High-Resolution Infrared Emission Spectrum of NaF

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The high-resolution infrared emission spectrum of sodium monofluoride has been recorded with a Fourier transform spectrometer. A total of 1131 of vibration–rotation transitions, from the $v = 1 \rightarrow 0$ to $v = 9 \rightarrow 8$ vibrational bands, have been assigned. The infrared data have been combined with existing microwave data in order to obtain improved spectroscopic constants, including Dunham Y_{ij} and U_{ij} coefficients, for the $X^1\Sigma^+$ electronic ground state of NaF.   © 1996 Academic Press, Inc.

INTRODUCTION

Alkali halides are the classical examples of ionic bonding. These molecules have been extensively studied by many different methods. A review of the spectroscopic literature on NaF was published by Douay *et al.* (*1*) in their diode laser measurements of the vibration–rotation first overtone spectrum. Since that time, some ab initio calculations have been published (*2, 3*), as well as a refit of the NaF data using analytical potential functions (*4*).

An electron diffraction study of alkali fluoride vapors (*5*) has also been completed. In addition, it should be mentioned that the spectroscopic constants of NaF are useful in the study of reaction dynamics, such as the Na + $FCH_3 \rightarrow NaF + CH_3$ system (*6*). This paper represents the first experimental study and analysis of the high-resolution Fourier-transform infrared emission spectrum of NaF. The previous diode laser work (*1*) generated a very small data set since only a few *R*-branch lines were measured for the $\Delta v = 2$ overtone bands.

FIG. 1. A portion of the *R* branch of vibration–rotation spectrum of NaF. The 1–0 and 2–1 bands are marked along with the J'' value.

TABLE 1
Observed Rovibrational Line Positions of the $X^1\Sigma^+$ State of NaF in cm^{-1} [Observed − Calculated Values Are Shown in the Column Labeled Δ (in units of cm^{-1})]

1-0 Band				2-1 Band				3-2 Band			
J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ
1	2	526.8200	2	1	2	519.8536	15	1	2	512.9940	18
2	3	525.9336	11	2	3	518.9735	-5	2	3	512.1225	-9
3	4	525.0361	-3	4	5	517.1914	-2	3	4	511.2458	0
4	5	524.1305	-9	5	6	516.2894	23	4	5	510.3581	-12
5	6	523.2171	-3	6	7	515.3738	-1	5	6	509.4644	1
6	7	522.2942	-4	7	8	514.4519	0	6	7	508.5606	0
7	8	521.3635	5	8	9	513.5213	0	7	8	507.6486	4
8	9	520.4181	-45	9	10	512.5842	23	8	9	506.7258	-15
9	10	519.4749	15	10	11	511.6341	2	9	10	505.7976	-1
10	11	518.5156	2	11	12	510.6774	1	10	11	504.8598	3
11	12	517.5486	-2	12	13	509.7121	0	11	12	503.9129	1
12	13	516.5733	-1	13	14	508.7384	1	12	13	502.9579	2
13	14	515.5895	1	14	15	507.7557	-4	13	14	501.9941	0
14	15	514.5968	-1	15	16	506.7652	-1	14	15	501.0218	-3
15	16	513.5962	6	16	17	505.7659	-2	15	16	500.0408	-8
16	17	512.5842	-16	17	18	504.7582	-1	16	17	499.0531	4
17	18	511.5674	-2	18	19	503.7422	-1	17	18	498.0556	1
18	19	510.5407	0	19	20	502.7176	-2	18	19	497.0499	-1
19	20	509.5055	0	20	21	501.6848	-1	19	20	496.0362	0
20	21	508.4616	-2	21	22	500.6436	-1	20	21	495.0141	-1
21	22	507.4083	-13	22	23	499.5940	-3	21	22	493.9842	4
22	23	506.3490	-2	23	24	498.5368	2	22	23	492.9452	-1
23	24	505.2803	0	24	25	497.4705	-1	23	24	491.8987	0
24	25	504.2030	-1	25	26	496.3966	1	24	25	490.8439	1
25	26	503.1174	-2	26	27	495.3141	-1	25	26	489.7814	4
26	27	502.0239	0	27	28	494.2236	-1	26	27	488.7102	2
27	28	500.9218	-2	28	29	493.1251	-1	27	28	487.6310	1
28	29	499.8118	0	29	30	492.0186	-1	28	29	486.5442	3
29	30	498.6940	6	30	31	490.9041	1	29	30	485.4489	0
30	31	497.5670	-1	31	32	489.7814	1	30	31	484.3459	0
31	32	496.4324	0	32	33	488.6506	-1	31	32	483.2351	1
32	33	495.2899	0	33	34	487.5119	-1	32	33	482.1162	0
33	34	494.1398	6	34	35	486.3653	-2	33	34	480.9894	-2
34	35	492.9808	3	35	36	485.2111	-1	34	35	479.8551	0
35	36	491.8137	-2	36	37	484.0488	-2	35	36	478.7127	-1
36	37	490.6393	-1	37	38	482.8788	-1	36	37	477.5627	-2
37	38	489.4578	9	38	39	481.7009	-2	37	38	476.4050	-2
38	39	488.2668	3	39	40	480.5155	0	38	39	475.2397	-1
39	40	487.0685	2	40	41	479.3220	-2	39	40	474.0664	-2
40	41	485.8624	0	41	42	478.1210	-2	40	41	472.8858	-2
41	42	484.6488	2	42	43	476.9123	-3	41	42	471.6975	-1
42	43	483.4271	0	43	44	475.6962	-2	42	43	470.5022	4
43	44	482.1980	2	44	45	474.4724	-1	43	44	469.2983	0
44	45	480.9611	1	45	46	473.2404	-8	44	45	468.0873	-2
45	46	479.7166	1	46	47	472.0022	-1	45	46	466.8694	3
46	47	478.4643	0	47	48	470.7557	-2	46	47	465.6433	-1
47	49	477.2045	-2	48	49	469.5018	-3	47	48	464.4117	15
48	49	475.9373	-1	49	50	466.9721	-2	48	49	463.1698	1
49	50	474.6627	0	51	52	465.6961	-2	49	50	461.9217	-2
50	51	473.3803	-1	52	53	464.4117	-14	50	51	460.6669	2
51	52	472.0907	-1	53	54	463.1236	10	51	52	459.4044	0
52	53	470.7937	1	54	55	461.8245	-2	52	53	458.1347	-1
53	54	469.4895	2	55	56	460.5197	-2	53	54	456.8581	1
54	55	468.1777	0	56	57	459.2075	-2	54	55	455.5740	-2
55	56	466.8587	1	57	58	457.8884	-1	55	56	454.2832	1
56	57	465.5321	-2	58	59	456.5615	-6	56	57	452.9848	-3
57	58	464.1963	-26	59	60	455.2286	-2	57	58	451.6801	2
58	59	462.8583	1	60	61	453.8881	-2	58	59	450.3676	-2
59	60	461.5104	0	61	62	452.5407	-2	59	60	449.0482	-5
60	61	460.1553	-1	62	63	451.1863	-2	60	61	447.7227	0
61	62	458.7932	-2	63	64	449.8250	-3	61	62	446.3894	-3
62	63	457.4245	1	64	65	448.4567	-4	62	63	445.0504	4
63	64	456.0484	1	65	66	447.0819	-3	63	64	443.7016	-17
64	65	454.6655	1	66	67	445.7003	-1	64	65	442.3505	5
65	66	453.275	-4	67	68	444.3113	-5	65	66	440.9894	-4
66	67	451.8775	-10	68	69	442.9165	-2	66	67	439.6228	-2
67	68	450.4744	-5	69	70	441.5144	-3	67	68	438.2498	3
68	69	449.064	-4	70	71	440.1033	-29	68	69	436.8691	-2
69	70	447.6473	1	71	72	438.6905	-4	69	70	435.4818	-8
70	71	446.2231	-1	72	73	437.2695	3	70	71	434.0876	-17
71	72	444.7919	-5	73	74	435.8411	2	71	72	432.6905	10
72	73	443.3550	-1	74	75	434.4051	-10	72	73	431.2820	-12
73	74	441.9108	-3	75	76	432.9648	-1	73	74	429.8716	11
74	75	440.4612	7	76	77	431.5173	1	74	75	428.4522	9
75	76	439.0033	-1	77	78	430.0637	5	75	76	427.0256	-3
76	77	437.5394	-4	78	79	428.6029	1	76	77	425.5968	27
77	78	436.0699	2	79	80	427.1366	3	3	2	517.2045	1
78	79	434.5936	4	80	81	425.6638	4	4	3	518.0199	-4
79	80	433.1095	-9	81	82	424.1868	26	5	4	518.8281	10
80	81	431.6215	4	1	0	522.4299	-28	6	5	519.6255	6
81	82	430.1253	-3	2	1	523.2754	4	7	6	520.4181	43
83	84	427.1174	17	3	2	524.1074	-10	8	7	521.1941	5

1-0 Band				2-1 Band				3-2 Band			
J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ
2	1	530.2793	6	4	3	524.9329	2	9	8	521.9642	-2
3	2	531.1206	-2	5	4	525.7480	-1	10	9	522.7266	4
4	3	531.9545	8	6	5	526.5542	-1	11	10	523.4788	1
5	4	532.7747	-30	7	6	527.3516	2	12	11	524.2223	2
6	5	533.5920	-3	8	7	528.1395	0	13	12	524.9563	-2
7	6	534.3977	-1	9	8	528.9182	-1	14	13	525.6814	-2
8	7	535.1939	-3	10	9	529.6881	1	15	14	526.3974	-1
9	8	535.9781	-31	11	10	530.4487	2	16	15	527.1028	-14
10	9	536.7589	-1	12	11	531.2005	8	17	16	527.8019	2
11	10	537.5275	1	13	12	531.9422	4	18	17	528.4899	1
12	11	538.2866	0	14	13	532.6745	0	19	18	529.1684	-2
13	12	539.0363	-1	15	14	533.3995	16	20	19	529.8407	27
14	13	539.7753	-16	16	15	534.1121	0	21	20	530.4984	2
15	14	540.5079	0	17	16	534.8168	0	22	21	531.1489	0
16	15	541.2295	0	18	17	535.5123	1	23	22	531.7903	0
17	16	541.9431	15	19	18	536.1980	-1	24	23	532.4223	2
18	17	542.6445	2	21	20	537.5419	2	25	24	533.0449	3
19	18	543.3375	0	22	21	538.1995	2	26	25	533.6579	4
20	19	544.0212	1	23	22	538.8473	-1	27	26	534.2611	2
21	20	544.6951	-1	24	23	539.4860	1	28	27	534.8548	-1
22	21	545.3598	1	25	24	540.1149	1	29	28	535.4393	1
23	22	546.0144	-2	26	25	540.7345	2	30	29	536.0141	1
24	23	546.6601	2	27	26	541.3441	0	31	30	536.5794	3
25	24	547.2958	3	28	27	541.9431	-11	32	31	537.1347	1
26	25	547.9215	0	29	28	542.5347	0	33	32	537.6806	1
27	26	548.5380	3	30	29	543.1154	-2	34	33	538.2169	1
28	27	549.1442	0	31	30	543.6867	0	35	34	538.7406	-27
29	28	549.741	1	32	31	544.2485	4	36	35	539.2601	0
30	29	550.3282	3	33	32	544.7997	0	37	36	539.7670	-1
31	30	550.9053	3	34	33	545.3417	1	38	37	540.2643	-1
32	31	551.4727	2	35	34	545.8735	-1	39	38	540.7519	0
33	32	552.0300	1	36	35	546.3962	2	40	39	541.2295	-1
34	33	552.5776	0	37	36	546.9084	0	41	40	541.6973	-2
35	34	553.1154	1	38	37	547.4108	-2	42	41	542.1553	-1
36	35	553.6432	1	39	38	547.9039	3	43	42	542.6036	0
37	36	554.1611	1	40	39	548.3863	0	44	43	543.0416	-1
38	37	554.6689	1	41	40	548.8593	-2	45	44	543.4699	-2
39	38	555.1667	0	42	41	549.3218	-2	46	45	543.8885	1
40	39	555.6549	3	43	42	549.7748	-1	47	46	544.2968	0
41	40	556.1327	2	44	43	550.2175	-3	48	47	544.6951	-1
42	41	556.6005	2	45	44	550.6504	-3	49	48	545.0837	1
43	42	557.0581	1	46	45	551.0736	2	50	49	545.4618	-1
44	43	557.5058	2	47	46	551.4857	-5	51	50	545.8304	1
45	44	557.9432	1	48	47	551.8889	0	52	51	546.1883	-3
46	45	558.3706	1	49	48	552.2812	-1	53	52	546.5366	-1
47	46	558.7876	0	50	49	552.6638	0	54	53	546.8746	-2
48	47	559.1950	4	51	50	553.0362	1	55	54	547.2025	-2
49	48	559.5916	2	52	51	553.3980	-2	56	55	547.5204	-1
50	49	559.9779	0	53	52	553.7499	-2	57	56	547.8280	0
51	50	560.3542	0	54	53	554.0916	-1	58	57	548.1254	-1
52	51	560.7201	-1	55	54	554.4232	1	59	58	548.4124	-2
53	52	561.0761	2	56	55	554.7443	-1	60	59	548.6895	-1
54	53	561.4216	4	57	56	555.0550	-2	61	60	548.9565	2
55	54	561.7566	3	58	57	555.3556	-3	62	61	549.2128	0
56	55	562.0810	0	59	58	555.6460	-1	63	62	549.4590	1
57	56	562.3954	1	60	59	555.9258	-3	64	63	549.6944	-4
58	57	562.699	-1	61	60	556.1954	-3	65	64	549.9202	-1
59	58	562.9926	0	62	61	556.4549	0	66	65	550.1350	-5
60	59	563.2754	-2	63	62	556.7035	-2	67	66	550.3408	5
61	60	563.5480	-2	64	63	556.9423	1	68	67	550.5349	1
62	61	563.8106	4	65	64	557.1700	-2	69	68	550.7187	-1
63	62	564.0621	3	66	65	557.3874	-2	70	69	550.8931	7
64	63	564.3031	3	67	66	557.5946	-1	71	70	551.0568	12
65	64	564.5332	-1	68	67	557.7909	-3	72	71	551.2082	-2
66	65	564.7532	1	69	68	557.9779	6	73	72	551.3505	-2
67	66	564.9623	-3	70	69	558.1526	0	74	73	551.4857	33
68	67	565.1614	1	71	70	558.3176	-2	75	74	551.6043	7
69	68	565.3494	-1	72	71	558.4722	0	76	75	551.7144	0
70	69	565.5272	2	73	72	558.6160	-1	77	76	551.8151	5
71	70	565.6940	1	74	73	558.7494	1	78	77	551.9046	4
72	71	565.8499	-1	75	74	558.8720	1	79	78	551.9835	2
73	72	565.9958	3	76	75	558.9846	7	80	79	552.0510	-8
74	73	566.1308	2	77	76	559.0856	4	81	80	552.1081	-16
75	74	566.2544	2	78	77	559.1764	6	82	81	552.1546	-24
76	75	566.3674	-1	79	78	559.2560	2	83	82	552.1887	-48
78	77	566.5673	5	80	79	559.3229	-22				
80	79	566.7150	22	81	80	559.3814	-23				
81	80	566.7696	-25	82	81	559.4301	-13				
82	81	566.8184	-21	83	82	559.4679	-6				
83	82	566.8566	-15	84	83	559.4947	0				
85	84	566.9015	10	85	84	559.5113	9				

TABLE 1—*Continued*

4-3 Band				5-4 Band				6-5 Band			
J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ
2	3	505.3793	2	1	2	499.5940	33	2	3	492.2006	-28
3	4	504.5138	31	2	3	498.7384	-13	4	5	490.4938	0
4	5	503.6344	10	3	4	497.8815	13	5	6	489.6271	8
5	6	502.7475	-2	4	5	497.0124	2	6	7	488.7505	0
6	7	501.8530	-4	5	6	496.1355	-1	7	8	487.8680	17
7	8	500.9507	2	6	7	495.2503	-3	8	9	486.9745	8
8	9	500.0408	17	7	8	494.3577	7	9	10	486.0724	-4
9	10	499.1186	-5	8	9	493.4544	-7	10	11	485.1636	-1
10	11	498.1914	7	9	10	492.5442	-5	11	12	484.2459	-4
11	12	497.2542	3	10	11	491.6241	-19	12	13	483.3204	-3
12	13	496.3088	1	11	12	490.6991	2	13	14	482.3864	-5
13	14	495.3556	4	12	13	489.7648	11	14	15	481.4447	-2
14	15	494.3934	2	13	14	488.8196	-4	15	16	480.4945	-2
15	16	493.4236	7	14	15	487.8680	-1	16	17	479.5367	1
16	17	492.4444	0	15	16	486.9083	4	17	18	478.5699	-4
17	18	491.4576	0	16	17	485.9381	-15	18	19	477.5958	-1
18	19	490.4623	-3	17	18	484.9627	-4	19	20	476.6129	-6
19	20	489.4578	-16	18	19	483.9763	-21	20	21	475.6225	-6
20	21	488.4482	2	19	20	482.9858	1	21	22	474.6248	0
21	22	487.4284	0	20	21	481.9846	-2	22	23	473.6184	-2
22	23	486.4012	4	21	22	480.9764	4	23	24	472.6050	6
23	24	485.3656	5	22	23	479.9590	-1	24	25	471.5823	-1
24	25	484.3213	0	23	24	478.9340	-2	25	26	470.5525	0
25	26	483.2696	1	24	25	477.8949	-64	26	27	469.5142	-7
26	27	482.2101	4	25	26	476.8605	-1	27	28	468.4694	-1
27	28	481.1418	-2	26	27	475.8116	-3	28	29	467.4161	-1
28	29	480.0664	0	27	28	474.7552	-2	29	30	466.3553	0
30	31	477.8949	35	28	29	473.6917	7	30	31	465.2870	3
31	32	476.7923	1	29	30	472.6192	3	31	32	464.2108	3
32	33	475.6852	1	30	31	471.5386	-3	32	33	463.1236	-31
33	34	474.5701	-2	31	32	470.4513	1	33	34	462.0356	3
34	35	473.4479	1	32	33	469.3513	14	34	35	460.9361	-2
35	36	472.3174	-2	33	34	468.2528	0	35	36	459.8293	-4
36	37	471.1798	1	34	35	467.1424	3	36	37	458.7156	-1
37	38	470.0341	0	35	36	466.0238	0	37	38	457.5940	-3
38	39	468.8811	1	36	37	464.8978	-1	38	39	456.4655	1
39	40	467.7203	0	37	38	463.7645	0	39	40	455.3289	-3
40	41	466.5522	1	38	39	462.6239	4	40	41	454.1852	-3
41	42	465.3763	-1	39	40	461.4749	-1	41	42	453.0338	-7
42	43	464.1963	32	40	41	460.3195	3	42	43	451.8775	13
43	44	463.0024	-1	41	42	459.1563	4	43	44	450.7112	4
44	45	461.8046	1	42	43	457.9838	-15	44	45	449.5373	-7
45	47	460.5991	0	43	44	456.8075	3	45	46	448.3585	4
46	47	459.3863	1	44	45	455.6218	0	46	47	447.1712	2
47	48	458.1660	-2	45	46	454.4292	0	47	48	445.9760	-8
48	49	456.939	1	46	47	453.2297	3	48	49	444.7755	0
49	50	455.7044	0	47	48	452.0223	0	49	50	443.5670	-2
50	51	454.4627	1	48	49	450.8078	-2	52	53	439.9005	4
51	52	453.2137	0	49	50	449.5866	0	53	54	438.6679	40
52	53	451.9576	-1	50	51	448.3585	3	54	55	437.4228	20
53	54	450.6951	6	51	52	447.1218	-8	55	56	436.1711	3
54	55	449.4241	-3	52	53	445.8802	2	56	57	434.9149	8
55	56	448.1481	9	53	54	444.6303	-1	58	59	432.3797	-6
56	57	446.8627	-3	54	55	443.3737	-1	59	60	431.1031	-2
57	58	445.5724	6	55	56	442.1103	0	60	61	429.8212	15
58	59	444.2740	3	56	57	440.8391	-8	61	62	428.5294	-1
59	60	442.9686	-2	57	58	439.5617	-9	62	63	427.2314	-13
60	61	441.6566	-4	58	59	438.2785	0	2	1	496.3258	-28
61	62	440.3383	-2	59	60	436.9879	3	3	2	497.1281	2
62	63	439.0174	6	60	61	435.6898	-2	4	3	497.9190	5
63	64	437.6811	1	61	62	434.3851	-5	5	4	498.6940	-65
64	65	436.3425	2	62	63	433.0762	16	6	5	499.4740	1
65	66	434.9969	1	63	64	431.7572	3	7	6	500.2389	5
66	67	433.6469	21	64	65	430.4316	-11	8	7	500.9867	-75
67	68	432.2887	25	65	66	429.1021	3	9	8	501.7417	4
68	69	430.9214	3	66	67	427.7651	7	10	9	502.4799	3
69	70	429.5500	6	3	2	503.7167	9	11	10	503.2097	7
70	71	428.1730	17	4	3	504.5138	-10	12	11	503.9313	17
71	72	426.7877	10	5	4	505.3047	-3	13	12	504.6417	4
72	73	425.3957	-1	6	5	506.0859	-4	14	13	505.3438	-3
2	1	509.5896	-17	7	6	506.8590	1	15	14	506.0375	-5
3	2	510.4086	11	8	7	507.6227	1	16	15	506.7258	28
4	3	511.2142	-6	9	8	508.3780	4	17	16	507.4083	94
5	4	512.0158	26	10	9	509.1237	2	18	17	508.0648	-10
6	5	512.8027	-1	11	10	509.8605	-1	19	18	508.7231	-6
7	6	513.5838	3	12	11	510.5875	-12	20	19	509.3723	-4

4-3 Band				5-4 Band				6-5 Band			
J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ
8	7	514.3556	3	13	12	511.3050	-29	21	20	510.0125	1
9	8	515.1178	-2	14	13	512.0158	-22	22	21	510.6432	0
10	9	515.8723	5	15	14	512.7192	0	23	22	511.2642	-5
11	10	516.6168	2	16	15	513.4115	2	24	23	511.8775	3
12	11	517.3513	-11	17	16	514.0943	0	25	24	512.4811	6
13	12	518.0810	19	18	17	514.7680	-2	26	25	513.0763	18
14	13	518.7965	-2	19	18	515.4302	-28	27	26	513.6587	-7
15	14	519.5048	-3	20	19	516.0882	-5	28	27	514.2349	-1
16	15	520.2045	0	21	20	516.7355	3	29	28	514.8011	-3
17	16	520.8958	12	22	21	517.3741	16	30	29	515.3588	3
18	17	521.5754	-3	23	22	518.0019	13	31	30	515.9055	-6
19	18	522.2479	4	24	23	518.6194	0	32	31	516.4444	-2
20	19	522.9101	1	25	24	519.2290	0	33	32	516.9735	-2
21	20	523.5635	2	26	25	519.8296	3	34	33	517.4927	-6
22	21	524.2073	1	27	26	520.4181	-22	35	34	518.0019	-18
23	22	524.8417	-2	28	27	521.0016	-3	36	35	518.5047	2
24	23	525.4670	-2	29	28	521.5754	12	37	36	518.9959	0
25	24	526.0833	1	30	29	522.1371	0	38	37	519.4749	-30
26	25	526.6896	-1	31	30	522.6903	-2	39	38	519.9513	9
27	26	527.2869	0	32	31	523.2345	-1	40	39	520.4181	48
28	27	527.8747	1	33	32	523.7700	8	41	40	520.8659	-8
29	28	528.4527	-1	34	33	524.2942	-1	42	41	521.3110	4
30	29	529.0207	-10	35	34	524.8098	1	43	42	521.7445	-4
31	30	529.5809	0	36	35	525.3157	-3	44	43	522.1690	-6
32	31	530.1305	-2	37	36	525.8123	-2	45	44	522.5839	-7
33	32	530.6710	1	38	37	526.2996	1	46	45	522.9898	-2
34	33	531.2005	-10	39	38	526.7769	0	47	46	523.3854	-5
35	34	531.7223	-2	40	39	527.2446	-1	48	47	523.7700	-20
36	35	532.2339	0	41	40	527.7021	-8	49	48	524.1479	-5
37	36	532.7359	2	42	41	528.1510	-4	50	49	524.5148	-2
38	37	533.2280	2	43	42	528.5901	-1	51	50	524.8723	3
39	38	533.7093	-9	44	43	529.0207	14	52	51	525.2193	1
40	39	534.1829	0	45	44	529.4365	-22	53	52	525.5589	23
41	40	534.6457	-2	46	45	529.8407	-76	54	53	525.8845	2
42	41	535.0996	6	47	46	530.2484	1	55	54	526.2016	-5
43	42	535.5407	-18	48	47	530.6384	-1	56	55	526.5094	-6
44	43	535.9781	19	49	48	531.0186	-2	57	56	526.8081	0
45	44	536.3999	0	50	49	531.3887	-6	58	57	527.1028	65
46	45	536.8139	0	51	50	531.7502	3	59	58	527.3758	12
47	46	537.2184	3	52	51	532.0999	-8	60	59	527.6433	2
48	47	537.6114	-9	53	52	532.4417	0	61	60	527.9018	2
49	48	537.9968	2	55	54	533.0933	-5	62	61	528.1510	9
50	49	538.3709	-1	58	57	533.9968	-6	63	62	528.3884	-3
51	50	538.7406	5	59	58	534.2795	10	64	63	528.6163	-10
52	51	539.0897	-3	60	59	534.5505	7	65	64	528.8359	0
53	52	539.4342	-3	61	60	534.8100	-9	66	65	529.0450	5
54	53	539.767	-19	62	61	535.0621	0	67	66	529.2430	0
55	54	540.0934	0	63	62	535.3030	-1	68	67	529.4365	50
56	55	540.4080	2	65	64	535.7552	4	69	68	529.6105	6
57	56	540.7124	1	66	65	535.9648	-8	70	69	529.7775	-7
58	57	541.0067	2	67	66	536.1662	0	71	70	529.9351	-14
59	58	541.2907	1	68	67	536.3573	8	72	71	530.0847	2
60	59	541.5649	2	69	68	536.5367	0	73	72	530.2222	-4
61	60	541.8288	2	70	69	536.7067	-1	74	73	530.3509	6
62	61	542.0825	1	71	70	536.8655	-11	75	74	530.4679	-1
63	62	542.3262	2	72	71	537.0158	-3				
64	63	542.5594	1	74	73	537.2848	2				
65	64	542.7828	3	75	74	537.4037	4				
66	65	542.9955	2	76	75	537.5113	-5				
67	66	543.1983	3	77	76	537.6114	14				
68	67	543.3904	0	78	77	537.6963	-16				
69	68	543.5729	4	81	80	537.8980	-12				
70	69	543.7439	-4	82	81	537.9485	29				
71	70	543.9057	0								
72	71	544.0567	-2								
73	72	544.1985	9								
74	73	544.3279	-1								
75	74	544.4491	11								
76	75	544.5578	2								
77	76	544.6566	-1								
78	77	544.7454	0								
79	78	544.8237	0								
80	79	544.8918	4								
81	80	544.9483	-5								
82	81	544.9952	-3								

EXPERIMENTAL DETAILS

The high-resolution infrared emission spectrum of NaF has been recorded with a Bruker IFS 120 HR Fourier transform spectrometer. Gas-phase NaF was obtained by heating NaF powder in a commercial CM Rapid Temp Furnace. The NaF powder was placed in the central part of a mullite ($3Al_2O_3 \cdot 2SiO_2$) tube; its interior was protected by a carbon liner tube. The tube was heated slowly in order to prevent the cracking of the tube. The cell was

TABLE 1—*Continued*

7-6 Band				8-7 Band				9-8 Band				7-6 Band				8-7 Band				9-8 Band			
J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ	J'	J"	Observed	Δ
0	1	487.4284	17	5	6	476.9123	32	29	30	448.1463	-26	9	8	495.2063	-12	33	32	503.6932	-7				
1	2	486.6060	42	6	7	476.0534	21	28	29	449.1765	-1	10	9	495.9389	8	34	33	504.2030	-1				
5	6	483.2210	28	9	10	473.4309	17	27	28	450.1976	7	12	11	497.3755	24	35	34	504.7034	5				
6	7	482.3515	1	10	11	472.5392	3	24	25	453.2119	-8	13	12	498.0774	-1	36	35	505.1976	41				
7	8	481.4770	6	11	12	471.6400	-5	23	24	454.2037	8	14	13	498.7726	-4	37	36	505.6749	0				
8	9	480.5930	-2	13	14	469.8193	-3	21	22	456.1613	10	15	14	499.4594	-3	38	37	506.1459	-12				
9	10	479.7007	-9	14	15	468.8972	1	19	20	458.0877	5	16	15	500.1376	0	40	39	507.0634	0				
11	12	477.8949	8	15	16	467.9664	-4	22	21	491.0677	-8	17	16	500.8066	0	41	40	507.5083	8				
12	13	476.9781	0	16	17	467.0285	0	23	22	491.6758	48	18	17	501.4662	-4	42	41	507.9427	3				
13	14	476.0534	-6	17	18	466.0822	0	24	23	492.2646	-2	19	18	502.1151	-27	43	42	508.3686	8				
14	15	475.1234	15	18	19	465.1285	4	25	24	492.8493	-3	20	19	502.7594	-6	44	43	508.7837	-2				
15	16	474.1809	-8	19	20	464.1658	-4	28	27	494.5513	7	21	20	503.3933	1	45	44	509.1884	-21				
16	17	473.2404	69	20	21	463.1970	5	29	28	495.0984	-12	22	21	504.0188	14	46	45	509.5896	19				
17	18	472.2772	0	21	22	462.2186	-4	33	32	497.2058	0	23	22	504.6331	6	47	46	509.9753	-2				
18	19	471.3135	4	22	23	461.2386	48	34	33	497.7095	-2	24	23	505.2385	-1	49	48	510.7228	3				
19	20	470.3414	4	23	24	460.2408	1	35	34	498.2027	-17	25	24	505.8366	9	50	49	511.0813	-5				
20	21	469.3573	-37	24	25	459.2389	-12					26	25	506.4237	0	51	50	511.4322	7				
21	22	468.3725	-6	25	26	458.2317	0					27	26	507.0020	-4	52	51	511.7725	8				
22	23	467.3773	-1	26	27	457.2161	4					28	27	507.5720	-2	54	53	512.4240	7				
23	24	466.3736	-3	27	28	456.1947	26					29	28	508.1320	-7	55	54	512.7350	3				
24	25	465.3621	-5	28	29	455.1610	0					30	29	508.6834	-6	57	56	513.3278	-8				
25	26	464.3434	-1	29	30	454.1221	-3					31	30	509.2258	-3	58	57	513.6099	-12				
26	27	463.3168	0	31	32	452.0223	-2					32	31	509.7589	-1	59	58	513.8836	-3				
27	28	462.2825	2	33	34	449.8927	-2					33	32	510.2824	-2	60	59	514.1456	-13				
28	29	461.2386	-16	34	35	448.8161	-9					34	33	510.7962	-7	61	60	514.4024	20				
29	30	460.1913	9	35	36	447.7348	11					35	34	511.3050	30	62	61	514.6436	-4				
30	31	459.1336	4	36	37	446.6436	4					36	35	511.7977	1								
31	32	458.0679	-4	37	38	445.5453	-1					37	36	512.2840	0								
32	33	456.9944	-14	38	39	444.4408	5					38	37	512.7607	-3								
33	34	455.9160	1	39	40	443.3275	-5					39	38	513.2260	-26								
34	35	454.8282	-3	40	41	442.2090	4					40	39	513.6865	-4								
35	36	453.7327	-10	42	43	439.9497	15					41	40	514.1352	-4								
36	37	452.6297	-18	43	44	438.8099	26					42	41	514.5757	9								
37	38	451.5201	-18	44	45	437.6592	-2					43	42	515.0055	8								
38	39	450.4052	2	45	46	436.5069	23					44	43	515.4302	52								
39	40	449.2808	0	46	47	435.3404	-22					45	44	515.8354	-5								
40	41	448.1481	-12	47	48	434.1729	-9					47	46	516.6286	-3								
41	42	447.0102	-3	48	49	432.9983	2					48	47	517.0109	-2								
42	43	445.8620	-26	49	50	431.8151	-4					50	49	517.7456	-10								
43	44	444.7127	13	50	51	430.6260	0					51	50	518.0968	-31								
44	45	443.5524	13	52	53	428.2292	25					52	51	518.4431	-4								
45	46	442.3844	5	53	54	427.0256	88					53	52	518.7777	2								
47	48	440.0286	6	14	13	492.3032	3					54	53	519.1022	4								
48	49	438.8398	3	15	14	492.9808	-17					55	54	519.4141	-23								
49	50	437.6441	0	17	16	494.3170	16					56	55	519.7227	15								
50	51	436.4419	2	18	17	494.9694	7					57	56	520.0189	26								
51	52	435.2326	2	20	19	496.2491	4					58	57	520.3027	12								
52	53	434.0169	6	21	20	496.8731	-22					60	59	520.8420	-8								
53	54	432.7924	-10	22	21	497.4925	-6					61	60	521.0989	2								
54	55	431.5637	1	23	22	498.1023	3					62	61	521.3437	-11								
55	56	430.3272	1	25	24	499.2937	9					64	63	521.8079	7								
56	57	429.0831	-9	26	25	499.8744	-3					65	64	522.0221	-16								
57	58	427.8359	19	27	26	500.4466	-10					66	65	522.2299	-3								
58	59	426.5810	35	28	27	501.0073	-41					67	66	522.4299	31								
3	2	490.6393	-25	29	28	501.5662	1					69	68	522.7887	-14								
5	4	492.2006	24	30	29	502.1151	33					70	69	522.9565	-3								
7	6	493.7176	-25	31	30	502.6489	6					71	70	523.1148	13								
8	7	494.4683	2	32	31	503.1753	-5																

TABLE 2

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

v	T_v	B_v	$10^6\,D_v$	$10^{13}\,H_v$
0	0	0.434627775(51)	1.16032(12)	-3.84(16)
1	528.567232(80)	0.430115926(71)	1.15518(11)	-3.45(15)
2	1050.14884(11)	0.42565039(11)	1.14974(11)	-3.26(15)
3	1564.85266(16)	0.42123145(22)	1.14408(13)	-3.20(15)
4	2072.78559(19)	0.41685868(30)	1.13822(15)	-3.19(17)
5	2574.05211(22)	0.41253280(35)	1.13251(16)	-2.90(19)
6	3068.75650(26)	0.40825187(49)	1.12613(26)	-3.39(38)
7	3557.00013(32)	0.40401600(74)	1.11911(47)	-4.89(86)
8	4038.88260(39)	0.39982572(91)	1.11184(58)	-6.88(102)
9	4514.5009(16)	0.3956837(42)	1.1081(24)	-

TABLE 3

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

Dunham Coefficient	This work(cm⁻¹)	Previous work[a]
Y_{10}	535.65805(21)	535.6594(15)
Y_{20}	-3.57523(13)	-3.57636(68)
$10^2\ Y_{30}$	1.8453(34)	1.878(11)
$10^5\ Y_{40}$	-4.85(40)	-8.55(64)
$10^7\ Y_{50}$	-9.71(172)	-
Y_{01}	0.436901534(71)	0.43690108(12)
$10^6\ Y_{02}$	-1.16296(12)	-1.16349(47)
$10^{13}\ Y_{03}$	-3.88(16)	-
$10^3\ Y_{11}$	-4.559178(74)	-4.55801(21)
$10^9\ Y_{12}$	5.124(22)	5.491(50)
$10^{14}\ Y_{13}$	2.59(25)	-
$10^5\ Y_{21}$	2.3598(17)	2.3006(98)
$10^{11}\ Y_{22}$	6.16(18)	-
$10^8\ Y_{31}$	-3.74(10)	3.7(11)

[a] Ref. 1.

pumped to remove the impurities up to a temperature of approximately 800°C. Above this temperature, the pumping port was sealed and about 5 Torr of argon buffer gas was added to prevent deposition of material onto the cell windows. In this type of experiment, a partial pressure of about 1 Torr of the high-temperature gas-phase molecule is desirable in order to obtain a high signal-to-noise ratio. The NaF partial pressure is 1 Torr at 1077°C (7), so the spectrum was recorded at 1100°C and the signal-to-noise ratio was approximately 15:1. The resolution of the spectrum was 0.005 cm⁻¹ over the range 400–750 cm⁻¹. A liquid-helium-cooled Si:B detector, a KBr beamsplitter, and KRS-5 cell windows were used. The final recording consisted of 50 coadded scans. A portion of the spectrum showing part of the R branches of the 1–0 and 2–1 bands with the J'' value marked is displayed in Fig. 1.

RESULTS AND DISCUSSION

A total of 1131 transitions was observed and analyzed. The line positions were measured using the PC-Decomp program. This program, developed by J. Brault, determines the line centers by fitting the measured line profiles to Voigt lineshape functions. The assignment of the bands was carried out using an interactive color Loomis–Wood program. The assignment of the rotational lines was based on the previous constants found in the literature (1). The

position of the lines was calibrated in accordance with the strong pure rotational HF lines (8) that appeared in the spectrum. Nine vibrational bands from $v = 1 \rightarrow 0$ to $v = 9 \rightarrow 8$ were observed and the lines positions are reported in Table 1. In order to obtain improved spectroscopic constants for NaF that can describe both the infrared and microwave data, all of the lines reported in Table 1 were fitted together with three microwave transitions (9) and ten millimeter-wave transitions (10). The diode laser measurements (1) were not included, since the present measurements should be superior in precision. The customary spectroscopic constants for the $X^1\Sigma^+$ ground state of NaF are given in Table 2. A reduced standard

TABLE 4

Dunham U_{ij} Coefficients for the $X^1\Sigma^+$ Ground State of NaF

Dunham U coefficients		Value(cm⁻¹)
	U_{10}	1727.62629(51)
	U_{20}	-37.1887(10)
	U_{30}	0.61805(89)
10^3	U_{40}	-4.91(33)
10^4	U_{50}	-3.83(45)
	U_{01}	4.54472982(33)
	U_{11}	-0.15294864(94)
10^3	U_{21}	2.54458(95)
10^5	U_{31}	-1.073(26)
10^4	U_{02}	-1.25801145
10^6	U_{12}	1.76150219
10^8	U_{22}	7.88933921
10^9	U_{32}	2.26004943
10^9	U_{42}	-1.46885511
10^{10}	U_{03}	-4.60356676
10^{10}	U_{13}	1.13037121
10^{12}	U_{23}	-2.19013631
10^{13}	U_{33}	-7.05296243
10^{15}	U_{04}	-7.33487005
10^{15}	U_{14}	4.46605805
10^{15}	U_{24}	1.04780907
10^{16}	U_{34}	-4.28405194
10^{18}	U_{05}	1.06825225
10^{20}	U_{15}	5.72565475
10^{19}	U_{25}	-1.49005919
10^{23}	U_{06}	7.89775842
10^{23}	U_{16}	4.67287807
10^{23}	U_{26}	-3.06742788
10^{27}	U_{07}	3.80267673
10^{27}	U_{17}	-3.17125957
10^{31}	U_{08}	3.84703495
10^{31}	U_{18}	-7.18475571
10^{36}	U_{09}	4.84313730
10^{39}	U_{010}	-2.41947816

deviation of the fit of 0.587 was obtained with 38 parameters.

Dunham Y_{ij} coefficients, listed in Table 3, were obtained by fitting the data set to the energy level expression (11)

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

A total of 14 Dunham Y_{ij} constants were necessary to reproduce the data with a reduced standard deviation of 0.539. These constants are in agreement with, but superior to, those reported by Douay et al. (1). Finally, to minimize the number of free parameters, a mass-reduced Dunham fit (m_{Na} = 22.98977, m_F = 18.998403) was carried out, varying only the U_{i0} and U_{i1} constants (12). All higher order U_{ij} ($j > 1$) constants were constrained by analytical relationships (12). In this case, nine parameters reproduced the data with a standard deviation of 0.741 (see Table 4).

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