Boron and Nitrogen Hyperfine Structure in the Rotational Spectrum of Aminodifluoroborane

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The boron and nitrogen hyperfine structure in the rotational spectra of aminodifluoroborane has been investigated and the quadrupole coupling constants of ^{11}B and nitrogen have been determined. We get the following results for the nuclear quadrupole coupling constants: $\chi_{aa}(^{11}B) = -1.971\,(6)$ MHz, $\chi_{bb}(^{11}B) = -0.500\,(11)$ MHz, $\chi_{cc}(^{11}B) = 2.471\,(11)$ MHz, and $\chi_{aa}(^{14}N) = 0.890\,(5)$ MHz, $\chi_{bb}(^{14}N) = 2.303\,(7)$ MHz, $\chi_{cc}(^{14}N) = -3.193\,(8)$ MHz. Additionally we determined rotational and centrifugal distortion constants according to Watson's A reduction.

Key words: Microwave spectroscopy, nuclear quadrupole hyperfine structure, aminodifluoroborane.

Introduction

Several types of aminoboranes, general formula $R_2N-BR'_2$ can often be prepared by pyrolysis of borane-ammonia complexes:

$$R_3NBR'_3 \xrightarrow{\Delta} R_2N-BR'_2 + RR'.$$

For example aminoborane, NH_2BH_2 ($R = R' = H$), which is isoelectronic with ethylene CH_2CH_2 is prepared by pyrolysis of the precursor molecule ammonia borane NH_3BH_3 [1]. Gaseous aminodifluoroborane, NH_2BF_2, which is isoelectronic with CH_2CF_2 may be prepared using the same preparation method. In this case ammonia-boron trifluorid NH_3BF_3 is the precursor molecule. Both aminoborane compounds mentioned above are unstable in opposition to their organic analogs.

The microwave spectra of 6 isotopomers of aminodifluoroborane, $^{14}NH_2{}^{11}BF_2$, $^{14}NH_2{}^{10}BF_2$, $^{15}NH_2{}^{11}BF_2$, $^{15}NH_2{}^{10}BF_2$, $^{14}ND_2{}^{11}BF_2$ and $^{14}ND_2{}^{10}BF_2$, were first observed and assigned by Lovas and Johnson [2]. They determined the structure and the dipole moment of the planar molecule, which belongs to the point group C_{2v}.

The nitrogen and the boron nucleus in aminodifluoroborane have nuclear spins I larger than 1/2, $I(^{14}N) = 1$ and $I(^{11}B) = 3/2$, which give rise to a hyperfine structure (hfs) of the rotational transitions due to quadrupole coupling of both nuclei. Lovas et al. were not able to resolve these hyperfine structures. Therefore they could not determine the nuclear quadrupole coupling constants of both nuclei.

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Experimental

Gaseous NH_2BF_2 was prepared by pyrolysis of solid ammonia-boron trifluoride NH_3BF_3.

$$H_3NBF_3 \xrightarrow{400-410\,K} H_2N-BF_2 + HF.$$

The precursor substance amonia-boron trifluoride was prepared by the reaction of ammonia and boron trifluoride. 100 Torr of gaseous ammonia was filled in an evacuated glass bulb and frozen at $-196\,^{\circ}C$ (liquid nitrogen). Then 100 Torr of gaseous boron trifluoride was filled in the cooled glass bulb. The mixture was allowed to warm to room temperature. During this time both substances, ammonia and boron trifluoride, react and build the white solid reaction product ammonia-boron trifluoride. This procedure was repeated several times until we gathered about 1 g of ammonia-boron trifluoride. This substance was used as precursor for the pyrolysis without further purification.

The lifetime of NH_2BF_2 was only about 1 min in the brass cells of the microwave Fourier transform (MWFT) spectrometers [3–6]. So we had to use a flow-system to measure the spectra. The rotational transitions of NH_2BF_2 were recorded in the frequency range between 5 and 18 GHz at room temperature and pressures between 0.13 and 0.65 Pa. We measured only transitions of the main isotopomer $^{14}NH_2{}^{11}BF_2$. These transitions are listed in Table 1. The frequencies of all hyperfine components were determined by a

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Table 1. Rotational transitions of $^{14}NH_2{}^{11}BF_2$, ν_c: hypothetical center frequency, δ_c: difference between calculated and hypothetical center frequency, ν_{obs}: frequency of the hyperfine component, $\Delta\nu_{exp}$: experimental hfs-splitting referred to the hypothetical center frequency, $\Delta\nu_{calc}$: calculated hfs-splitting referred to the center frequency, δ: difference between experimental and calculated hfs-splitting. Transitions marked with *, are used for the hfs-analysis.

$J\,K_-\,K_+ - J'\,K'_-\,K'_+$				ν_c [MHz]			δ_c [MHz]
F	I	F'	I'	ν_{obs} [MHz]	$\Delta\nu_{exp}$ [MHz]	$\Delta\nu_{calc}$ [MHz]	δ [MHz]
$1_{01} - 0_{00}$*				14 483.216			−0.049
0.5	0.5	0.5	0.5	14 482.985	−0.231	−0.230	−0.001
0.5	1.5	0.5	0.5	14 483.726	0.510	0.506	0.004
1.5	0.5	0.5	0.5	14 483.198	−0.018	−0.017	−0.001
1.5	2.5	0.5	0.5	14 483.799	0.583	0.583	−0.000
0.5	0.5	1.5	1.5	14 482.985	−0.231	−0.230	−0.001
0.5	1.5	1.5	1.5	14 483.726	0.510	0.506	0.004
1.5	1.5	1.5	1.5	14 482.575	−0.641	−0.636	−0.005
1.5	2.5	1.5	1.5	14 483.799	0.583	0.583	−0.000
2.5	1.5	1.5	1.5	14 483.483	0.267	0.265	0.002
2.5	2.5	1.5	1.5	14 482.826	−0.390	−0.383	−0.007
1.5	1.5	2.5	2.5	14 482.575	−0.641	−0.636	−0.005
1.5	2.5	2.5	2.5	14 483.799	0.583	0.583	−0.000
2.5	1.5	2.5	2.5	14 483.483	0.267	0.265	0.002
2.5	2.5	2.5	2.5	14 482.826	−0.390	−0.383	−0.007
3.5	2.5	2.5	2.5	14 483.274	0.058	0.054	0.004
$2_{21} - 2_{02}$*				15 407.711			0.020
2.5	1.5	2.5	1.5	15 408.865	1.154	1.151	0.003
2.5	2.5	2.5	2.5	15 406.937	−0.774	−0.768	−0.006
3.5	1.5	3.5	1.5	15 406.462	−1.249	−1.240	−0.009
3.5	2.5	3.5	2.5	15 408.719	1.008	1.006	0.002
4.5	2.5	4.5	2.5	15 407.680	−0.031	−0.035	0.004
$3_{21} - 3_{22}$*				13 466.795			0.041
1.5	1.5	1.5	1.5	13 465.838	−0.957	−0.948	−0.009
1.5	2.5	2.5	2.5	13 467.418	0.623	0.624	−0.001
2.5	0.5	2.5	0.5	13 466.875	0.080	0.083	−0.003
2.5	1.5	2.5	1.5	13 467.571	0.776	0.781	−0.005
3.5	2.5	2.5	2.5	13 466.158	−0.637	−0.635	−0.002
3.5	0.5	3.5	0.5	13 467.127	0.332	0.329	0.003
3.5	1.5	3.5	0.5	13 467.356	0.561	0.559	0.002
3.5	2.5	3.5	0.5	13 466.158	−0.637	−0.635	−0.002
3.5	0.5	3.5	1.5	13 467.127	0.332	0.329	0.003
3.5	1.5	3.5	1.5	13 467.356	0.561	0.559	0.002
3.5	2.5	3.5	2.5	13 466.158	−0.637	−0.635	−0.002
3.5	2.5	4.5	2.5	13 466.158	−0.637	−0.635	−0.002
4.5	1.5	4.5	1.5	13 465.955	−0.840	−0.845	0.005
4.5	2.5	4.5	1.5	13 467.220	0.425	0.427	−0.002
4.5	1.5	4.5	2.5	13 465.955	−0.840	−0.845	0.005
4.5	2.5	4.5	2.5	13 467.220	0.425	0.427	−0.002
5.5	2.5	4.5	2.5	13 466.955	0.160	0.162	−0.002
5.5	2.5	5.5	2.5	13 466.955	0.160	0.162	−0.002
$4_{41} - 4_{22}$*				17 341.294			−0.007
1.5	2.5	1.5	2.5	17 340.991	−0.303	−0.310	0.007
2.5	1.5	2.5	1.5	17 340.850	−0.444	−0.450	0.006
2.5	2.5	2.5	2.5	17 341.481	0.187	0.195	−0.008
3.5	0.5	3.5	0.5	17 341.168	−0.126	−0.128	0.002
3.5	1.5	3.5	1.5	17 341.681	0.387	0.392	−0.005
3.5	0.5	3.5	2.5	17 341.548	0.254	0.257	−0.003
3.5	2.5	3.5	2.5	17 341.141	−0.153	−0.147	−0.006
4.5	1.5	4.5	0.5	17 341.520	0.226	0.227	−0.001
4.5	2.5	4.5	0.5	17 341.296	0.002	0.011	−0.009
4.5	1.5	4.5	1.5	17 341.481	0.187	0.194	−0.007
4.5	2.5	4.5	1.5	17 341.268	−0.026	−0.022	−0.004
4.5	0.5	4.5	2.5	17 341.390	0.096	0.099	−0.003
5.5	1.5	5.5	1.5	17 341.023	−0.271	−0.279	0.008
5.5	2.5	5.5	2.5	17 341.646	0.352	0.362	−0.010
6.5	2.5	6.5	2.5	17 341.141	−0.153	−0.158	0.005
$5_{41} - 5_{42}$				11 646.350			0.045
2.5	2.5	2.5	2.5	11 646.615	0.264	0.256	0.008
3.5	1.5	3.5	1.5	11 645.955	−0.396	−0.405	0.009
3.5	2.5	3.5	2.5	11 646.615	0.264	0.267	−0.003
4.5	0.5	4.5	0.5	11 646.503	0.152	0.131	0.021
4.5	1.5	4.5	1.5	11 646.615	0.264	0.275	−0.011
4.5	2.5	4.5	2.5	11 645.955	−0.396	−0.381	−0.015
5.5	0.5	5.5	0.5	11 646.615	0.264	0.249	0.015
5.5	1.5	5.5	1.5	11 646.503	0.152	0.163	−0.011
5.5	2.5	5.5	2.5	11 645.955	−0.396	−0.383	−0.013
6.5	1.5	6.5	1.5	11 645.955	−0.396	−0.403	0.007
6.5	2.5	6.5	2.5	11 646.503	0.152	0.160	−0.008
7.5	2.5	7.5	2.5	11 646.503	0.152	0.148	0.004
$6_{51} - 6_{52}$				10 490.786			0.049
3.5	2.5	3.5	2.5	10 490.988	0.201	0.225	−0.024
4.5	1.5	4.5	1.5	10 490.473	−0.314	−0.301	−0.013
4.5	2.5	4.5	2.5	10 490.988	0.201	0.192	0.009
5.5	0.5	5.5	0.5	10 490.913	0.126	0.135	−0.009
5.5	1.5	5.5	1.5	10 490.988	0.201	0.186	0.015
5.5	2.5	5.5	2.5	10 490.473	−0.314	−0.319	0.005
6.5	0.5	6.5	0.5	10 490.988	0.201	0.208	−0.007
6.5	1.5	6.5	1.5	10 490.913	0.126	0.117	0.009
6.5	2.5	6.5	2.5	10 490.473	−0.314	−0.332	0.018
7.5	1.5	7.5	1.5	10 490.473	−0.314	−0.309	−0.005
7.5	2.5	7.5	2.5	10 490.913	0.126	0.109	0.017
8.5	2.5	8.5	2.5	10 490.913	0.126	0.141	0.015

Table 1 (continued)

$J\ K_-\ K_+ - J'\ K'_-\ K'_+$				ν_c [MHz]			δ_c [MHz]
F	I	F'	I'	ν_{obs} [MHz]	$\Delta\nu_{exp}$ [MHz]	$\Delta\nu_{calc}$ [MHz]	δ [MHz]
$7_{61} - 7_{62}$				9 214.365			0.043
4.5	2.5	4.5	2.5	9 214.552	0.187	0.199	−0.012
5.5	1.5	5.5	1.5	9 214.123	−0.242	−0.233	−0.009
5.5	2.5	5.5	2.5	9 214.500	0.135	0.143	−0.008
6.5	0.5	6.5	0.5	9 214.500	0.135	0.131	0.004
6.5	1.5	6.5	1.5	9 214.500	0.135	0.132	0.003
6.5	2.5	6.5	2.5	9 214.078	−0.287	−0.276	−0.011
7.5	0.5	7.5	0.5	9 214.552	0.187	0.179	0.008
7.5	1.5	7.5	1.5	9 214.448	0.083	0.088	−0.005
7.5	2.5	7.5	2.5	9 214.078	−0.287	−0.291	0.004
8.5	1.5	8.5	1.5	9 214.123	−0.242	−0.245	0.003
8.5	2.5	8.5	2.5	9 214.448	0.083	0.077	0.006
9.5	2.5	9.5	2.5	9 214.500	0.135	0.133	0.002
$9_{81} - 9_{82}$				6 502.249			0.029
6.5	2.5	6.5	2.5	6 502.367	0.119	0.149	−0.030
7.5	1.5	7.5	1.5	6 502.099	−0.149	−0.146	−0.003
7.5	2.5	7.5	2.5	6 502.309	0.061	0.082	−0.021
8.5	0.5	8.5	0.5	6 502.367	0.119	0.109	0.010
8.5	1.5	8.5	1.5	6 502.309	0.061	0.071	−0.010
8.5	2.5	8.5	2.5	6 502.045	−0.203	−0.204	0.001
9.5	0.5	9.5	0.5	6 502.367	0.119	0.131	−0.012
9.5	1.5	9.5	1.5	6 502.309	0.061	0.052	0.009
9.5	2.5	9.5	2.5	6 502.045	−0.203	−0.217	0.014
10.5	1.5	10.5	1.5	6 502.099	−0.149	−0.157	0.008
10.5	2.5	10.5	2.5	6 502.309	0.061	0.041	0.020
11.5	2.5	11.5	2.5	6 502.367	0.119	0.109	0.010
$11_{92} - 11_{93}$				16 174.118			0.011
8.5	2.5	8.5	2.5	16 174.267	0.150	0.173	−0.023
9.5	1.5	9.5	1.5	16 173.912	−0.205	−0.200	−0.005
9.5	2.5	9.5	2.5	16 174.204	0.087	0.108	−0.021
10.5	0.5	10.5	0.5	16 174.267	0.150	0.138	0.012
10.5	1.5	10.5	1.5	16 174.204	0.087	0.099	−0.012
10.5	2.5	10.5	2.5	16 173.850	−0.267	−0.261	−0.006
11.5	0.5	11.5	0.5	16 174.267	0.150	0.161	−0.011
11.5	1.5	11.5	1.5	16 174.204	0.087	0.076	0.011
11.5	2.5	11.5	2.5	16 173.850	−0.267	−0.271	0.004
12.5	1.5	12.5	1.5	16 173.912	−0.205	−0.209	0.004
12.5	2.5	12.5	2.5	16 174.204	0.087	0.068	0.019
13.5	2.5	13.5	2.5	16 174.267	0.150	0.133	0.017

$J\ K_-\ K_+ - J'\ K'_-\ K'_+$				ν_c [MHz]			δ_c [MHz]
F	I	F'	I'	ν_{obs} [MHz]	$\Delta\nu_{exp}$ [MHz]	$\Delta\nu_{calc}$ [MHz]	δ [MHz]
$12_{102} - 12_{103}$				14 199.503			−0.015
9.5	2.5	9.5	2.5	14 199.648	0.145	0.163	−0.018
10.5	1.5	10.5	1.5	14 199.324	−0.179	−0.174	−0.005
10.5	2.5	10.5	2.5	14 199.576	0.073	0.090	−0.017
11.5	0.5	11.5	0.5	14 199.648	0.145	0.133	0.012
11.5	1.5	11.5	1.5	14 199.567	0.064	0.081	−0.017
11.5	2.5	11.5	2.5	14 199.252	−0.251	−0.244	−0.007
12.5	0.5	12.5	0.5	14 199.648	0.145	0.151	−0.006
12.5	1.5	12.5	1.5	14 199.567	0.064	0.064	−0.000
12.5	2.5	12.5	2.5	14 199.252	−0.251	−0.253	0.002
13.5	1.5	13.5	1.5	14 199.324	−0.179	−0.183	0.004
13.5	2.5	13.5	2.5	14 199.576	0.073	0.055	0.018
14.5	2.5	14.5	2.5	14 199.648	0.145	0.128	0.017
$14_{122} - 14_{123}$				10 155.498			−0.074
11.5	2.5	11.5	2.5	10 155.618	0.120	0.134	−0.014
12.5	1.5	12.5	1.5	10 155.367	−0.131	−0.128	−0.003
12.5	2.5	12.5	2.5	10 155.545	0.047	0.061	−0.014
13.5	0.5	13.5	0.5	10 155.618	0.120	0.114	0.006
13.5	1.5	13.5	1.5	10 155.545	0.047	0.054	−0.007
13.5	2.5	13.5	2.5	10 155.295	−0.203	−0.198	−0.005
14.5	0.5	14.5	0.5	10 155.618	0.120	0.124	−0.004
14.5	1.5	14.5	1.5	10 155.545	0.047	0.044	0.003
14.5	2.5	14.5	2.5	10 155.295	−0.203	−0.206	0.003
15.5	1.5	15.5	1.5	10 155.367	−0.131	−0.136	0.005
15.5	2.5	15.5	2.5	10 155.545	0.047	0.036	0.011
16.5	2.5	16.5	2.5	10 155.618	0.120	0.109	0.011
$15_{132} - 15_{133}$				8 235.192			−0.100
12.5	2.5	12.5	2.5	8 235.295	0.103	0.116	−0.013
13.5	1.5	13.5	1.5	8 235.085	−0.107	−0.107	−0.001
13.5	2.5	13.5	2.5	8 235.230	0.038	0.049	−0.011
14.5	0.5	14.5	0.5	8 235.295	0.103	0.099	0.004
14.5	1.5	14.5	1.5	8 235.230	0.038	0.043	−0.005
14.5	2.5	14.5	2.5	8 235.022	−0.170	−0.171	0.001
15.5	0.5	15.5	0.5	8 235.295	0.103	0.107	−0.004
15.5	1.5	15.5	1.5	8 235.230	0.038	0.035	0.003
15.5	2.5	15.5	2.5	8 235.022	−0.170	−0.178	0.008
16.5	1.5	16.5	1.5	8 235.085	−0.107	−0.113	0.006
16.5	2.5	16.5	2.5	8 235.230	0.038	0.029	0.009
17.5	2.5	17.5	2.5	8 235.295	0.103	0.095	0.008

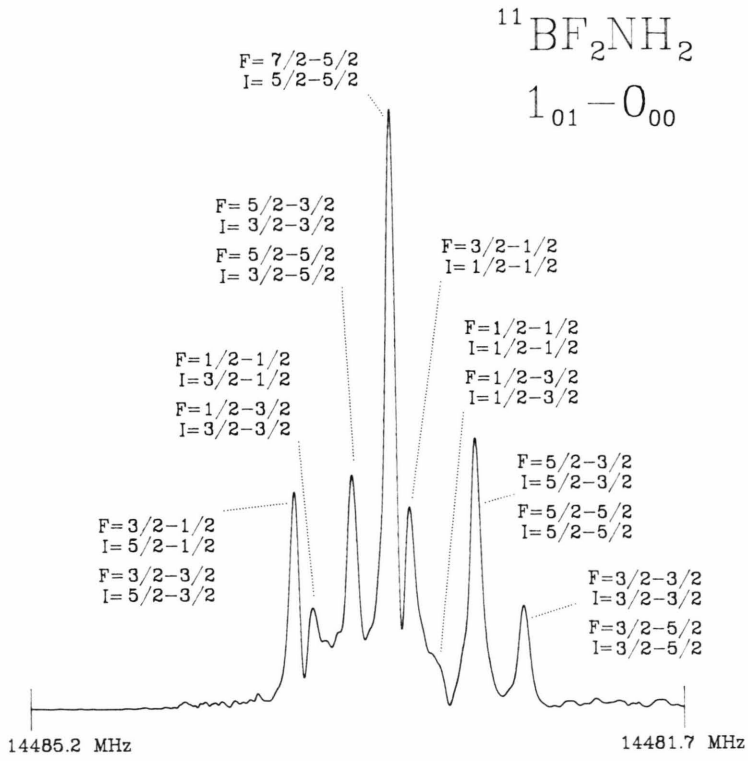

Fig. 1. Rotational transition $J K_- K_+ - J' K'_- K'_+ = 1\,0\,1 - 0\,0\,0$ of aminodifluoroborane, first the nuclear spins of the boron and the nitrogen are coupled to the spin I, and then I is coupled with rotational angular momentum of the molecule J to F. The I- and F-quantum numbers are given. Sample interval: 20 ns, polarizing frequency: 14 484.2 MHz, 1024 data points, $6.5 \cdot 10^6$ averaging cycles, pressure: 0.2 Pa, temperature: 293 K.

Table 2. Rotational and centrifugal distortion constants of NH_2BF_2, standard errors of the constants are given in brackets, Φ_{KJ}, Φ_K, φ_J, φ_{JK} and φ_K are fixed to zero, Φ_{JK} constrained by planarity relations σ: standard deviation of the fit, N: number of rotational transitions, $K_{max}|*,*|$: highest correlation coefficient.

A	10019.504 (15) MHz	$[\Phi_{KJ}$	0.0 Hz]
B	9590.311 (15) MHz	$[\Phi_K$	0.0 Hz]
C	4892.801 (16) MHz	$[\varphi_J$	0.0 Hz]
Δ_J	10.38 (36) kHz	$[\varphi_{JK}$	0.0 Hz]
Δ_{JK}	−16.810 (37) kHz	$[\varphi_K$	0.0 Hz]
Δ_K	6.62 (17) kHz	$\varkappa$	0.83256592
δ_J	0.6357 (50) kHz	σ	101 kHz
δ_K	33.43 (16) kHz	N	45
Φ_J	0.64 (11) Hz	$K_{max}\|A,B\|$	0.978
Φ_{JK}	−0.601 (86) Hz		

Table 3. Boron (^{11}B) and nitrogen quadrupole coupling constants, standard errors given in brackets, σ: standard deviation, N: number of components, $K_{max}|*,*|$: highest correlation coefficient.

nitrogen:		boron:	
χ_+	−0.890 (5) MHz	χ_+	1.971 (6) MHz
χ_-	5.496 (9) MHz	χ_-	−2.971 (14) MHz
χ_{aa}	0.890 (5) MHz	χ_{aa}	−1.971 (6) MHz
χ_{bb}	2.303 (7) MHz	χ_{bb}	−0.500 (11) MHz
χ_{cc}	−3.193 (7) MHz	χ_{cc}	2.471 (11) MHz
		σ	0.005 MHz
$K_{max}\|\chi_+(^{14}N), \chi_+(^{11}B)\|$	0.375	N	53

least squares fit of the signal in the time domain to minimize overlapping effects in the frequency domain [7, 8].

Results and Discussion

NH_2BF_2 is a slightly asymmetric oblate top rotor ($\varkappa = 0.833$) with the dipole moment vector along the a-axis of inertia. Our first calculations of the rotational transitions were based on the rotational and centrifugal distortion constants given in [2]. For the final fit of the rotational parameters we made use of all our transitions. Additionally the transitions which are listed in [2] with the exception of the transition $J K_- K_+ - J' K'_- K'_+ = 4\,1\,3 - 3\,1\,2$ were included. The difference between the calculated and the measured center frequency of the transition mentioned above was about 400 kHz. Therefore it was omitted in the final fit which had a standard deviation of 101 kHz. This rather high standard deviation results from the two sets of transitions with different accuracy. We were able to determine the rotational constants, centrifugal distortion constants according to

Watson's A reduction of fourth order [9] and two of the sextic constants, Φ_J and Φ_{JK}. The other sextic constants were fixed to zero. Additionally we had to use the planarity relation for the sextic constants [10]. The results of the fit are listed in Table 2.

The hyperfine structure of the rotational transitions of NH_2BF_2 were analysed by first order approximation [11]. First calculations of the hyperfine structure of transitions were based on the principal boron coupling constants of BF_2OH (χ_z, χ_x, χ_y) [12] and the nitrogen coupling constants of aminoborane [13]. The assignment and analysis of the hyperfine pattern of the transition $J K_- K_+ - J' K'_- K'_+ = 1\,0\,1 - 0\,0\,0$ (see Fig. 1) yields the coupling constants χ_{aa} of both boron and nitrogen. The determined value of the boron coupling constant $\chi_{aa} = -1.971$ MHz is rather similar to the initial assumption, the coupling constant $\chi_z(BF_2OH) = -1.835$ MHz. The determined value of the nitrogen coupling constant $\chi_{aa} = 0.890$ MHz differs strongly from our initial assumed value $\chi_{aa}(^{11}BH_2{}^{14}NH_2) = 0.095$ MHz.

The four transitions which are marked with * in Table 1 were used for the hyperfine structure analysis. The results are listed in Table 3.

The interpretation of the boron coupling constants of aminodifluoroborane is similar to the discussion of coupling constants of trivalent bonded boron compounds given in [13]. In this paper we listed in Table 5 some trivalent boron compounds and their quadrupole coupling constants. These boron compounds were classified in three groups by the order of magnitude of their coupling constants χ_{cc}. In the picture we use in [13] the boron bonding orbitals are sp^2-hybrids, the orbital perpendicular to the sp^2-plane is a pure p-orbital. The unbalanced occupation of this p-orbital is approximately described by the coupling constant χ_{cc}. The higher the occupation of this orbital, the lower is the coupling constant χ_{cc}. Aminodifluoroborane belongs to the third group of molecules in Table 5 containing $C_6H_5BF_2$ and BF_2OH. These boron compounds have three bonding partners possessing π-electrons. In case of aminodifluoroborane the bonding partners are the two fluorine atoms and the NH_2-group which provide all back donation of π-electrons into the p-orbital of boron. Consequently the value of coupling constant χ_{cc} of NH_2BF_2 is as low as the other χ_{cc} values of the boron compounds of the third group.

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