17	16	1	0	809.85275	3	50
75	76	1	0	682.78345	2	50	18	17	1	0	810.77071	0	50
73	74	1	0	686.31002	11	50	19	18	1	0	811.67840	4	50
72	73	1	0	688.06226	94	100	20	19	1	0	812.57575	12	50
71	72	1	0	689.80437	−44	50	21	20	1	0	813.46176	−76	100
70	71	1	0	691.54065	31	50	22	21	1	0	814.33893	−6	50
68	69	1	0	694.98805	63	100	23	22	1	0	815.20506	5	50
67	68	1	0	696.69845	−46	50	24	23	1	0	816.06076	18	50
65	66	1	0	700.09838	73	100	25	24	1	0	816.90581	16	50
64	65	1	0	701.78458	−26	50	26	25	1	0	817.74025	4	50
63	64	1	0	703.46277	−111	150	27	26	1	0	818.56431	8	50
62	63	1	0	705.13485	12	50	28	27	1	0	819.37905	136	150
61	62	1	0	706.79775	38	50	29	28	1	0	820.18051	−6	50
59	60	1	0	710.09783	−5	50	30	29	1	0	820.97300	16	50
58	59	1	0	711.73608	38	50	31	30	1	0	821.75436	−11	50
57	58	1	0	713.36489	−31	50	32	31	1	0	822.52545	0	50
56	57	1	0	714.98618	−16	50	33	32	1	0	823.28725	150	150
55	56	1	0	716.59894	−15	50	34	33	1	0	824.03544	9	50
54	55	1	0	718.20357	14	50	35	34	1	0	824.77426	4	50
53	54	1	0	719.79962	29	50	36	35	1	0	825.50247	14	50
52	53	1	0	721.38672	−5	50	37	36	1	0	826.21959	−9	50
51	52	1	0	722.96571	1	50	38	37	1	0	826.92619	−3	50
50	51	1	0	724.53589	−22	50	39	38	1	0	827.62204	9	50
49	50	1	0	726.09784	−13	50	40	39	1	0	828.30644	−38	50
48	49	1	0	727.65116	−9	50	41	40	1	0	828.98091	8	50
47	48	1	0	729.19609	16	50	42	41	1	0	829.64395	0	50
46	47	1	0	730.73200	4	50	43	42	1	0	830.29634	18	50
45	46	1	0	732.25917	−17	50	44	43	1	0	830.93756	14	50
43	44	1	0	735.28783	−15	50	45	44	1	0	831.56781	9	50
42	43	1	0	736.78884	−36	50	46	45	1	0	832.18705	1	50
41	42	1	0	738.28170	5	50	47	46	1	0	832.79553	18	50
40	41	1	0	739.76560	31	50	48	47	1	0	833.39272	9	50
39	40	1	0	741.24232	221	250	49	48	1	0	833.97872	−13	50
38	39	1	0	742.70607	−1	50	50	49	1	0	834.55407	7	50
37	38	1	0	744.16322	6	50	51	50	1	0	835.11818	13	50
36	37	1	0	745.61144	11	50	52	51	1	0	835.67093	−4	50
35	36	1	0	747.05044	−13	50	53	52	1	0	836.21271	−4	50
34	35	1	0	748.48096	12	50	54	53	1	0	836.74328	−8	50
33	34	1	0	749.90226	13	50	55	54	1	0	837.26243	−34	50
32	33	1	0	751.31430	−9	50	56	55	1	0	837.77058	−39	50
31	32	1	0	752.71774	12	50	57	56	1	0	838.26800	7	50
30	31	1	0	754.11184	7	50	58	57	1	0	838.75368	4	50
29	30	1	0	755.49681	−2	50	59	58	1	0	839.22807	2	50
28	29	1	0	756.87290	14	50	60	59	1	0	839.69117	0	50
26	27	1	0	759.59695	−19	50	61	60	1	0	840.14289	−6	50
25	26	1	0	760.94616	61	100	62	61	1	0	840.58354	16	50
24	25	1	0	762.28481	9	50	63	62	1	0	841.01219	−25	50
22	23	1	0	764.93689	163	200	64	63	1	0	841.42990	−20	50
20	21	1	0	767.54652	−206	200	65	64	1	0	841.83637	3	50
19	20	1	0	768.84123	3	50	66	65	1	0	842.23102	−12	50
18	19	1	0	770.12428	−16	50	67	66	1	0	842.61446	−2	50
17	18	1	0	771.39831	4	50	68	67	1	0	842.98617	−16	50
16	17	1	0	772.66288	22	50	69	68	1	0	843.34669	2	50
15	16	1	0	773.91731	−27	50	71	70	1	0	844.03287	13	50
14	15	1	0	775.16327	26	50	74	73	1	0	844.97470	−26	50
13	14	1	0	776.39882	−10	50	75	74	1	0	845.26516	−61	100
12	13	1	0	777.62537	8	50	76	75	1	0	845.54396	−97	100
11	12	1	0	778.84203	−6	50	77	76	1	0	845.81285	46	50
10	11	1	0	780.04886	−43	50	78	77	1	0	846.06778	−37	50
9	10	1	0	781.24686	−2	50	79	78	1	0	846.31167	−50	50
8	9	1	0	782.43485	3	50	80	79	1	0	846.54466	22	50
7	8	1	0	783.61295	−14	50	81	80	1	0	846.76431	−63	100
4	5	1	0	787.08965	4	50	83	82	1	0	847.17019	−32	50
3	4	1	0	788.22892	−1	50	87	86	1	0	847.83937	−2	50
1	2	1	0	790.47809	−7	50	88	87	1	0	847.97724	39	50
2	1	1	0	794.85781	−43	50	89	88	1	0	848.10364	129	150
3	2	1	0	795.92846	1	50	90	89	1	0	848.21811	223	200
4	3	1	0	796.98884	16	50	91	90	1	0	848.31932	191	200
6	5	1	0	799.07704	−208	200	76	77	2	1	672.45038	23	50
7	6	1	0	800.10952	24	50	74	75	2	1	675.96306	116	150
8	7	1	0	801.12946	10	50	73	74	2	1	677.70613	3	50
9	8	1	0	802.13956	21	50	72	73	2	1	679.44225	−22	50
10	9	1	0	803.13938	17	50	70	71	2	1	682.89188	24	50
11	10	1	0	804.12905	12	50	69	70	2	1	684.60413	−24	50
13	12	1	0	806.07772	−9	50	67	68	2	1	688.00680	81	100
14	13	1	0	807.03715	22	50	66	67	2	1	689.69453	−29	50
15	14	1	0	807.98443	−138	150	65	66	2	1	691.37525	−37	50

TABLE I—*Continued*

J'	J''	v'	v''	observed $/\mathrm{cm}^{-1}$	obs.-calc. $/10^{-5}\mathrm{cm}^{-1}$	uncertainty $/10^{-5}\mathrm{cm}^{-1}$	J'	J''	v'	v''	observed $/\mathrm{cm}^{-1}$	obs. calc. $/10^{-5}\mathrm{cm}^{-1}$	uncertainty $/10^{-5}\mathrm{cm}^{-1}$
64	65	2	1	693.04865	29	50	34	33	2	1	814.21690	75	100
63	64	2	1	694.71342	40	50	35	34	2	1	814.94776	15	50
62	63	2	1	696.36976	19	50	36	35	2	1	815.66849	11	50
61	62	2	1	698.01830	33	50	38	37	2	1	817.07793	13	50
60	61	2	1	699.65774	−47	50	39	38	2	1	817.76653	13	50
59	60	2	1	701.29036	12	50	40	39	2	1	818.44479	57	50
58	59	2	1	702.91398	−7	50	41	40	2	1	819.11044	−82	100
57	58	2	1	704.52975	15	50	42	41	2	1	819.76737	−10	50
56	57	2	1	706.13673	−13	50	43	42	2	1	820.41286	2	50
55	56	2	1	707.73557	−25	50	44	43	2	1	821.04748	13	50
53	54	2	1	710.90866	−1	50	45	44	2	1	821.66970	−128	150
52	53	2	1	712.48210	−42	50	46	45	2	1	822.28378	9	50
51	52	2	1	714.04762	−32	50	47	46	2	1	822.88535	−12	50
50	51	2	1	715.60477	−13	50	48	47	2	1	823.47610	−19	50
49	50	2	1	717.15297	−42	50	49	48	2	1	824.05620	7	50
48	49	2	1	718.69321	−15	50	50	49	2	1	824.62522	24	50
47	48	2	1	720.22452	−28	50	51	50	2	1	825.18288	9	50
45	46	2	1	723.26203	8	50	52	51	2	1	825.72958	2	50
44	45	2	1	724.76759	−2	50	53	52	2	1	826.26558	32	50
43	44	2	1	726.26461	−2	50	54	53	2	1	826.78997	10	50
42	43	2	1	727.75314	18	50	55	54	2	1	827.30330	−6	50
40	41	2	1	730.70357	7	50	56	55	2	1	827.80566	−5	50
39	40	2	1	732.16551	−14	50	58	57	2	1	828.77687	−3	50
38	39	2	1	733.61902	1	50	59	58	2	1	829.24562	−9	50
37	38	2	1	735.06345	−11	50	60	59	2	1	829.70345	17	50
36	37	2	1	736.49933	6	50	61	60	2	1	830.14943	−17	50
35	36	2	1	737.92630	19	50	62	61	2	1	830.58371	−93	100
34	35	2	1	739.34403	−3	50	63	62	2	1	831.00869	30	50
33	34	2	1	740.75277	−32	50	64	63	2	1	831.42067	−16	50
32	33	2	1	742.15332	14	50	66	65	2	1	832.21145	−20	50
31	32	2	1	743.54412	−17	50	67	66	2	1	832.58987	−12	50
30	31	2	1	744.92638	−1	50	68	67	2	1	832.95700	7	50
29	30	2	1	746.29964	17	50	69	68	2	1	833.31209	−35	50
28	29	2	1	747.66353	3	50	70	69	2	1	833.65620	−29	50
26	27	2	1	750.36431	3	50	72	71	2	1	834.30979	−37	50
25	26	2	1	751.70105	7	50	73	72	2	1	834.61865	−108	100
24	25	2	1	753.02864	12	50	74	73	2	1	834.91828	52	50
23	24	2	1	754.34697	9	50	75	74	2	1	835.20413	−9	50
22	23	2	1	755.65608	6	50	77	76	2	1	835.74396	158	150
21	22	2	1	756.95600	8	50	79	78	2	1	836.23467	64	50
19	20	2	1	759.52805	15	50	82	81	2	1	836.88363	−29	50
18	19	2	1	760.79984	−9	50	87	86	2	1	837.73384	179	200
17	18	2	1	762.06247	−14	50	70	71	3	2	674.35579	89	100
16	17	2	1	763.31584	−8	50	69	70	3	2	676.05402	116	150
15	16	2	1	764.55975	−8	50	68	69	3	2	677.74320	25	50
14	15	2	1	765.79438	6	50	67	68	3	2	679.42516	2	50
13	14	2	1	767.01948	11	50	66	67	3	2	681.09914	−27	50
12	13	2	1	768.23504	10	50	64	65	3	2	684.42469	64	100
11	12	2	1	769.44077	−23	50	63	64	3	2	686.07388	−49	50
10	11	2	1	770.63774	19	50	62	63	3	2	687.71653	−12	50
9	10	2	1	771.82397	−57	50	61	62	3	2	689.35063	−23	50
8	9	2	1	773.00242	46	50	60	61	3	2	690.97715	17	50
7	8	2	1	774.17008	31	50	59	60	3	2	692.59578	82	100
6	7	2	1	775.32756	−40	50	58	59	3	2	694.20516	37	50
3	4	2	1	778.74449	0	50	57	58	3	2	695.80650	6	50
2	3	2	1	779.86366	−25	50	56	57	3	2	697.39945	−42	50
3	2	2	1	786.37378	−93	100	55	56	3	2	698.98493	−13	50
6	5	2	1	789.49700	27	50	54	55	3	2	700.56180	−18	50
7	6	2	1	790.51745	−3	50	53	54	3	2	702.13048	−13	50
8	7	2	1	791.52866	44	50	52	53	3	2	703.69052	−39	50
9	8	2	1	792.52885	−9	50	51	52	3	2	705.24344	59	50
12	11	2	1	795.47065	−1	50	50	51	3	2	706.78537	−105	100
13	12	2	1	796.43114	13	50	49	50	3	2	708.32135	−22	50
14	13	2	1	797.38225	104	100	47	48	3	2	711.36678	25	50
15	14	2	1	798.32116	−8	50	46	47	3	2	712.87613	−15	50
17	16	2	1	800.17100	34	50	45	46	3	2	714.37776	24	50
18	17	2	1	801.07990	−11	50	44	45	3	2	715.87025	5	50
19	18	2	1	801.97920	11	50	43	44	3	2	717.35418	−13	50
20	19	2	1	802.86794	7	50	42	43	3	2	718.83004	23	50
21	20	2	1	803.74630	−3	50	41	42	3	2	720.29672	4	50
22	21	2	1	804.61392	−53	50	39	40	3	2	723.20460	19	50
23	22	2	1	805.47231	12	50	38	39	3	2	724.64604	82	100
24	23	2	1	806.31954	0	50	37	38	3	2	726.07705	−23	50
25	24	2	1	807.15658	11	50	36	37	3	2	727.50052	−6	50
27	26	2	1	808.79909	10	50	35	36	3	2	728.91460	−48	50
28	27	2	1	809.60458	5	50	34	35	3	2	730.32057	−19	50
29	28	2	1	810.39970	15	50	33	34	3	2	731.71751	−7	50
30	29	2	1	811.18411	7	50	32	33	3	2	733.10552	−1	50
31	30	2	1	811.95798	1	50	31	32	3	2	734.48458	0	50
32	31	2	1	812.72130	−1	50	30	31	3	2	735.85486	17	50
33	32	2	1	813.47359	−46	50	29	30	3	2	737.21579	−6	50

TABLE I—*Continued*

J'	J''	v'	v''	observed /cm^{-1}	obs.-calc. /10^{-5}cm^{-1}	uncertainty /10^{-5}cm^{-1}
28	29	3	2	738.56832	30	50
27	28	3	2	739.91264	146	150
25	26	3	2	742.57026	−10	50
24	25	3	2	743.88636	3	50
23	24	3	2	745.19298	−20	50
22	23	3	2	746.49095	6	50
21	22	3	2	747.77927	−16	50
20	21	3	2	749.05838	−39	50
19	20	3	2	750.32875	−13	50
18	19	3	2	751.59103	128	150
17	18	3	2	752.84140	5	50
16	17	3	2	754.08369	5	50
15	16	3	2	755.31684	23	50
14	15	3	2	756.54018	−4	50
13	14	3	2	757.75528	82	100
12	13	3	2	758.95904	−25	50
11	12	3	2	760.15536	67	100
10	11	3	2	761.34027	−37	50
9	10	3	2	762.51723	13	50
8	9	3	2	763.68384	−22	50
7	8	3	2	764.84196	48	50
5	6	3	2	767.12741	−22	50
3	4	3	2	769.37474	−60	100
3	2	3	2	776.93717	42	50
5	4	3	2	779.00917	15	50
7	6	3	2	781.04257	83	100
10	9	3	2	784.01576	−51	50
11	10	3	2	784.98779	−1	50
13	12	3	2	786.90061	−13	50
14	13	3	2	787.84212	3	50
16	15	3	2	789.69435	−12	50
17	16	3	2	790.60513	−32	50
18	17	3	2	791.50637	13	50
19	18	3	2	792.39723	40	50
20	19	3	2	793.27717	−3	50
21	20	3	2	794.14719	−12	50
22	21	3	2	795.00646	−70	100
23	22	3	2	795.85660	−10	50
24	23	3	2	796.69606	13	50
25	24	3	2	797.52497	16	50
26	25	3	2	798.34362	30	50
27	26	3	2	799.15164	21	50
28	27	3	2	799.94932	19	50
30	29	3	2	801.51430	111	150
31	30	3	2	802.27938	−12	50
32	31	3	2	803.03525	−5	50
33	32	3	2	803.78054	−2	50
34	33	3	2	804.51530	3	50
35	34	3	2	805.24087	148	150
36	35	3	2	805.95316	25	50
37	36	3	2	806.65564	−17	50
38	37	3	2	807.34783	−22	50
39	38	3	2	808.02969	7	50
40	39	3	2	808.70122	73	100
41	40	3	2	809.36083	18	50
42	41	3	2	810.00993	−12	50
43	42	3	2	810.64848	−22	50
44	43	3	2	811.27665	10	50
45	44	3	2	811.89350	−9	50
46	45	3	2	812.49943	−37	50
47	46	3	2	813.09517	2	50
48	47	3	2	813.67923	−39	50
50	49	3	2	814.81565	−17	50
52	51	3	2	815.90804	−19	50
53	52	3	2	816.43823	27	50
54	53	3	2	816.95678	11	50
56	55	3	2	817.96088	−7	50
57	56	3	2	818.44479	−169	200
58	57	3	2	818.92125	35	50
60	59	3	2	819.83597	−36	50
61	60	3	2	820.27786	56	50
62	61	3	2	820.70707	−1	50
63	62	3	2	821.12589	26	50
64	63	3	2	821.53326	31	50
65	64	3	2	821.92875	−26	50
66	65	3	2	822.31400	22	50
67	66	3	2	822.68807	82	100
68	67	3	2	823.04887	−52	50
65	66	4	3	674.26592	−129	150
58	59	4	3	685.60578	−141	150
57	58	4	3	687.19437	−60	100
56	57	4	3	688.77412	−49	50
55	56	4	3	690.34589	−19	50
54	55	4	3	691.90964	28	50
52	53	4	3	695.01118	−2	50
51	52	4	3	696.54947	−24	50
50	51	4	3	698.07969	−23	50
49	50	4	3	699.60197	19	50
48	49	4	3	701.11450	−78	100
47	48	4	3	702.62049	11	50
46	47	4	3	704.11752	46	50
45	46	4	3	705.60530	1	50
44	45	4	3	707.08496	−8	50
43	44	4	3	708.55671	42	50
42	43	4	3	710.01889	−11	50
41	42	4	3	711.47306	−9	50
40	41	4	3	712.91884	13	50
39	40	4	3	714.35579	13	50
38	39	4	3	715.78388	−8	50
37	38	4	3	717.20358	−1	50
36	37	4	3	718.61503	50	50
35	36	4	3	720.01628	−45	50
34	35	4	3	721.41019	0	50
33	34	4	3	722.79466	−20	50
32	33	4	3	724.17057	−16	50
31	32	4	3	725.53813	36	50
30	31	4	3	726.89643	49	50
29	30	4	3	728.24516	−7	50
28	29	4	3	729.58562	2	50
27	28	4	3	730.91683	−20	50
26	27	4	3	732.23928	−22	50
25	26	4	3	733.55288	−9	50
24	25	4	3	734.85776	34	50
23	24	4	3	736.15302	20	50
22	23	4	3	737.43936	21	50
21	22	4	3	738.71672	34	50
20	21	4	3	739.98448	0	50
19	20	4	3	741.24232	−111	150
18	19	4	3	742.49312	−8	50
17	18	4	3	743.73367	−10	50
15	16	4	3	746.18751	32	50
14	15	4	3	747.39976	−23	50
12	13	4	3	749.79783	20	50
11	12	4	3	750.98130	−113	150
10	11	4	3	752.15799	15	50
9	10	4	3	753.32391	7	50
8	9	4	3	754.48018	−22	50
6	7	4	3	756.76573	62	100
7	6	4	3	771.68220	83	100
9	8	4	3	773.65600	−6	50
10	9	4	3	774.62886	32	50
12	11	4	3	776.54358	−10	50
13	12	4	3	777.48636	8	50
14	13	4	3	778.41879	−9	50
17	16	4	3	781.15662	25	50
19	18	4	3	782.93097	9	50
20	19	4	3	783.80271	−20	50
21	20	4	3	784.66476	−1	50
22	21	4	3	785.51632	−11	50
23	22	4	3	786.35760	−26	50
25	24	4	3	788.00991	−4	50
26	25	4	3	788.82034	−22	50
27	26	4	3	789.62131	45	50
28	27	4	3	790.41129	48	50
29	28	4	3	791.19056	16	50
30	29	4	3	791.95910	−49	50
31	30	4	3	792.71825	−12	50
32	31	4	3	793.46681	10	50
33	32	4	3	794.20482	22	50
34	33	4	3	794.93181	−19	50
35	34	4	3	795.64934	45	50
36	35	4	3	796.35529	3	50
37	36	4	3	797.05074	−33	50
38	37	4	3	797.73594	−36	50
39	38	4	3	798.41048	−46	50
41	40	4	3	799.72849	17	50
42	41	4	3	800.37091	−11	50
43	42	4	3	801.00353	50	50
45	44	4	3	802.23419	−70	100
46	45	4	3	802.83435	−34	50
47	46	4	3	803.42318	−53	50
48	47	4	3	804.00188	−5	50

TABLE I—*Continued*

J'	J''	v'	v''	observed /cm^{-1}	obs.-calc. /$10^{-5}cm^{-1}$	uncertainty /$10^{-5}cm^{-1}$
49	48	4	3	804.56925	−7	50
51	50	4	3	805.67146	−7	50
52	51	4	3	806.20624	−7	50
53	52	4	3	806.72980	−37	50
54	53	4	3	807.24320	11	50
55	54	4	3	807.74505	0	50
56	55	4	3	808.23530	−72	100
60	59	4	3	810.08994	28	50
62	61	4	3	810.95076	76	100
66	65	4	3	812.53725	38	50
68	67	4	3	813.26274	−30	50
69	68	4	3	813.60946	22	50
54	55	5	4	683.36754	−26	50
51	52	5	4	687.96765	−13	50
50	51	5	4	689.48564	98	100
49	50	5	4	690.99347	19	50
46	47	5	4	695.46905	−21	50
45	46	5	4	696.94490	37	50
42	43	5	4	701.32026	46	50
41	42	5	4	702.76167	38	50
40	41	5	4	704.19339	−86	100
38	39	5	4	707.03438	−13	50
35	36	5	4	711.22931	−104	100
34	35	5	4	712.61214	51	50
33	34	5	4	713.98411	−10	50
32	33	5	4	715.34709	−96	100
31	32	5	4	716.70303	−9	50
30	31	5	4	718.04953	12	50
29	30	5	4	719.38701	13	50
28	29	5	4	720.71452	−99	100
27	28	5	4	722.03565	38	50
24	25	5	4	725.94266	161	200
23	24	5	4	727.22482	−25	50
22	23	5	4	728.50129	122	150
17	18	5	4	734.73822	−94	100
13	14	5	4	739.56521	−50	50
11	12	5	4	741.92314	−36	50
10	11	5	4	743.08763	−81	100
9	10	5	4	744.24444	40	50

The spectral analysis program PC-DECOMP, developed by J. W. Brault, was used for data analysis. The rotational line profiles were fit to Voigt lineshape functions. The strong lines show a "ringing" caused by the sin x/x lineshape function of the

TABLE II

Dunham Coefficients for AlF in cm^{-1}

constant	this work	Ref. *(30)*
Y_{10}	802.323 85 (15)	802.324 30 (148)
Y_{20}	−4.849 536 (98)	−4.849 45 (90)
Y_{30}	0.019 497 (24)	0.019 312 (157)
$10^3\ Y_{40}$	−0.029 5 (20)	
Y_{01}	0.552 480 296 (49)	0.552 480 075 (151)
$10^3\ Y_{11}$	−4.984 214 (60)	−4.984 385 (248)
$10^3\ Y_{21}$	0.017 153 (22)	0.017 274 (124)
$10^6\ Y_{31}$	0.050 3 (24)	0.033 1 (178)
$10^6\ Y_{02}$	−1.048 280 (68)	−1.046 651 (424)
$10^9\ Y_{12}$	1.854 8 (80)	1.700 5 (289)
$10^9\ Y_{22}$	0.060 1 (19)	0.068 9 (37)
$10^{12}\ Y_{03}$	−0.305 0 (93)	

Fourier transform spectrometer. The ringing was eliminated by using the "filter fitting" routine available in PC-DECOMP. The signal-to-noise ratio for the strongest lines belonging to the fundamental band of AlF was about 50 and the resulting resolution-enhanced linewidth was 0.0005 cm^{-1}. Pure rotational lines of HF were used for absolute calibration ($\pm 0.0002\ \mathrm{cm}^{-1}$) of the spectrum (*34*). For this calibration the HF absorption lines, taken in a spectrum at lower temperature, were calibrated against CO_2 (*35*). The AlF line positions are listed in Table I.

Bands with $v = 1 \rightarrow 0$ to $v = 5 \rightarrow 4$ of AlF were picked out by using an interactive color Loomis–Wood program which runs on a 486/33 MHz microcomputer. Data reduction was made by using the well known Dunham equation (*36*)

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

Pure rotational transitions (*16*, *17*) were corrected for the effect of hyperfine structure and included in the final fit. The Dunham coefficients are shown in Table II.

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REFERENCES

1. P. GROSS, C. HAYMAN, AND D. L. LEVY, *Trans. Faraday Soc.* **50**, 477–480 (1954).
2. T. YUASA, *Soc. Reports Tokyo Bunrika Daigaku* **3**, 239 (1938).
3. H. C. ROWLINSON AND R. F. BARROW, *Proc. Phys. Soc. London, Sect. A* **66**, 437–446 (1953).
4. H. C. ROWLINSON AND R. F. BARROW, *Proc. Phys. Soc. London, Sect. A* **66**, 772–773 (1953).
5. P. G. DODSWORTH AND R. F. BARROW, *Proc. Phys. Soc. London, Sect. A* **68**, 824–828 (1955).
6. J. M. BROWN, I. KOPP, C. MALMBERG, AND B. RYDH, *Phys. Scr.* **17**, 55–67 (1978).
7. R. F. BARROW, J. W. C. JOHNS, AND F. J. SMITH, *Trans. Faraday Soc.* **52**, 913–916 (1956).
8. G. D. ROCHESTER, *Phys. Rev.* **56**, 305–307 (1939).
9. S. M. NAUDÉ AND T. J. HUGO, *Can. J. Phys.* **31**, 1106–1114 (1953).
10. S. M. NAUDÉ AND T. J. HUGO, *Can. J. Phys.* **32**, 246–258 (1954).
11. S. M. NAUDÉ AND T. J. HUGO, *Can. J. Phys.* **33**, 573–574 (1955).
12. S. M. NAUDÉ AND T. J. HUGO, *Can. J. Phys.* **35**, 64–70 (1957).
13. R. F. BARROW, I. KOPP, AND C. MALMBERG, *Phys. Scr.* **10**, 86–102 (1974).
14. D. R. LIDE, JR., *J. Chem. Phys.* **38**, 2027 (1963).
15. D. R. LIDE, JR., *J. Chem. Phys.* **42**, 1013–1018 (1964).
16. F. C. WYSE, W. GORDY, AND E. F. PEARSON, *J. Chem. Phys.* **52**, 3887–3889 (1970).
17. J. HOEFT, F. J. LOVAS, E. TIEMANN, AND T. TÖRRING, *Z. Naturforsch. A: Astrophys. Phys. Phys. Chem.* **25**, 1029–1035 (1970).
18. R. HONERJÄGER AND R. TISCHER, *Z. Naturforsch. A: Phys. Phys. Chem. Kosmophys.* **29**, 342–345 (1974).
19. G. HERZBERG AND K. P. HUBER, "Molecular Spectra and Molecular Structure IV. Constants of Diatomic Molecules," Van Nostrand–Reinhold, New York, 1979.
20. W. W. RICE AND R. J. JENSEN, *Appl. Phys. Lett.* **22**, 67–68 (1973).
21. S. ROSENWAKS, R. E. STEELE, AND H. P. BROIDA, *Chem. Phys. Lett.* **38**, 121–124 (1976).
22. S. ROSENWAKS, *J. Chem. Phys.* **65**, 3668–3673 (1976).

23. T. Ishikawa and J. M. Parson, *J. Chem. Phys.* **79,** 4261-4270 (1983).

24. J. M. Dyke, C. Kirby, A. Morris, B. W. J. Gravenor, R. Klein, and P. Rosmus, *Chem. Phys.* **88,** 289-298 (1984).

25. D. V. Dearden, R. D. Johnson III, and J. W. Hudgens, *J. Phys. Chem.* **95,** 4291-4296 (1991).

26. R. Klein and P. Rosmus, *Theor. Chim. Acta* **66,** 21-29 (1984).

27. D. M. Hirst, *J. Mol. Spectrosc.* **121,** 189-198 (1987).

28. S. R. Langhoff, C. W. Bauschlicher, Jr., and P. R. Taylor, *J. Chem. Phys.* **88,** 5715-5725 (1988).

29. A. Snelson, *J. Phys. Chem.* **71,** 3202-3207 (1967).

30. A. G. Maki and F. J. Lovas, *J. Mol. Spectrosc.* **95,** 80-91 (1982).

31. C. I. Frum, R. Engleman, Jr., and P. F. Bernath, *J. Chem. Phys.* **93,** 5457-5461 (1990).

32. A. G. Maki, *J. Mol. Spectrosc.* **102,** 361-367 (1983).

33. H. G. Hedderich, C. I. Frum, R. Engleman, Jr., and P. F. Bernath, *Can. J. Chem.*, **69,** 1659-1671 (1991).

34. H. G. Hedderich, K. Walker, and P. F. Bernath, *J. Mol. Spectrosc.* **149,** 314-316 (1991).

35. G. Guelachvili and K. Narahari Rao, "Handbook of Infrared Standards," Academic Press, Orlando, FL, 1986.

36. J. L. Dunham, *Phys. Rev.* **41,** 721-731 (1932).