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Infrared Emission Spectrum of KF

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The high-resolution infrared emission spectrum of potassium monofluoride has been recorded with a Fourier transform spectrometer. Over 900 vibration–rotation transitions, from the $v = 1 \rightarrow 0$ to the $v = 8 \rightarrow 7$ vibrational bands, have been assigned. Improved spectroscopic constants have been obtained for the KF ground electronic state by combining the infrared measurements with the existing microwave data.

INTRODUCTION

The KF molecule has been extensively studied by many different spectroscopic methods. Early high resolution studies include molecular beam electric resonance experiments (*1–4*), and millimeter-wave molecular beam spectroscopy (*5*). The low resolution infrared absorption measurements of KF vapor (*6, 7*) and matrix isolation spectra of the monomer and dimer were published (*8, 9*). Improved vibrational constants were obtained in an infrared diode laser study (*10*) of the $v = 2 \leftarrow 0$, $3 \leftarrow 1$ and $4 \leftarrow 2$ overtones. By combining a small number of infrared measurements with the existing microwave data, Maki and Lovas (*10*) obtained a reliable set of Dunham constants. Recent experimental measurements on KF include a measurement of the spontaneous vibrational decay rates (*11*), electron diffraction (*12*), and a more extensive measurement of the hyperfine structure (*13*).

The KF molecule has also been the target of several *ab initio* calculations of molecular properties such as the dissociation energy (*14*). More recently, Modisette *et al.* (*15*), reported a calculation of the electronic structure using the increasingly popular density functional approach, while Garcia–Cuesta *et al.* (*16*) used large basis sets and extensive electron correlation. Dyall and Partridge (*17*) explored the effects of relativistic corrections to the properties of alkali fluorides.

In the work reported here we have made the first high resolution measurements of the fundamental ($v = 1 \rightarrow 0$) vibration–rotation band and related hot bands by infrared emission spectroscopy with a Fourier transform spectrometer. High resolution Fourier transform data are now available for the entire nonradioactive alkali fluoride family, LiF (*18*), NaF (*19*), KF (this work), RbF (*20*), and CsF (*20*).

EXPERIMENTAL DETAILS

The high resolution infrared emission spectrum of KF has been recorded with a Bruker IFS 120 HR Fourier transform spectrometer. The technique used has been described previously in, for example, our paper on NaF (*19*). The KF spectrum was recorded at 900°C with a resolution of 0.01 cm^{-1} over the range 350–750 cm^{-1} with a 3.5-μm-thick Mylar beamsplitter. The final recording consisted of 50 coadded scans. A portion of the spectrum is displayed in Fig. 1.

RESULTS AND DISCUSSION

Although potassium has three natural isotopes, ^{39}K (93.26%), ^{40}K (0.01%), and ^{41}K (6.73%), only the main isotope was observed in this experiment. Over 900 transitions were observed and analyzed. The assignment of the rotational lines was based on the previous constants found in the literature (*10*). The position of the lines was calibrated in accordance with the strong pure rotational HF lines (*21, 22*) that appeared in the spectrum. Eight vibrational bands

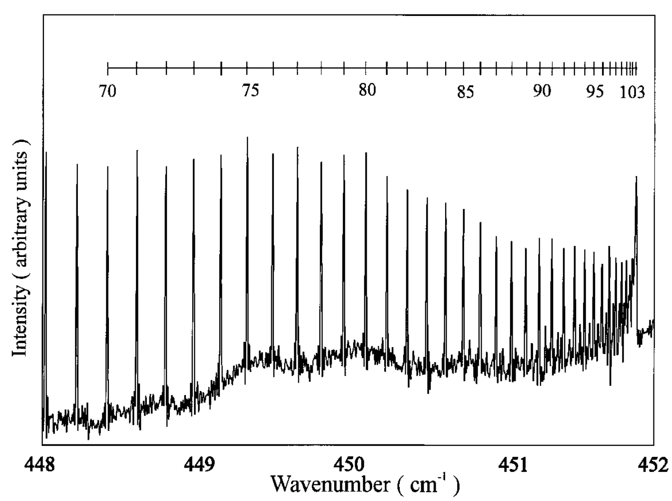

FIG. 1. A portion of the *R* branch of the vibration–rotation spectrum of KF. The lines of the 1–0 band are marked with their J'' values.

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TABLE 1

Observed Rovibrational Line Positions of the $X\ ^1\Sigma^+$ State of KF in cm^{-1} (Observed—Calculated Values in Units of $10^{-3}\ cm^{-1}$ Are Shown in the Column Labeled Δ)

1-0 band				2-1 band				3-2 band			
J'	J''	Observed	Δ	J'	J''	Observed	Δ	J'	J''	Observed	Δ
57	58	381.7618	0.46	52	53	381.2055	-0.17	46	47	381.2909	-3.62
56	57	382.5647	0.52	51	52	381.9823	0.01	45	46	382.0413	0.13
55	56	383.3612	-1.77	50	51	382.7548	-0.18	44	45	382.7844	0.73
54	55	384.1579	0.03	49	50	383.5227	-1	43	44	383.5227	0.58
53	54	384.9471	-1.65	47	48	385.0486	-0.35	42	43	384.2564	-0.08
52	53	385.7347	-0.89	46	47	385.8068	1.29	41	42	384.9876	0.77
51	52	386.5179	-0.47	45	46	386.5578	-0.26	40	41	385.7131	0.04
50	51	387.3011	3.92	43	44	388.0510	0.15	39	40	386.4368	1.59
49	50	388.0706	-1.34	42	43	388.7908	-0.21	38	39	387.1530	-0.15
48	49	388.8426	0	41	42	389.5284	1.21	37	38	387.8674	0.32
47	48	389.6101	0.8	40	41	390.2600	0.75	36	37	388.5773	0.46
46	47	390.3720	0.16	39	40	390.9874	0.32	35	36	389.2811	-1.25
45	46	391.1304	0.12	38	39	391.7109	0.03	34	35	389.9848	1.01
44	45	391.8847	0.06	37	38	392.4298	-0.61	33	34	390.6799	-1.2
43	44	392.6352	0.36	36	37	393.1462	0.34	32	33	391.3750	0.84
42	43	393.3800	-0.95	35	36	393.8566	-0.49	31	32	392.0627	-0.33
41	42	394.1229	-0.08	34	35	394.5643	0.14	30	31	392.7474	-0.26
40	41	394.8616	0.78	33	34	395.2675	0.51	29	30	393.4279	-0.22
39	40	395.5934	-1.04	32	33	395.9655	-0.08	28	29	394.1034	-0.89
38	39	396.3238	-0.09	31	32	396.6592	-0.8	27	28	394.7766	0.38
37	38	397.0487	-0.49	30	31	397.3497	-0.48	26	27	395.4450	1.04
36	37	397.7705	0.14	29	30	398.0348	-1.22	25	26	396.1078	0.41
35	36	398.4877	0.52	28	29	398.7179	0.19	24	25	396.7658	-0.71
34	35	399.2001	0.23	27	28	399.3953	0.29	23	24	397.4207	-0.65
33	34	399.9078	-0.52	26	27	400.0679	-0.23	22	23	398.0721	0.19
32	33	400.6129	0.34	25	26	400.7371	0.14	21	22	398.7179	-0.23
31	32	401.3129	0.39	24	25	401.4019	0.52	20	21	399.3608	0.76
30	31	402.0083	0.18	23	24	402.0617	0.16	19	20	399.9975	-0.07
29	30	402.7000	0.49	22	23	402.7167	-0.63	18	19	400.6296	-1.17
28	29	403.3858	-0.87	21	22	403.3692	0.34	17	18	401.2601	0.47
27	28	404.0694	-0.06	20	21	404.0156	-0.34	16	17	401.8842	0.1
26	27	404.7476	-0.34	19	20	404.6592	0.57	15	16	402.5049	0.76
25	26	405.4221	0.05	18	19	405.2969	-0.09	14	15	403.1195	-0.28
24	25	406.0913	-0.58	17	18	405.9307	-0.31	13	14	403.7317	0.64
23	24	406.7569	-0.47	16	17	406.5607	0.14	12	13	404.3383	0.35
22	23	407.4185	0.06	15	16	407.1857	-0.02	11	12	404.9406	0.29
21	22	408.0750	-0.11	14	15	407.8071	0.64	10	11	405.5385	0.23
20	21	408.7276	0.06	13	14	408.4235	0.82	9	10	406.1316	-0.18
19	20	409.3754	-0.03	12	13	409.0337	-0.8	8	9	406.7202	-0.63
18	19	410.0191	0.17	11	12	409.6421	0.2	7	8	407.3062	0.84
17	18	410.6582	0.16	10	11	410.2448	-0.03	6	7	407.8831	-2.39
16	17	411.2944	1.64	9	10	410.8431	-0.09	5	6	408.4615	0.46
15	16	411.9235	0.46	8	9	411.4370	-0.14	4	5	409.0337	1.69
14	15	412.5479	-0.86	7	8	412.0271	0.56	3	4	409.5975	-1.08
13	14	413.1671	-3.04	6	7	412.6110	-0.43	2	3	410.1631	2.56
12	13	413.7869	-0.02	5	6	413.1918	0.07	2	1	412.9019	-0.03
11	12	414.3984	-0.9	4	5	413.7660	-1.54	3	2	413.4350	-1.41
10	11	415.0087	1.58	3	4	414.3379	-0.86	4	3	413.9693	3.03
9	10	415.6102	-0.19	2	3	414.9049	-0.49	5	4	414.4909	-0.6
8	9	416.2090	-0.22	1	2	415.4689	1.32	6	5	415.0087	-3.42
7	8	416.7998	-3.65	3	2	418.2085	-0.39	7	6	415.5280	-0.09
6	7	417.3930	-0.16	4	3	418.7436	0.38	8	7	416.0397	0.43
5	6	417.9784	0.01	5	4	419.2728	-0.13	9	8	416.5465	0.58
4	5	418.5588	-0.18	6	5	419.7978	-0.26	10	9	417.0474	-0.37
3	4	419.1361	1.14	7	6	420.3181	-0.23	11	10	417.5451	0.05
2	3	419.7059	-0.42	8	7	420.8340	-0.01	12	11	418.0342	-3.3
0	1	420.8340	-1.27	10	9	421.8513	0.12	13	12	418.5257	0.39
3	2	423.0385	0.92	11	10	422.3526	-0.08	14	13	419.0083	-0.02
4	3	423.5756	-0.86	12	11	422.8494	-0.03	15	14	419.4901	3.47
5	4	424.1103	-0.37	13	12	423.3415	0.05	16	15	419.9602	0.08
6	5	424.6397	-0.51	14	13	423.8293	0.56	17	16	420.4297	0.82
7	6	425.1641	-0.88	15	14	424.3110	-0.17	18	17	420.8932	0.4
8	7	425.6789	-6.19	16	15	424.7891	0.22	19	18	421.3494	-2.56
9	8	426.1955	-4.94	17	16	425.2647	2.92	20	19	421.8066	0.2
10	9	426.7109	-0.12	18	17	425.7299	0.05	21	20	422.2559	-0.01
11	10	427.2166	-0.25	19	18	426.1955	2.41	22	21	422.7005	-0.11

1-0 band				2-1 band				3-2 band			
J'	J''	Observed	Δ	J'	J''	Observed	Δ	J'	J''	Observed	Δ
12	11	427.7177	-0.21	20	19	426.6514	-0.03	23	22	423.1407	0.14
13	12	428.2142	-0.02	21	20	427.1051	0.08	24	23	423.5756	0.02
14	13	428.7057	-0.01	22	21	427.5538	0.03	25	24	424.0063	0.59
15	14	429.1938	1.39	23	22	427.9975	-0.07	26	25	424.4311	0.09
16	15	429.6726	-1.64	24	23	428.4362	-0.36	27	26	424.8511	-0.38
17	16	430.1525	1.22	25	24	428.8707	0.06	28	27	425.2647	-2.32
18	17	430.6235	-0.06	26	25	429.2998	0.05	29	28	425.6789	1.28
19	18	431.0910	0.15	27	26	429.7238	-0.23	30	29	426.0831	-0.18
20	19	431.5535	0.09	28	27	430.1443	0.91	31	30	426.4839	-0.15
21	20	432.0108	-0.23	29	28	430.5595	1.74	32	31	426.8799	-0.03
22	21	432.4636	-0.1	30	29	430.9673	0.05	33	32	427.2710	0.21
23	22	432.9114	-0.11	31	30	431.3714	-0.29	34	33	427.6566	-0.02
24	23	433.3544	-0.06	32	31	431.7711	-0.06	35	34	428.0376	0.02
25	24	433.7923	-0.15	33	32	432.1652	-0.54	36	35	428.4144	0.87
26	25	434.2258	0.23	34	33	432.5551	-0.15	37	36	428.7843	-0.17
27	26	434.6536	-0.15	35	34	432.9398	0.03	38	37	429.1504	-0.01
28	27	435.0765	-0.44	36	35	433.3192	-0.07	39	38	429.5120	0.64
30	29	435.9066	-1.7	37	36	433.6940	0.17	40	39	429.8670	-0.23
31	30	436.3166	-0.01	38	37	434.0632	-0.05	41	40	430.2194	1.38
32	31	436.7206	0.74	39	38	434.4276	-0.04	42	41	430.5653	1.45
33	32	437.1185	0.43	40	39	434.7870	0.02	43	42	430.9045	0
34	33	437.5112	-0.05	41	40	435.1388	-2.4	44	43	431.2404	0.2
35	34	437.8994	-0.11	42	41	435.4871	-3.33	45	44	431.5700	-0.73
36	35	438.2823	-0.34	43	42	435.8348	0.28	46	45	431.8963	0.12
37	36	438.6605	-0.16	44	43	436.1733	-0.12	47	46	432.2162	-0.25
38	37	439.0337	0.01	45	44	436.5079	0.62	48	47	432.5316	-0.08
39	38	439.3995	-2.15	46	45	436.8360	0.01	49	48	432.8418	-0.03
40	39	439.7645	0	47	46	437.1602	0.54	50	49	433.1468	0.1
41	40	440.1222	-0.01	48	47	437.4782	0.14	51	50	433.4464	-0.09
42	41	440.4749	0.04	49	48	437.7915	0.16	52	51	433.7411	-0.04
43	42	440.8222	-0.12	50	49	438.0996	0.18	53	52	434.0302	-0.35
44	43	441.1650	0.38	51	50	438.4033	0.97	54	53	434.3148	0
45	44	441.5019	0.04	52	51	438.7000	0	55	54	434.5938	0
46	45	441.8340	0.13	53	52	438.9926	0.07	56	55	434.8653	-2.39
47	46	442.1608	0.02	54	53	439.2799	0.11	56	55	434.8698	2.09
48	47	442.4837	1.2	55	54	439.5621	0.22	57	56	435.1388	2.57
49	48	442.7989	-0.05	56	55	439.8406	2.01	58	57	435.3980	-1.6
50	49	443.1103	0.03	57	56	440.1099	-0.29	59	58	435.6579	0.1
51	50	443.4163	0.01	58	57	440.3756	-0.87	60	59	435.9109	0.29
52	51	443.7172	0.02	59	58	440.6375	0.06	61	60	436.1586	0.33
53	52	444.0128	0	60	59	440.8932	0.01	62	61	436.4006	0
54	53	444.3032	0.08	61	60	441.1440	0.38	63	62	436.6373	-0.26
55	54	444.5850	-3.2	62	61	441.3888	0.03	64	63	436.8688	-0.51
56	55	444.8681	0.04	63	62	441.6293	0.8	65	64	437.0959	0.12
57	56	445.1425	-0.09	64	63	441.8629	-0.11	66	65	437.3165	-0.38
58	57	445.4128	1.03	65	64	442.0937	1.63	67	66	437.5325	-0.1
59	58	445.6756	-0.17	66	65	442.3167	0.84	68	67	437.7429	-0.14
60	59	445.9343	0.01	67	66	442.5341	-0.13	69	68	437.9477	-0.34
61	60	446.1877	0.12	68	67	442.7474	0.12	70	69	438.1475	-0.26
62	61	446.4352	-0.33	69	68	442.9547	-0.14	71	70	438.3420	-0.06
63	62	446.6782	0.08	70	69	443.1570	-0.13	72	71	438.5308	-0.21
64	63	446.9155	0.17	71	70	443.3537	-0.2	73	72	438.7147	0.19
65	64	447.1472	0.04	72	71	443.5451	-0.19	74	73	438.8926	-0.08
66	65	447.3737	0.04	73	72	443.7313	0.01	75	74	439.0650	-0.32
67	66	447.5948	0.13	74	73	443.9117	-0.08	76	75	439.2324	-0.16
68	67	447.8103	0	75	74	444.0866	-0.26	78	77	439.5499	-0.81
69	68	448.0207	0.12	76	75	444.2561	-0.36	79	78	439.7015	-0.09
70	69	448.2220	-3.3	77	76	444.4205	-0.07	80	79	439.8406	-6.4
71	70	448.4249	0.2	79	78	444.7321	-0.29	81	80	439.9868	-0.15
72	71	448.6185	-0.06	80	79	444.8802	0.27	82	81	440.1222	0.8
73	72	448.8069	-0.1	81	80	445.0216	-0.47	83	82	440.2502	-0.1
74	73	448.9900	0.07	82	81	445.1584	-0.25	84	83	440.3756	1.92
75	74	449.1676	0.26	83	82	445.2892	-0.49	85	84	440.4914	-0.14
76	75	449.3395	0.14	84	83	445.4128	-2.31	86	85	440.6042	0.4
77	76	449.5059	0.1	85	84	445.5344	-0.7	87	86	440.7106	0.04
78	77	449.6667	-0.01	86	85	445.6484	-0.96	88	87	440.8108	-1

TABLE 1—*Continued*

1-0 band

J	J	Observed	Δ
79	78	449.8220	-0.05
80	79	449.9719	0.02
81	80	450.1163	0.12
82	81	450.2551	0.23
83	82	450.3880	-0.01
84	83	450.5154	-0.2
85	84	450.6377	0.14
86	85	450.7539	0.06
87	86	450.8646	0.01
88	87	450.9696	-0.04
89	88	451.0693	0.2
90	89	451.1629	0.1
91	90	451.2509	-0.01
92	91	451.3334	-0.01
93	92	451.4100	-0.05
94	93	451.4809	-0.18
95	94	451.5467	0.29
96	95	451.6065	0.52
97	96	451.6601	0.22
98	97	451.7077	-0.24
99	98	451.7501	-0.16
100	99	451.7876	0.71
101	100	451.8180	0.3
102	101	451.8409	-1.8
103	102	451.8647	2.86
104	103	451.8814	6.17

2-1 band

J	J	Observed	Δ
87	86	445.7575	-0.63
88	87	445.8606	-0.71
89	88	445.9582	-0.59
90	89	446.0506	-0.15
91	90	446.1368	-0.19
92	91	446.2174	-0.18
93	92	446.2928	0.2
94	93	446.3623	0.35
95	94	446.4239	-1.62
96	95	446.4837	0.19
97	96	446.5365	0.73
98	97	446.5834	1.03
99	98	446.6244	1.23
100	99	446.6593	1
101	100	446.6895	1.88
102	101	446.7115	0.31
103	102	446.7289	-0.13
104	103	446.7440	2.9

3-2 band

J	J	Observed	Δ
89	88	440.9080	0.59
90	89	440.9969	-0.55
91	90	441.0816	-0.26
92	91	441.1590	-1.72
93	92	441.2346	0.67
94	93	441.3009	-0.59
95	94	441.3632	-0.15
96	95	441.4198	0.19
97	96	441.4710	0.7
98	97	441.5166	1.43
99	98	441.5548	0.33
100	99	441.5869	-1.09
101	100	441.6133	-2.53
109	108	441.6293	-2.6
103	102	441.6543	-0.12
105	104	441.6683	-1.69

4-3 band

J	J'	Observed	Δ
8	7	411.2944	-6.01
9	8	411.8036	0.96
10	9	412.3003	0.04
11	10	412.7928	-0.45
12	11	413.2816	0.18
13	12	413.7660	0.97
14	13	414.2443	0.46
15	14	414.7184	0.38
16	15	415.1880	0.66
17	16	415.6522	0.19
18	17	416.1121	0.14
19	18	416.5657	-1.33
20	19	417.0183	0.9
21	20	417.4639	0.91
22	21	417.9035	-0.32
23	22	418.3386	-1.18
24	23	418.7716	0.66
25	24	419.1970	-0.23
26	25	419.6186	-0.12
27	26	420.0352	-0.1
28	27	420.4472	0.17
29	28	420.8538	-0.09
30	29	421.2559	0.01
31	30	421.6531	0.19
32	31	422.0454	0.27
33	32	422.4322	-0.13
34	33	422.8131	-1.53
35	34	423.1922	0.23
36	35	423.5640	-0.37
37	36	423.9340	2.1
38	37	424.2945	0.24
39	38	424.6520	0.22
40	39	425.0043	0.02
41	40	425.3514	-0.26
42	41	425.6937	-0.42
43	42	426.0322	0.72
44	43	426.3628	-1.04
45	44	426.6898	-1.28
46	45	427.0133	-0.05
47	46	427.3305	0.06
48	47	427.6423	-0.21
49	48	427.9495	0.03
50	49	428.2515	0.25
51	50	428.5481	0.09
52	51	428.8397	0.1
53	52	429.1263	0.35
54	53	429.4070	-0.2
55	54	429.6835	0.22
56	55	429.9557	1.48
57	56	430.2194	-0.55
58	57	430.4805	0.02
59	58	430.7357	-0.09
60	59	430.9853	-0.56
61	60	431.2301	-0.59
62	61	431.4710	0.7
63	62	431.7034	-1.29
64	63	431.9341	0.38
65	64	432.1573	-0.25
66	65	432.3758	-0.27
67	66	432.5890	-0.26
68	67	432.7972	0.04
69	68	432.9996	-0.05
70	69	433.1971	0.12
71	70	433.3884	-0.46
72	71	433.5753	-0.02
73	72	433.7567	0.13

5-4 band

J	J	Observed	Δ
43	42	421.2156	-0.09
44	43	421.5462	1.5
45	44	421.8687	-0.07
46	45	422.1879	0.07
47	46	422.5015	-0.25
48	47	422.8131	2.45
49	48	423.1138	-0.71
50	49	423.4135	0.23
51	50	423.7071	0.17
52	51	423.9949	-0.58
53	52	424.2788	-0.09
54	53	424.5571	-0.2
55	54	424.8307	0.29
56	55	425.0997	1.23
57	56	425.3629	1.53
58	57	425.6195	0.44
59	58	425.8716	-0.03
60	59	426.1198	0.9
61	60	426.3628	1.74
62	61	426.5976	-0.42
63	62	426.8294	-0.26
64	63	427.0565	0.33
65	64	427.2773	-0.03
66	65	427.4925	-0.78
67	66	427.7037	-0.27
68	67	427.9094	-0.02
69	68	428.1089	-0.62
70	69	428.3043	-0.07
71	70	428.4939	-0.06
72	71	428.6777	-0.45
73	72	428.8563	-0.68
74	73	429.0308	0.24
76	75	429.3624	0.88
78	77	429.6726	1.64
79	78	429.8169	-0.76
80	79	429.9557	-3.18
81	80	430.0949	0.14
82	81	430.2194	-5.74
83	82	430.3492	-0.96
84	83	430.4695	-0.11
85	84	430.5832	-0.53
86	85	430.6916	-0.69
87	86	430.7955	0.14
88	87	430.8920	-1.07
89	88	430.9853	0.16
90	89	431.0724	0.66
92	91	431.2301	1.72
93	92	431.2969	-1.54
95	94	431.4207	-1.04
97	96	431.5241	1.23
99	98	431.6014	-0.06
100	99	431.6322	-0.23
101	100	431.6586	0.92
103	102	431.6912	-0.23

6-5 band

J	J'	Observed	Δ
38	37	414.7536	0.53
39	38	415.1032	-0.55
40	39	415.4493	-0.17
41	40	415.7901	-0.16
42	41	416.1260	-0.1
43	42	416.4571	0.17
44	43	416.7827	-0.1
45	44	417.1038	0.21
46	45	417.4197	0.25
47	46	417.7300	-0.38
48	47	418.0342	-1.94
49	48	418.3386	1.66
50	49	418.6325	-0.16
51	50	418.9230	-0.33
52	51	419.2089	0.02
53	52	419.4901	0.67
54	53	419.7650	0.25
55	54	420.0352	0.08
56	55	420.3014	1.1
57	56	420.5616	1.26
58	57	420.8153	0.02
59	58	421.0646	-0.47
60	59	421.3096	-0.09
61	60	421.5462	-2.9
62	61	421.7835	0.06
63	62	422.0136	1.08
64	63	422.2375	1.16
65	64	422.4549	-0.08
66	65	422.6689	0.47
67	66	422.8767	0.01
68	67	423.0795	-0.17
69	68	423.2778	0.41
70	69	423.4697	-0.1
71	70	423.6573	0.31
73	72	424.0188	3.39
74	73	424.1872	0.52
75	74	424.3524	-0.24
76	75	424.5134	0.06
77	76	424.6685	-0.05
78	77	424.8187	0.18
79	78	424.9646	1.5
81	80	425.2364	0.24
83	82	425.4880	0.39
84	83	425.6055	0.32
85	84	425.7161	-1.3
86	85	425.8248	0.64
87	86	425.9258	0.32
88	87	426.0273	5.95
89	88	426.1141	2.38
90	89	426.1955	-1.21
92	91	426.3628	12.74
93	92	426.4203	1.83
94	93	426.4839	2.5
95	94	426.5397	0.92
96	95	426.5976	6.91
97	96	426.6370	0.04
98	97	426.6768	-0.92
99	98	426.7109	-2

4-3 band

J	J	Observed	Δ
40	41	381.2243	2.9
39	40	381.9397	1.91
38	39	382.6438	-6.28
37	38	383.3612	2.98
36	37	384.0622	-0.13
35	36	384.7612	-1.1
34	35	385.4601	1.96
33	34	386.1486	-1.24
32	33	386.8381	0.71
31	32	387.5214	0.67
30	31	388.2006	0.73
29	30	388.8760	1.15
28	29	389.5454	-0.26
27	28	390.2112	-0.99
26	27	390.8742	-0.36
25	26	391.5328	0.14
24	25	392.1862	-0.27
23	24	392.8374	1.32
22	23	393.4822	0.85
21	22	394.1229	0.52
20	21	394.7586	-0.42
19	20	395.3922	0.77
18	19	396.0207	1.12
17	18	396.6434	0.14
16	17	397.2634	0.73
15	16	397.8787	1.01
14	15	398.4877	-0.62
13	14	399.0937	-0.9
12	13	399.6963	-0.24
11	12	400.2889	-5.07
9	10	401.4758	0.11
3	2	408.7276	7.99
4	3	409.2434	-1.58
5	4	409.7654	-0.4
6	5	410.2826	0.62
7	6	410.7941	0.63

5-4 band

J	J	Observed	Δ
7	6	406.1171	2.06
8	7	406.6180	0.37
9	8	407.1126	-3.05
10	9	407.6084	-0.55
11	10	408.0977	0.04
12	11	408.5815	-0.16
13	12	409.0615	0.41
14	13	409.5359	0.17
15	14	410.0050	-0.75
16	15	410.4703	-0.77
17	16	410.9317	0.04
18	17	411.3882	0.69
19	18	411.8388	0.15
20	19	412.2856	0.64
21	20	412.7263	-0.29
22	21	413.1671	3.6
23	22	413.5950	-0.49
24	23	414.0226	-0.19
25	24	414.4452	-0.07
26	25	414.8631	0.17
27	26	415.2758	0.01
28	27	415.6839	0.12
29	28	416.0871	0.15
30	29	416.4851	-0.06
31	30	416.8786	-0.03
32	31	417.2671	-0.05
33	32	417.6505	-0.27
34	33	418.0342	4.66
35	34	418.4037	0.36
36	35	418.7716	-0.71
37	36	419.1361	-0.14
38	37	419.4901	-5.17
39	38	419.8491	-0.21
40	39	420.1985	0.19
41	40	420.5425	0.08
42	41	420.8818	0.21

6-5 band

J	J	Observed	Δ
27	28	381.2512	1.91
26	27	381.9030	2.06
25	26	382.5495	1.05
23	24	383.8307	-0.16
19	20	386.3440	-0.99
16	17	388.1837	-2.2
15	16	388.7908	-0.05
13	14	389.9848	-3.16
12	13	390.5844	4.37
10	11	391.7518	0.74
9	10	392.3268	-3.27
7	8	393.4635	-11
3	4	395.7068	-4.66
11	10	403.4564	-1.62
15	14	405.3489	-0.66
17	16	406.2605	-6.83
18	17	406.7202	1.03
19	18	407.1647	-1.6
20	19	407.6084	-0.35
21	20	408.0470	0.59
22	21	408.4797	0.28
23	22	408.9078	0.21
24	23	409.3305	-0.62
25	24	409.7487	-1.1
26	25	410.1631	-0.56
27	26	410.5716	-1.18
28	27	410.9762	-0.84
29	28	411.3766	0.09
30	29	411.7698	-1.33
31	30	412.1603	-0.61
32	31	412.5479	2.02
33	32	412.9262	0.25
34	33	413.3008	-0.42
35	34	413.6713	-0.18
36	35	414.0365	-0.45
37	36	414.3984	0.9

TABLE 1—*Continued*

4-3 band

J	J	Observed	Δ
74	73	433.9318	-0.54
75	74	434.1030	0.24
76	75	434.2675	-0.22
77	76	434.4276	0.29
78	77	434.5811	-0.43
79	78	434.7298	-0.46
80	79	434.8698	-3.77
81	80	435.0111	-0.24
82	81	435.1388	-4.92
83	82	435.2704	-0.21
84	83	435.3980	5.97
85	84	435.5077	-0.27
86	85	435.6181	-0.31
87	86	435.7239	0.54
88	87	435.8219	-0.82
89	88	435.9109	-5.59
90	89	436.0042	-0.62
91	90	436.0882	0.66
92	91	436.1586	-6.08
93	92	436.2358	-0.43
94	93	436.3016	-0.62
95	94	436.3626	0.03
96	95	436.4163	-1.06
98	97	436.5079	-2

5-4 band

J	J	Observed	Δ

6-5 band

J	J'	Observed	Δ

7-6 band

J	J	Observed	Δ
40	39	410.7553	-1.15
41	40	411.0935	-0.51
42	41	411.4257	-0.85
43	42	411.7535	-0.77
44	43	412.0759	-1.03
45	44	412.3944	-0.3
46	45	412.7072	-0.22
47	46	413.0152	-0.03
48	47	413.3169	-1.14
49	48	413.6165	0.66
50	49	413.9079	-0.69
51	50	414.1966	0.32
52	51	414.4781	-0.84
54	53	415.0296	0.39
55	54	415.2971	0.46
56	55	415.5603	1.22
57	56	415.8162	-0.19
58	57	416.0688	0.15
59	58	416.3154	-0.39
60	59	416.5657	8.03
61	60	416.7998	5.29
62	61	417.0183	-7.91
63	62	417.2523	-0.51
64	63	417.4639	-10
65	64	417.6910	0.68
66	65	417.9035	2.16
67	66	418.1073	0.22
68	67	418.3083	0.59
69	68	418.5044	1.36
70	69	418.6947	1.55
71	70	418.8781	0.03
72	71	419.0574	-0.29
73	72	419.2330	0.96
75	74	419.5670	2.15
76	75	419.7236	0.22
77	76	419.8825	5.91
78	77	420.0229	-1.51
79	78	420.1669	-0.12
81	80	420.4297	-6.4
85	84	420.9107	0.9

8-7 band

J	J	Observed	Δ
58	57	411.3766	-2.15
60	59	411.8615	-1.01
61	60	412.0968	0.15
62	61	412.3264	0.59
63	62	412.5479	-1.9
64	63	412.7697	0.98
65	64	412.9824	-0.05
66	65	413.1918	0.76
67	66	413.3942	-0.26
68	67	413.5950	2.28
69	68	413.7869	1.05
70	69	413.9693	-4.47
71	70	414.1577	1.23
72	71	414.3379	3.91
73	72	414.5063	0.02

J	J'	Observed	Δ

7-6 band

J	J	Observed	Δ
26	25	405.5181	-1.19
28	27	406.3243	-1.1
30	29	407.1126	0.3
31	30	407.4984	-0.11
32	31	407.8831	3.13
33	32	408.2548	-1.77
34	33	408.6275	-0.81
35	34	408.9958	0.61
36	35	409.3572	0.01
37	36	409.7139	-0.45
38	37	410.0659	-0.7
39	38	410.4142	0.24

8-7 band

J	J	Observed	Δ
34	33	404.0156	1.42
38	37	405.4363	-2.18
40	39	406.1171	-4.4
41	40	406.4537	-2.03
43	42	407.1126	3.21
48	47	408.6563	-0.89
50	49	409.2434	1.74
51	50	409.5252	-1.13
52	51	409.8061	0.03
53	52	410.0787	-2.04
54	53	410.3508	0.3
57	56	411.1310	1.73

TABLE 2
Dunham Y_{ij} Coefficients for the $X\ ^1\Sigma^+$ Ground State of KF

Dunham coefficients	Value (cm^{-1})	Previous work[a]
Y_{10}	426.261872(98)	426.26119(84)
Y_{20}	-2.449801(44)	-2.449513(400)
$10^3\ Y_{30}$	9.4357(79)	9.3447(564)
$10^5\ Y_{40}$	-1.048(53)	-
Y_{01}	0.279937682(52)	0.279937548(64)
$10^3\ Y_{11}$	-2.335154(42)	-2.335296(97)
$10^6\ Y_{21}$	6.933(10)	7.057(25)
$10^8\ Y_{31}$	1.873(89)	-
$10^7\ Y_{02}$	-4.84117(78)	-4.8320(50)
$10^{10}\ Y_{12}$	1.254(59)	[0.633771][b]
$10^{11}\ Y_{22}$	3.720(77)	3.72(25)

[a] Ref. 10.
[b] The value of Y_{12}, and also the values of Y_{03} and Y_{13}, were fixed at the values calculated from the Dunham a_i potential parameters.

TABLE 3
Spectroscopic Constants for the $X\ ^1\Sigma^+$ Ground State of KF (in cm^{-1})

v	T_v	B_v	$10^7\ D_v$
0	0	0.278771826(43)	4.84025(74)
1	421.392834(50)	0.276450649(48)	4.83832(71)
2	837.970760(65)	0.274143387(56)	4.83549(69)
3	1249.789858(88)	0.271850416(73)	4.83222(67)
4	1656.90571(11)	0.269571722(92)	4.82813(65)
5	2059.37425(13)	0.26730728(11)	4.82306(64)
6	2457.25102(20)	0.26505730(14)	4.81735(63)
7	2850.58980(55)	0.26282242(32)	4.81143(73)
8	3239.4513(24)	0.2605997(14)	4.8017(19)

from $v = 1 \rightarrow 0$ to $v = 8 \rightarrow 7$ were observed; the line positions are reported in Table 1. In order to obtain improved spectroscopic constants for KF that can describe both the infrared and microwave data, all of the lines reported in Table 1 were fitted, together with the hyperfine-corrected microwave (*1*, *4*) and millimeter-wave transitions (*5*) belonging to the first three vibrational levels. Dunham Y_{ij} coefficients, listed in Table 2, were obtained by fitting the data set to the energy level expression (*23*)

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

The customary spectroscopic constants for the $X\,^1\Sigma^+$ ground state of KF are given in Table 3. From the Y_{01} equilibrium constant, the equilibrium internuclear separation $r_e = 2.1714558(2)$ Å was calculated.

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