The Microwave Ground State Spectra of Methylphosphine-Borane-(^{11}B) and Methylphosphine-Trideuteroborane-(^{11}B)

W. Kasten and H. Dreizler
Abteilung Chemische Physik im Institut für Physikalische Chemie der Universität Kiel

R. L. Kuczkowski and M. Soltis LaBarge
Department of Chemistry, University of Michigan, Ann Arbor, MI 48 109

Z. Naturforsch. **41 a**, 835–854 (1986); received March 15, 1986

The microwave ground state spectra of methylphosphine-borane-(^{11}B) and methylphosphine-trideuteroborane-(^{11}B) have been measured by microwave Fourier transform spectroscopy and analysed for ^{11}B-nuclear quadrupole hyperfine splittings and CH_3 and BH_3 torsion fine structure. As high J transitions were measured a centrifugal distortion analysis was necessary. The B–P bond order is discussed.

I. Introduction

This paper presents an investigation of the rotational spectrum of methylphosphine-borane-(^{11}B), $CH_3PH_2BH_3$, and methylphosphine-trideuteroborane-(^{11}B), $CH_3PH_2BD_3$, in the torsional and vibrational ground state.

Some time ago Bryan and Kuczkowski [1] determined the rotational constants, the dipole moment and the r_s-structure of methylphosphine-borane. The barriers hindering internal rotation of the methyl and borane group were subsequently determined from the rotational transitions of the first excited torsional states of the methyl and borane group by Durig et al. [2], since the barriers were too high to resolve splittings in the ground state. We reinvestigated the spectrum of $CH_3PH_2BH_3$ with the higher resolution of microwave Fourier transform (MWFT) spectroscopy to resolve the CH_3 and BH_3 torsion fine structure and the boron-hfs in the ground state.

Additionally, we investigated the spectrum of $CH_3PH_2BD_3$ in the ground state to assign the methyl torsion splittings, because the moment of inertia of the BD_3 group is too high to provide resolvable BD_3 torsion splittings and therefore the spectrum simplifies to the spectrum of a molecule with effectively one top and boron-hfs.

Reprint requests to Prof. Dr. H. Dreizler, Abteilung Chemische Physik im Institut für Physikalische Chemie, Christian-Albrechts-Universität, Olshausenstr. 40, D-2300 Kiel, F.R.G., or Prof. Dr. R. L. Kuczkowski, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109.

II. Experimental

$CH_3PH_2BH_3$ was prepared according to [1] by the reaction of methylphosphine, CH_3PH_2, with diborane, B_2H_6, and $CH_3PH_2BD_3$ by the reaction of CH_3PH_2 with perdeuterodiborane, B_2D_6, respectively.

The MWFT measurements were made at Kiel with a spectrometer described in [3, 4, 5].

The spectra of $CH_3PH_2BD_3$ were recorded in the range of 8 to 18 GHz and the spectra of $CH_3PH_2BH_3$ in the range of 8 to 26 GHz, respectively. Sample pressures were around 0.2 mTorr and the cell temperature was around $-60\,^{\circ}C$.

The measurements at the University of Michigan were made with a conventional spectrometer with Stark effect modulation in the range of 18 to 40 GHz to assign the low J transitions.

III. Spectra

The frequencies and their assignments are listed in Table 1a and 1b for $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$, respectively. The lines measured with a conventional Stark spectrometer are indicated in these tables by "S". Because of the better resolution of a MWFT spectrometer the lines measured by Stark spectroscopy are only used for a first determination of the rotational and fourth order centrifugal constants to prepare the high resolution measurements due to boron-hfs and torsional splitting. For the fine structure analyses these measurements are not used.

0340-4811 / 86 / 0600-0835 $ 01.30/0. – Please order a reprint rather than making your own copy.

Fig. 1. $J_{K_-K_+} = 33_{726} - 33_{727}$ transition of $CH_3PH_2BD_3$ with ^{11}B-hfs and CH_3 torsion splitting. A section of 1.1 MHz out of a 5 MHz range of the power spectrum is given. The small hfs-splitting is about 20 kHz, see Table 1 a. Frequency increases from right to left. Sample interval 100 ns, 6400 k cycles, 1024 data points supplemented by 3072 zeros, pressure 0.1 mTorr, temperature − 50 °C.

Figure 1 gives an example of the MWFT recordings. The measurements of narrow split multiplets were refined by a contour analysis [6].

The assignment was checked by the consistency of the analysis of centrifugal distortion, hfs and torsional fine structure. The three perturbation effects were calculated separately. The calculated spectra were refined by an iterative procedure to fit the measured ones.

The ^{11}B-hfs was analysed by first order perturbation theory to give the nuclear quadrupole coupling constants (program HT1NQ and DH14KS). The deviations from the rigid rotor lines were added to the observed frequencies ν_{obs} of the hfs-components. The hypothetical hfs-unsplit line $\nu_{hfs,\,unsplit}$ was then calculated as a mean value. We proved that no line within the range of our spectrometer is sensitive enough to the off diagonal element χ_{ab} of the quadrupole coupling tensor. The results for the hfs-analyses are given in Table 2 a and 2 b for $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$, respectively. The standard deviations of the fits are 6 kHz for $CH_3PH_2BD_3$ and 9 kHz for $CH_3PH_2BH_3$ for a mean splitting of 88 kHz.

The frequencies $\nu_{hfs,\,unsplit}$ were used to analyse the torsional fine structure by the internal axis method (IAM) in a two top approximation by a program written by Woods [7, 8] and modified by W. Kasten (program AC3IAM).

The following Hamiltonian is used:

$$H = H_R + \sum_{l=1}^{2} [F_l p'^2_{\alpha_l} + \tfrac{1}{2} V_3^{(l)} (1 - 3\cos\alpha_l)] \quad (1)$$

with

$$\begin{aligned} F_l &= (2 I_\alpha^{(l)} r_l^0)^{-1}; \\ r_l^0 &= r_l - \frac{I_\alpha^{(l)} I_\alpha^{(l')} \left(\sum_g \lambda_g^{(l)} \lambda_g^{(l')} / I_g \right)^2}{r_{l'}}, \\ r_l &= 1 - \sum_g \lambda_g^{(l)2} I_\alpha^{(l)} / I_g, \end{aligned} \quad (2)$$

and

$$\begin{aligned} p'_{\alpha_l} &= I_\alpha^{(l)} r_l \dot{\alpha}_l - \sum_g I_g \varrho_g^{(l)} \varrho_g^{(l')} \dot{\alpha}_{l'}, \\ \varrho_g^{(l)} &= \lambda_g^{(l)} I_\alpha^{(l)} / I_g; \\ \lambda_g^{(l)} &= \cos(g, i_l); \quad l \neq l', \end{aligned} \quad (3)$$

where H_R is the rotational Hamiltonian, F_l is the reduced internal rotational constant of the lth top, p'_{α_l} is the angular momentum operator for the internal rotation of the lth top, $V_3^{(l)}$ is the threefold expansion coefficient of the potential barrier in the internal rotation angle α_l of the lth top, $I_\alpha^{(l)}$ is the moment of inertia of the lth top, i_l is the internal rotation axis of the lth top, I_g are the components of the inertia tensor, and $g = a, b, c$ are the principal axes.

For $CH_3PH_2BH_3$ the Fourier coefficients $w_1(s^{(l)})$, $s^{(l)}$ the reduced barrier, the angles $\measuredangle(a, i_l)$ and the moments of inertia $I_\alpha^{(l)}$ of the methyl and borane group could be fitted.

For $CH_3PH_2BD_3$ the internal rotation parameters of the BD_3 group had to be assumed, because no BD_3 torsional splittings could be resolved.

A single top approximation for $CH_3PH_2BD_3$ was not used, because structural parameters of the BD_3 top modify the reduced internal rotational constant F_l of the CH_3 top, see (2).

Table 1a. Measured frequencies ν_{obs} with ^{11}B-hfs and CH_3 torsion of methylphosphine-trideuteroborane-(^{11}B) refined by a contour analysis. $\nu_{hfs,\,unsplit}$: hypothetical frequency without hfs-splitting, Γ: symmetry species, $\nu_{unsplit}$: hypothetical frequency without hfs and torsion-splitting, S: measured by Stark-spectroscopy, not used for the analyses. Frequencies in MHz. The F-quantumnumbers are doubled. * indicates dipole forbidden transitions.

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\,unsplit}$	Γ	$\nu_{unsplit}$
		1a.1. A-transitions :							
		1a.1.1. R-branch :							
1	0	1 - 0	0	0	1-3	9 563.663	9 563.932	A, E	9 563.932
					5-3	9 563.880			
					3-3	9 564.143			
2	0	2 - 1	0	1	S	19 081.88	19 081.88		19 081.88
2	1	2 - 1	1	1	S	18 335.39	18 335.39		18 335.39
2	1	1 - 1	1	0	S	19 920.33	19 920.33		19 920.33
3	0	3 - 2	0	2	S	28 508.91	28 508.91		28 508.91
3	1	3 - 2	1	2	S	27 475.17	27 475.17		27 475.17
3	1	2 - 2	1	1	S	29 850.70	29 850.70		29 850.70
3	2	2 - 2	2	1	S	28 692.27	28 692.27		28 692.27
3	2	1 - 2	2	0	S	28 874.24	28 874.24		28 874.24
4	0	4 - 3	0	3	S	37 804.95	37 804.95		37 804.95
4	1	4 - 3	1	3	S	36 583.10	36 583.10		36 583.10
4	1	3 - 3	1	2	S	39 742.69	39 742.69		39 742.69
4	2	3 - 3	2	2	S	38 219.97	38 219.97		38 219.97
4	2	2 - 3	2	1	S	38 669.38	38 669.38		38 669.38
4	3	2 - 3	3	1	S	38 343.93	38 343.93		38 343.93
4	3	1 - 3	3	0	S	38 353.51	38 353.51		38 353.51
		1a.1.2. Q-branch :							
5	1	4 - 5	1	5	11-11	11 840.164	11 840.279	A	11 840.042
					13-13	11 840.349			
					11-11	11 839.807	11 839.924	E	
					13-13	11 840.003			
6	1	5 - 6	1	6	13-13;11-11	16 501.743	16 501.848	A	16 501.522
					15-15; 9- 9	16 501.943			
					13-13;11-11	16 501.261	16 501.359	E	
					15-15; 9- 9	16 501.447			
7	1	6 - 7	1	7	S	21 842.62	21 842.62		21 842.62
8	1	7 - 8	1	8	S	27 780.35	27 780.35		27 780.35
8	2	6 - 8	2	7	17-17;15-15	8 158.438	8 158.481	A	8 158.314
					19-19;13-13	8 158.524			
					17-17;15-15	8 158.187	8 158.230	E	
					19-19;13-13	8 158.273			
9	1	8 - 9	1	9	S	34 200.91	34 200.91		34 200.91
9	2	7 - 9	2	8	19-19;17-17	11 971.932	11 971.981	A	11 971.734
					21-21;15-15	11 972.027			
					19-19;17-17	11 971.560	11 971.610	E	
					21-21;15-15	11 971.657			
10	2	8 -10	2	9	21-21;19-19	16 612.919	16 612.974	A	16 612.631
					23-23;17-17	16 613.028			
					21-21;19-19	16 612.405	16 612.460	E	
					23-23;17-17	16 612.514			
12	2	10 -12	2	11	S	28 178.76	28 178.76		28 178.76
13	3	10 -13	3	11	27-27;25-25	10 133.217	10 133.248	A	10 133.038
					29-29;23-23	10 133.278			
					27-27;25-25	10 132.901	10 132.933	E	
					29-29;23-23	10 132.965			
14	3	11 -14	3	12	29-29;27-27	14 356.255	14 356.290	A	14 355.993
					31-31;25-25	14 356.325			
					29-29;27-27	14 355.811	14 355.844	E	
					31-31;25-25	14 355.876			
18	4	14 -18	4	15	37-37;35-35	11 141.867	11 141.885	A	11 141.651
					39-39;33-33	11 141.903			
					37-37;35-35	11 141.513	11 141.534	E	
					39-39;33-33	11 141.554			
19	4	15 -19	4	16	39-39;37-37	15 568.634	15 568.656	A	15 568.317
					41-41;35-35	15 568.677			
					39-39;37-37	15 568.126	15 568.148	E	
					41-41;35-35	15 568.170			
23	5	18 -23	5	19	47-47;45-45	11 444.577	11 444.594	A	11 444.339
					49-49;43-43	11 444.610			
					47-47;45-45	11 444.196	11 444.211	E	
					49-49;43-43	11 444.225			
24	5	19 -24	5	20	49-49;47-47	15 901.426	15 901.447	A	15 901.086
					51-51;45-45	15 901.467			
					49-49;47-47	15 900.884	15 900.906	E	
					51-51;45-45	15 900.927			

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
28	6	22 -28	6	23	57-57;55-55	11 227.019	11 227.033	A	11 226.756
					59-59;53-53	11 227.046			
					57-57;55-55	11 226.604	11 226.617	E	
					59-59;53-53	11 226.630			
29	6	23 -29	6	24	59-59;57-57	15 569.096	15 569.107	A	15 568.718
					61-61;55-55	15 569.118			
					59-59;57-57	15 568.512	15 568.524	E	
					61-61;55-55	15 568.536			
33	7	26 -33	7	27	67-67;65-65	10 634.662	10 634.671	A	10 634.378
					69-69;63-63	10 634.680			
					67-67;65-65	10 634.221	10 634.232	E	
					69-69;63-63	10 634.243			
34	7	27 -34	7	28		14 745.498	14 745.498	A	14 745.091
						14 744.888	14 744.888	E	
38	8	30 -38	8	31	77-77;75-75	9 786.098	9 786.105	A	9 785.794
					79-79;73-73	9 786.111			
					77-77;75-75	9 785.631	9 785.638	E	
					79-79;73-73	9 785.645			
39	8	31 -39	8	32		13 577.771	13 577.771	A	13 577.340
						13 577.125	13 577.125	E	
	1a.2. B-transitions :								
	1a.2.1. Q-branch :								
2	1	1 - 2	0	2	5-5	11 492.069	11 492.243	A	11 492.009
					7-7	11 492.311			
					5-5	11 491.719	11 491.892	E	
					7-7	11 491.961			
2	2	1 - 2	1	2	S	31 959.13	31 959.13		31.959.13
2	2	0 - 2	1	1	S	29 627.73	29 627.73		29 627.73
3	1	2 - 3	0	3	7-7	12 833.983	12 834.103	A	12 833.855
					5-5	12 834.064			
					9-9	12 834.158			
					3-3	12 834.256			
					7-7	12 833.613	12 833.731	E	
					5-5	12 833.692			
					9-9	12 833.787			
					3-3	12 833.879			
3	2	2 - 3	1	3	S	33 176.41	33 176.41		33 176.41
3	2	1 - 3	1	2	S	28 651.43	28 651.43		28 651.43
4	1	3 - 4	0	4	9-9	14 771.861	14 771.962	A	14 771.689
					11-11	14 772.025			
					9-9	14 771.449	14 771.553	E	
					11-11	14 771.605			
4	2	2 - 4	1	3	S	27 578.44	27 578.44		27 578.44

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
4	2	3 - 4	1	4	S	34 813.33	34 813.33		34 813.33
5	1	4 - 5	0	5	11-11	17 408.408	17 408.508	A	17 408.175
					13-13	17 408.570			
					11-11	17 407.913	17 408.008	E	
					13-13	17 408.067			
5	2	3 - 5	1	4	S	26 588.49	26 588.49		26 588.49
6	1	5 - 6	0	6	S	20 829.51	20 829.51		20 829.51
6	2	4 - 6	1	5	S	25 878.65	28 878.65		28.878.65
6	2	5 - 6	1	6	S	39 372.04	39 372.04		39 372.04
7	1	6 - 7	0	7	S	25 073.54	25 073.54		25 073.54
7	2	5 - 7	1	6	S	25 634.63	25 634.63		25 634.63
8	1	7 - 8	0	8	S	30 108.49	30 108.49		30 108.49
8	2	6 - 8	1	7	S	26 016.53	26 016.53		26 016.53
9	1	8 - 9	0	9	S	35 829.91	35 829.91		35 829.91
9	2	7 - 9	1	8	S	27 153.51	27 153.51		27 153.51
10	2	8 -10	1	9	S	29 147.98	29 147.98		29 147.98
11	2	9 -11	1	10	S	32 075.34	32 075.34		32 075.34
12	3	9 -12	2	10	S	39 559.27	39 559.27		39 559.27
13	3	10 -13	2	11	S	38 970.62	38 970.62		38 970.62
14	3	11 -14	2	12	S	39 206.29	39 206.29		39 206.29
	1a.2.2. R-branch :								
1	1	1 - 0	0	0	S	19 424.85	19 424.85		19 424.85
2	0	2 - 1	1	1	7-5	9 220.692	9 220.779	A	9 220.957
					7-5	9 220.958	9 221.045	E	
2	1	2 - 1	0	1	S	28 196.17	28 196.17		28 196.17
3	0	3 - 2	1	2	S	19 394.76	19 394.76		19 394.76
4	0	4 - 3	1	3	S	29 724.54	29 724.54		29 724.54
6	1	5 - 5	2	4	S	34 305.28	34 305.28		34 305.28
6	1	6 - 5	2	3	15-13; 9- 7	16 251.334	16 251.445	A	16 252.170
					13-11;11- 9	16 251.566			
					15-13; 9- 7	16 252.417	16 252.528	E	
					13-11;11- 9	16 252.649			

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\,unsplit}$	Γ	$\nu_{unsplit}$
6	2	4 - 5	3	3	15-13; 9- 7	8 507.292	8 507.342	A	8 508.182
					13-11;11- 9	8 507.401			
					15-13; 9- 7	8 509.511	8 509.565	E	
					13-11;11- 9	8 509.629			
7	2	6 - 6	3	3	17-15;11- 9	14 358.438	14 358.507	A	14 359.392
					15-13;13-11	14 358.580			
					17-15;11- 9	14 359.444	14 359.514	E	
					15-13;13-11	14 359.589			
9	3	6 - 8	4	5	21-19;15-13	16 419.262	16 419.300	A	16 420.437
					19-17;17-15	16 419.338			
					21-19;15-13	16 423.680	16 423.714	E	
					19-17;17-15	16 423.748			
9	3	7 - 8	4	4	21-19;15-13	14 952.933	14 952.983	A	14 954.146
					19-17;17-15	14 953.034			
					21-19;15-13	14 951.966	14 952.018	E	
					19-17;17-15	14 952.072			
11	4	7 -10	5	6	25-23;19-17	14 459.515	14 459.554	A	14 460.990
					23-21;21-19	14 459.592			
					25-23;19-17	14 470.194	14 470.235	E	
					23-21;21-19	14 470.276			
					25-23;19-17	14 163.030	14 163.071	E*	
					23-21;21-19	14 163.112			
11	4	8 -10	5	5	25-23;19-17	14 148.761	14 148.802	A	14 150.240
					23-21;21-19	14 148.842			
					25-23;19-17	14 142.394	14 142.432	E	
					23-21;21-19	14 142.470			
					25-23;19-17	14 449.560	14 449.597	E*	
					23-21;21-19	14 449.634			
13	5	8 -12	6	7	29-27;23-21	13 027.300	13 027.333	A	13 029.014
					27-25;25-23	13 027.366			
					29-27;23-21	13 042.504	13 042.535	E	
					27-25;25-23	13 042.566			
					29-27;23-21	12 982.412	12 982.443	E*	
					27-25;25-23	12 982.473			
13	5	9 -12	6	6	29-27;23-21	12 969.785	12 969.819	A	12 971.492
					27-25;25-23	12 969.853			
					29-27;23-21	12 959.615	12 959.647	E	
					27-25;25-23	12 959.679			
					29-27;23-21	13 019.702	13 019.738	E*	
					27-25;25-23	13 019.774			
15	6	9 -14	7	8	33-31;27-25	11 736.533	11 736.566	A	11 738.432
					31-29;29-27	11 736.599			
					33-31;27-25	11 734.834	11 734.866	E*	
					31-29;29-27	11 734.898			
15	6	10 -14	7	7	33-31;27-25	11 726.699	11 726.732	A	11 728.606
					31-29;29-27	11 726.765			
					33-31;27-25	11 734.009	11 734.042	E*	
					31-29;29-27	11 734.075			

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\,unsplit}$	Γ	$\nu_{unsplit}$
17	7	10 -16	8	9	37-35;31-29	10 488.837	10 488.864	A	10 490.871
					35-33;33-31	10 488.890			
					37-35;31-29	10 492.211	10 492.241	E*	
					35-33;33-31	10 492.270			
17	7	11 -16	8	8	37-35;31-29	10 487.229	10 487.257	A	10 489.278
					35-33;33-31	10 487.284			
					37-35;31-29	10 489.886	10 489.917	E*	
					35-33;33-31	10 489.947			
19	8	11 -18	9	10	41-39;35-33	9 262.467	9 262.488	A	9 264.585
					39-37;37-35	9 262.510			
					41-39;35-33	9 266.398	9 266.427	E*	
					39-37;37-35	9 266.456			
19	8	12 -18	9	9	41-39;35-33	9 262.198	9 262.221	A	9 264.337
					39-37;37-35	9 262.243			
					41-39;35-33	9 264.566	9 264.595	E*	
					39-37;37-35	9 264.624			
21	9	12 -20	10	11	45-43;39-37	8 052.619	8 052.641	A	8 054.795
					43-41;41-39	8 052.664			
					45-43;39-37	8 056.480	8 056.510	E*	
					43-41;41-39	8 056.539			
21	9	13 -20	10	10	45-43;39-37	8 052.619	8 052.641	A	8 054.782
					43-41;41-39	8 052.664			
					45-43;39-37	8 055.178	8 055.207	E*	
					43-41;41-39	8 055.236			
22	9	13 -21	10	12	47-45;41-39	17 882.914	17 882.936	A	17 885.021
					45-43;43-41	17 882.957			
					47-45;41-39	17 886.668	17 886.686	E*	
					45-43;43-41	17 886.703			
22	9	14 -21	10	11	47-45;41-39	17 882.857	17 882.882	A	17 884.957
					45-43;43-41	17 882.906			
					47-45;41-39	17 885.337	17 885.360	E*	
					45-43;43-41	17 885.383			
24	10	14 -23	11	13	51-49;45-43	16 668.765	16 668.783	A	16 670.852
					49-47;47-45	16 668.800			
					51-49;45-43	16 672.259	16 672.285	E*	
					49-47;47-45	16 672.310			
24	10	15 -23	11	12	51-49;45-43	16 668.765	16 668.783	A	16 670.852
					49-47;47-45	16 668.800			
					51-49;45-43	16 671.451	16 671.476	E*	
					49-47;47-45	16 671.501			
26	11	15 -25	12	14		15 471.939	15 471.939	A	15 473.960
						15 475.131	15 475.131	E*	
26	11	16 -25	12	13		15 471.939	15 471.939	A	15 473.960
						15 474.799	15 474.799	E*	
28	12	16 -27	13	15		14 292.529	14 292.529	A	14 294.453
						14 295.335	14 295.335	E*	

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
28	12	17 −27	13	14		14 292.529	14 292.529	A	14 294.453
						14 295.481	14 295.481	E*	
30	13	17 −29	14	16		13 131.079	13 131.079	A	13 132.869
						13 133.523	13 133.523	E*	
30	13	18 −29	14	15		13 131.079	13 131.079	A	13 132.869
						13 133.982	13 133.982	E*	
32	14	18 −31	15	17		11 988.389	11 988.389	A	11 990.022
						11 990.428	11 990.428	E*	
32	14	19 −31	15	16		11 988.389	11 988.389	A	11 990.022
						11 991.220	11 991.220	E*	
34	15	19 −33	16	18		10 865.407	10 865.407	A	10 866.874
						10 867.069	10 867.069	E*	
34	15	20 −33	16	17		10 865.407	10 865.407	A	10 866.874
						10 868.118	10 868.118	E*	
36	16	20 −35	17	19		9 763.196	9 763.196	A	9 764.477
						9 764.491	9 764.491	E*	
36	16	21 −35	17	18		9 763.196	9 763.196	A	9 764.477
						9 765.716	9 765.716	E*	
38	17	21 −37	18	20		8 682.877	8 682.877	A	8 683.980
						8 683.848	8 683.848	E*	
38	17	22 −37	18	19		8 682.877	8 682.877	A	8 683.980
						8 685.190	8 685.190	E*	
					1a.2.3. P-branch :				
7	5	3 − 8	4	4	15-17;13-15	15 236.570	15 236.655	A	15 235.120
					17-19;11-13	15 236.742			
					15-17;13-15	15 250.971	15 251.062	E*	
					17-19;11-13	15 251.154			
7	5	2 − 8	4	5	15-17;13-15	15 261.065	15 261.152	A	15 259.625
					17-19;11-13	15 261.241			
					15-17;13-15	15 242.066	15 242.158	E*	
					17-19;11-13	15 242.252			
9	6	4 −10	5	5	19-21;17-19	16 473.739	16 473.805	A	16 472.013
					21-23;15-17	16 473.871			
					19-21;17-19	16 471.579	16 471.642	E*	
					21-23;15-17	16 471.704			
9	6	3 −10	5	6	19-21;17-19	16 477.774	16 477.840	A	16 476.043
					21-23;15-17	16 477.906			
					19-21;17-19	16 474.554	16 474.617	E*	
					21-23;15-17	16 474.680			

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
11	7	5 −12	6	6	23-25;21-23	17 689.956	17 690.014	A	17 688.008
					25-27;19-21	17 690.072			
					23-25;21-23	17 685.827	17 685.882	E*	
					25-27;19-21	17 685.951			
11	7	4 −12	6	7	23-25;21-23	17 690.582	17 690.636	A	17 688.635
					25-27;19-21	17 690.690			
					23-25;21-23	17 688.691	17 688.755	E*	
					25-27;19-21	17 688.805			
14	8	7 −15	7	8	29-31;27-29	9 136.608	9 136.642	A	9 134.537
					31-33;25-27	9 136.675			
					29-31;27-29	9 132.399	9 132.440	E*	
					31-33;25-27	9 132.480			
14	8	6 −15	7	9	29-31;27-29	9 136.881	9 136.919	A	9 134.799
					31-33;25-27	9 136.956			
					29-31;27-29	9 134.750	9 134.788	E*	
					31-33;25-27	9 134.825			
16	9	8 −17	8	9	33-35;31-33	10 332.101	10 332.137	A	10 329.917
					35-37;29-31	10 332.173			
					33-35;31-33	10 327.884	10 327.920	E*	
					35-37;29-31	10 327.955			
16	9	7 −17	8	10	33-35;31-33	10 332.101	10 332.137	A	10 329.928
					35-37;29-31	10 332.173			
					33-35;31-33	10 329.683	10 329.718	E*	
					35-37;29-31	10 329.753			
18	10	9 −19	9	10	37-39;35-37	11 513.972	11 514.004	A	11 511.742
					39-41;33-35	11 514.035			
					37-39;35-37	11 509.960	11 509.992	E*	
					39-41;33-35	11 510.023			
18	10	8 −19	9	11	37-39;35-37	11 513.972	11 514.004	A	11 511.742
					39-41;33-35	11 514.035			
					37-39;35-37	11 511.209	11 511.241	E*	
					39-41;33-35	11 511.273			
20	11	10 −21	10	11	41-43;39-41	12 681.294	12 681.323	A	12 679.067
					43-45;37-39	12 681.351			
					41-43.39-41	12 677.566	12 677.593	E*	
					43-45;37-39	12 677.620			
20	11	9 −21	10	12	41-43;39-41	12 681.294	12 681.323	A	12 679.067
					43-45;37-39	12 681.351			
					41-43;39-41	12 678.269	12 678.297	E*	
					43-45;37-39	12 678.324			
22	12	11 −23	11	12	45-47;43-45	13 832.892	13 832.920	A	13 830.713
					47-49;41-43	13 832.947			
					45-47;43-45	13 829.490	13 829.517	E*	
					47-49;41-43	13 829.544			

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
22	12	10	-23	11	13	45-47;43-45	13 832.892	13 832.920	A	13 830.713
						47-49;41-43	13 832.947		
						45-47;43-45	13 829.692	13 829.719	E*	
						47-49;41-43	13 829.745		
24	13	12	-25	12	13	49-51;47-49	14 967.520	14 967.547	A	14 965.432
						51-53;45-47	14 967.573		
						49-51;47-49	14 964.501	14 964.530	E*	
						51-53;45-47	14 964.558		
24	13	11	-25	12	14	49-51;47-49	14 967.520	14 967.547	A	14 965.432
						51-53;45-47	14 967.573		
						49-51;47-49	14 964.207	14 964.236	E*	
						51-53;45-47	14 964.264		
26	14	13	-27	13	14	53-55;51-53	16 083.882	16 083.909	A	16 081.927
						55-57;49-51	16 083.935		
						53-55;51-53	16 081.277	16 081.299	E*	
						55-57;49-51	16 081.320		
26	14	12	-27	13	15	53-55;51-53	16 083.882	16 083.909	A	16 081.927
						55-57;49-51	16 083.935		
						53-55;51-53	16 080.570	16 080.594	E*	
						55-57;49-51	16 080.618		

Table 1 a (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
28	15	14	-29	14	15	57-59;55-57	17 180.719	17 180.738	A	17 178.918
						59-61;53-55	17 180.757		
						57-59;55-57	17 178.532	17 178.554	E*	
						59-61;53-55	17 178.575		
28	15	13	-29	14	16	57-59;55-57	17 180.719	17 180.738	A	17 178.918
						59-61;53-55	17 180.757		
						57-59;55-57	17 177.464	17 177.487	E*	
						59-61;53-55	17 177.509		
31	16	16	-32	15	17		8 562.618	8 562.618	A	8 561.041
							8 560.908	8 560.908	E*	
31	16	15	-32	15	18		8 562.618	8 562.618	A	8 561.041
							8 559.626	8 559.626	E*	
33	17	17	-34	16	18		9 630.904	9 630.904	A	9 629.509
							9 629.570	9 629.570	E*	
33	17	16	-34	16	19		9 630.904	9 630.904	A	9 629.509
							9 628.072	9 628.072	E*	
35	18	18	-36	17	19		10 676.427	10 676.427	A	10 675.235
							10 675.446	10 675.446	E*	
35	18	17	-36	17	20		10 676.427	10 676.427	A	10 675.235
							10 673.854	10 673.854	E*	

Table 1 b. Measured frequencies ν_{obs} with ^{11}B-hfs and CH_3 and BH_3 torsion of methylphosphine-borane-(^{11}B). See Table 1 a.

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
1b.1. A-transitions :									
1b.1.1. Q-branch :									
4	1	3	- 4	1	4	9-9	9 938.460	9 938.577	AA	9 938.358
						7-7	9 938.521			
						11-11	9 938.648			
						5-5	9 938.708			
						9-9	9 938.123	9 938.249	EE	
						7-7	9 938.199			
						11-11	9 938.311			
						5-5	9 938.392			
5	1	4	- 5	1	5	11-11	14 865.580	14 865.697	AA	14 865.385
						9-9	14 865.638			
						13-13	14 865.765			
						7-7	14 865.825			
						11-11	14 865.112	14 865.229	EE	
						9-9	14 865.168			
						13-13	14 865.297			
						7-7	14 865.357			

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
6	1	5	- 6	1	6	13-13;11-11	20 706.192	20 706.286	AA	20 705.851
						15-15; 9- 9	20 706.374			
						13-13;11-11	20 705.541	20 705.633	EE	
						15-15; 9- 9	20 705.719			
8	1	7	- 8	1	8	S	34 779.35	34 779.35	AA	34 778.64
						S.	34 778.29	34 778.29	EE	
8	2	6	- 8	2	7	17-17;15-15	10 714.942	10 714.991	AA	10 714.812
						19-19;13-13	10 715.038			
						17-17;15-15	10 714.672	10 714.722	EE	
						19-19;13-13	10 714.771			
9	2	7	- 9	2	8	19-19;17-17	15 643.062	15 643.112	AA	15 642.843
						21-21;15-15	15 643.161			
						19-19;17-17	15 642.659	15 642.708	EE	
						21-21;15-15	15 642.756			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
10	2	8 −10	2	9	21-21;19-19	21 598.424	21 598.478	AA	21 598.110
					23-23;17-17	21 598.532			
					21-21;19-19	21 597.871	21 597.926	EE	
					23-23;17-17	21 597.981			
11	2	9 −11	2	10	S	28 514.31	28 514.31	AA	28 513.85
					S	28 513.62	28 513.62	EE	
12	2	10 −12	2	11	S	36 289.78	36 289.78	AA	36 289.13
					S	36 288.81	36 288.81	EE	
12	3	9 −12	3	10	25-25;23-23	9 423.234	9 423.264	AA	9 423.155
					27-27;21-21	9 423.294			
					25-25;23-23	9 423.072	9 423.101	EE	
					27-27;21-21	9 423.130			
13	3	10 −13	3	11	27-27;25-25	13 902.042	13 902.075	AA	13 901.902
					29-29;23-23	13 902.107			
					27-27;25-25	13 901.782	13 901.815	EE	
					29-29;23-23	13 901.848			
14	3	11 −14	3	12	29-29;27-27	19 523.016	19 023.053	AA	19 522.795
					31-31;25-25	19 523.090			
					29-29;27-27	19 522.627	19 522.666	EE	
					31-31;25-25	19 522.704			
15	3	12 −15	3	13	S	26 266.68	26 266.68		26 266.68
17	4	13 −17	4	14	35-35;33-33	11 116.432	11 116.453	AA	11 116.360
					37-37;31-31	11 116.474			
					35-35;33-33	11 116.295	11 116.314	EE	
					37-37;31-31	11 116.333			
18	4	14 −18	4	15	37-37;35-35	15 976.443	15 976.467	AA	15 976.310
					39-39;33-33	15 976.490			
					37-37;35-35	15 976.206	15 976.231	EE	
					39-39;33-33	15 976.256			
19	4	15 −19	4	16	39-39;37-37	22 063.278	22 063.314	AA	22 063.079
					41-41;35-35	22 063.349			
					39-39;37-37	22 062.924	22 062.961	EE	
					41-41;35-35	22 062.997			
21	5	16 −21	5	17	43-43;41-41	8 245.251	8 245.265	AA	8 245.228
					45-45;39-39	8 245.278			
					43-43;41-41	8 245.196	8 245.210	EE	
					45-45;39-39	8 245.224			
22	5	17 −22	5	18	45-45;43-43	12 107.672	12 107.687	AA	12 107.601
					47-47;41-41	12 107.701			
					45-45;43-43	12 107.540	12 107.558	EE	
					47-47;41-41	12 107.575			
23	5	18 −23	5	19	47-47;45-45	17 164.144	17 164.166	AA	17 164.012
					49-49;43-43	17 164.187			
					47-47;45-45	17 163.916	17 163.935	EE	
					49-49;43-43	17 163.954			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
24	5	19 −24	5	20	49-49;47-47	23 515.914	23 515.945	AA	23 515.715
					51-51;45-45	23 515.975			
					49-49;47-47	23 515.568	23 515.600	EE	
					51-51;45-45	23 515.631			
26	6	20 −26	6	21	53-53;51-51	8 641.753	8 641.764	AA	8 641.715
					55-55;49-49	8 641.774			
					53-53;51-51	8 641.679	8 641.690	EE	
					55-55;49-49	8 641.701			
27	6	21 −27	6	22	55-55;53-53	12 526.647	12 526.660	AA	12 526.559
					57-57;51-51	12 526.673			
					55-55;53-53	12 526.495	12 526.509	EE	
					57-57;51-51	12 526.523			
28	6	22 −28	6	23	57-57;55-55	17 620.288	17 620.303	AA	17 620.123
					59-59;53-53	17 620.318			
					57-57;55-55	17 620.014	17 620.033	EE	
					59-59;53-53	17 620.052			
29	6	23 −29	6	24	59-59;57-57	24 053.990	24 054.011	AA	24 053.761
					61-61;55-55	24 054.031			
					59-59;57-57	24 053.616	24 053.636	EE	
					61-61;55-55	24 053.656			
31	7	24 −31	7	25	63-63;61-61	8 681.029	8 681.038	AA	8 680.950
					65-65;59-59	8 681.046			
					63-63;61-61	8 680.899	8 680.906	EE	
					65-65;59-59	8 680.913			
32	7	25 −32	7	26	65-65;63-63	12 476.720	12 476.731	AA	12 476.578
					67-67;61-61	12 476.741			
					65-65;63-63	12 476.491	12 476.502	EE	
					67-67;61-61	12 476.513			
33	7	26 −33	7	27	67-67;65-65	17 469.273	17 469.285	AA	17 469.050
					69-69;63-63	17 469.296			
					67-67;65-65	17 468.920	17 468.933	EE	
					69-69;63-63	17 468.945			
34	7	27 −34	7	28		23 818.371	23 818.371	AA	23 818.022
						23 817.848	23 817.848	EE	
36	8	28 −36	8	29		8 432.719	8 432.719	AA	8 432.577
						8 432.506	8 432.506	EE	
37	8	29 −37	8	30		12 047.737	12 047.737	AA	12 047.522
						12 047.415	12 047.415	EE	
38	8	30 −38	8	31		16 821.472	16 821.472	AA	16 821.147
						16 820.984	16 820.984	EE	
39	8	31 −39	8	32		22 937.155	22 937.155	AA	22 936.681
						22 936.444	22 936.444	EE	

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
1b.1.2. R-branch :									
1	0	1 - 0	0	0	1-3	10 950.352	10 950.590		10 950.590
					5-3	10 950.549			
					3-3	10 950.772			
2	0	2 - 1	0	1		21 839.739	21 839.739	AA	21 839.692
						21 839.666	21 839.666	EE	
2	1	1 - 1	1	0		22 896.801	22 896.801	AA	22 896.734
						22 896.688	22 896.688	EE	
2	1	2 - 1	1	1	7-5	20 905.546	20 905.612		20 905.612
					5-3	20 905.763			
3	0	3 - 2	0	2	S	32 607.51	32 607.51		32 607.51
3	1	2 - 2	1	1	S	34 305.09	34 305.09		34 305.09
3	1	3 - 2	1	2	S	31 321.00	31 321.00		31 321.00
3	2	1 - 2	2	0	S	33 095.67	33 095.67		33 095.67
3	2	2 - 2	2	1	S	32 852.45	32 852.45		32 852.45
1b.2. B-transitions :									
1b.2.1. Q-branch :									
1	1	0 - 1	0	1	3-5;5-3	12 611.430	12 611.552	AA	12 611.226
					5-5	12 611.644			
					3-5;5-3	12 610.934	12 611.063	EE	
					5-5	12 611.155			
2	1	1 - 2	0	2	5-5	13 668.473	13 668.633	AA	13 668.285
					3-3	13 668.628			
					7-7	13 668.702			
					1-1	-			
					5-5	13 667.948	13 668.111	EE	
					3-3	13 668.107			
					7-7	13 668.180			
					1-1	13 668.353			
3	1	2 - 3	0	3	7-7	15 366.138	15 366.248	AA	15 365.867
					5-5	15 366.206			
					9-9	15 366.307			
					3-3	15 366.387			
					7-7	15 365.562	15 365.676	EE	
					5-5	15 365.643			
					9-9	15 365.732			
					3-3	15 365.814			
3	2	1 - 3	1	2	S	33 697.57	33 697.57	AA	33 696.88
					S	33 696.54	33 696.54	EE	
3	2	2 - 3	1	3	S	39 363.61	39 363.61	AA	39 362.63
					S	39 362.14	39 362.14	EE	

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
4	1	3 - 4	0	4	9-9	17 826.634	17 826.741	AA	17 826.304
					11-11	17 826.801			
					5-5	17 826.860			
					9-9	17 825.989	17 826.085	EE	
					11-11	17 826.149			
					5-5	17 826.214			
4	2	2 - 4	1	3	S	32 389.15	32 389.15	AA	32 388.42
					S	32 388.05	32 388.05	EE	
5	1	4 - 5	0	5	11-11; 9- 9	21 182.432	21 182.515	AA	21 182.010
					13-13; 7- 7	21 182.590			
					11-11; 9- 9	21 181.677	21 181.758	EE	
					13-13; 7- 7	21 181.832			
5	2	3 - 5	1	4	S	31 219.94	31 219.94	AA	31 219.26
					S	31 218.92	31 218.92		
6	1	5 - 6	0	6	13-13;11-11	25 537.682	25 537.769	AA	25 537.185
					15-15; 9- 9	25 537.853			
					13-13;11-11	25 536.812	25 536.893	EE	
					15-15; 9- 9	25 536.970			
6	2	4 - 6	1	5	S	30 443.64	30 443.64	AA	30 442.91
					S	30 442.54	30 442.54	EE	
7	1	6 - 7	0	7	S	30 926.47	30 926.47	AA	30 925.80
					S	30 925.46	30 925.46		
7	2	5 - 7	1	6	S	30 296.29	30 296.29	AA	30 295.58
					S	30 295.22	30 295.22	EE	
8	1	7 - 8	0	8	S	37 286.15	37 286.15	AA	37 285.34
					S	37 284.94	37 284.94	EE	
8	2	6 - 8	1	7	S	30 975.84	30 975.84	AA	30 975.13
					S	30 974.77	30 974.77	EE	
9	2	7 - 9	1	8	S	32 640.84	32 640.84	AA	32 640.12
					S	32 639.76	32 639.76	EE	
10	2	8 -10	1	9	S	35 414.79	35 414.79	AA	35 413.97
					S	35 413.56	35 413.56	EE	
11	2	9 -11	1	10	S	39 381.33	39 381.33	AA	39 380.48
					S	39 380.06	39 380.06	EE	
1b.2.2. R-branch :									
1	1	1 - 0	0	0		22 566.497	22 566.497	AA	22 566.169
						22 566.000	22 566.000	EE	
2	0	2 - 1	1	1	7-5	10 223.770	10 223.844	AA	10 224.111
					5-3	10 224.040			
					7-5	10 224.172	10 224.249	EE	
					5-3	10 224.422			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
2	1	2 - 1	0	1	s	32 521.26	32 521.26		32 521.26
3	0	3 - 2	1	2	9-7	21 925.788	21 925.814	AA	21 926.035
					7-5	21 925.834			
					9-7	21 926.111	21 926.137	EE	
					7-5	21 926.157			
4	0	4 - 3	1	3	s	33 806.62	33 806.62		33 806.62
4	1	3 - 3	2	2	11- 9; 5- 3	12 269.373	12 269.431	AA	12 270.215
					9- 7; 7- 5	12 269.498			
					11- 9; 5- 3	12 270.665	12 270.723	EE	
					9- 7; 7- 5	12 270.791			
5	1	4 - 4	2	3		25 459.807	25 459.807	AA	25 460.507
						25 460.890	25 460.890	EE	
6	1	6 - 5	2	3	15-13; 9- 7	16 199.950	16 200.070	AA	16 201.151
					13-11;11- 9	16 200.197			
					15-13; 9- 7	16 201.560	16 201.666	EE	
					13-11;11- 9	16 201.782			
6	1	5 - 5	2	4	s	38 970.57	38 970.57	AA	38 971.14
					s	38 971.42	38 971.42	EE	
6	2	4 - 5	3	3	15-13; 9- 7	8 329.065	8 329.112	AA	8 330.515
					13-11;11- 9	8 329.134			
					15-13; 9- 7	8 329.134	8 329.155	EE	
					13-11;11- 9	8 329.207			
					15-13; 9- 7	8 332.238	8 332.281	EE, EA	
					13-11;11- 9	8 332.330			
					15-13; 9- 7	8 332.330	8 332.384	AE	
					13-11;11- 9	8 332.439			
7	2	6 - 6	3	3	17-15;11- 9	14 342.515	14 342.594	AA	14 344.015
					15-13;13-11	14 342.673			
					17-15;11- 9	14 344.267	14 344.346	EE	
					15-13;13-11	14 344.427			
7	2	5 - 6	3	4	17-15;11- 9	21 378.046	21 378.068	AA	21 379.409
					15-13;13-11	21 378.098			
					17-15;11- 9	21 378.098	21 378.124	EE	
					15-13;13-11	21 378.148			
					17-15;11- 9	21 380.385	21 380.407	EE	
					15-13;13-11	21 380.431			
					17-15;11- 9	21 380.431	21 380.458	AE, EA	
					15-13;13-11	21 380.482			
7	1	7 - 6	2	4	17-15;11- 9	21 347.306	21 347.394	AA	21 348.571
					15-13;13-11	21 347.492			
					17-15;11- 9	21 349.050	21 349.148	EE	
					15-13;13-11	21 349.255			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
8	2	7 - 7	3	4	19-17;13-11	23 888.225	23 888.281	AA	23 889.714
					17-15;15-13	23 888.339			
					19-17;13-11	23 888.272	23 888.326	EE	
					17-15;15-13	23 888.383			
					19-17;13-11	23 890.181	23 890.235	EE	
					17-15;15-13	-			
					19-17;13-11	-	23 890.292	AE, EA	
					17-15;15-13	23 890.349			
9	3	6 - 8	4	5	21-19;15-13	16 688.330	16 688.361	AA	16 690.241
					19-17;17-15	16 688.400			
					21-19;15-13	16 688.400	16 688.422	EE	
					19-17;17-15	16 688.455			
					21-19;15-13	16 694.023	16 694.049	EE, EA	
					19-17;17-15	16 694.075			
					21-19;15-13	16 694.185	16 694.209	AE	
					19-17;17-15	16 694.233			
9	3	7 - 8	4	4	21-19;15-13	14 620.160	14 620.206	EE, AE	14 622.270
					19-17;17-15	14 620.252			
					21-19;15-13	14 620.331	14 620.373	AA, EA	
					19-17;17-15	14 620.413			
					21-19;15-13	14 620.413	14 620.443	EE	
					19-17;17-15	14 620.487			
10	3	8 - 9	4	5	23-21;17-15	25 543.845	25 543.881	AA	25 545.735
					21-19;19-17	25 543.912			
					23-21;17-15	25 543.912	25 543.946	EE	
					21-19;19-17	25 543.982			
					23-21;17-15	25 545.386	25 545.422	EE, AE	
					21-19, 19-17	25 545.469			
					23-21;17-15	25 545.469	25 545.523	EA	
					21-19;19-17	25 545.559			
11	4	7 -10	5	6	25-23;19-17	13 577.630	13 577.664	AA	13 579.974
					23-21;21-19	13 577.701			
					25-23;19-17	13 577.701	13 577.739	EE	
					23-21;21-19	13 577.773			
					25-23;19-17	13 590.808	13 590.844	EA	
					23-21;21-19	13 590.879			
					25-23;19-17	13 590.927	13 590.959	EE	
					23-21;21-19	13 590.990			
					25-23;19-17	-	13 591.209	AE	
					23-21;21-19	13 591.243			
					25-23;19-17	13 129.835	13 129.869	EE*	
					23-21;21-19	-			
					25-23;19-17	-	13 130.137	AE*	
					23-21;21-19	13 130.171			
11	4	8 -10	5	5	25-23;19-17	13 110.572	13 110.608	AA	13 112.909
					23-21;21-19	13 110.638			
					25-23;19-17	13 110.638	13 110.669	EE	
					23-21;21-19	13 110.704			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
					25-23;19-17	13 103.933	13 103.969	AE	
					23-21;21-19	–			
					25-23;19-17	13 104.061	13 104.094	EE	
					23-21;21-19	13 104.126			
					25-23;19-17	–	13 104.356	EA	
					23-21;21-19	13 104.391			
					25-23;19-17	13 565.129	13 565.166	EE*, AE*	
					23-21;21-19	13 565.202			
					25-23;19-17	–	13 565.412	EA*	
					23-21;21-19	13 565.447			
12	4	8 -11	5	7	27-25;21-19	25 387.971	25 387.996	AA	25 390.230
					25-23;23-21	25 388.028			
					27-25;21-19	25 388.028	25 388.055	EE	
					25-23;23-21	25 388.080			
						24 496.569	24 496.569	EE*, EA*	
						24 496.812	24 496.812	AE*	
12	4	9 -11	5	6	27-25;21-19	24 469.894	24 469.923	AA	24 472.165
					25-23;23-21	24 469.954			
					27-25;21-19	24 469.954	24 469.987	EE	
					25-23;23-21	24 470.016			
					27-25;21-19	24 466.562	24 466.591	AE	
					25-23;23-21	24 466.647			
					27-25;21-19	24 466.647	24 466.671	EE	
					25-23;23-21	24 466.700			
					27-25;21-19	–	24 466.880	EA	
					25-23;23-21	24 466.909			
						25 367.882	25 367.882	EE*	
13	5	9 -12	6	6	29-27;23-21	11 091.298	11 091.329	AA	11 093.957
					27-25;25-23	11 091.359			
					29-27;23-21	11 091.359	11 091.388	EE	
					27-25;25-23	11 091.419			
					29-27;23-21	11 174.366	11 174.397	AE*	
					27-25;25-23	11 174.427			
					29-27;23-21	11 174.427	11 174.461	EE*	
					27-25;25-23	11 174.492			
					29-27;23-21	11 174.619	11 174.650	EA*	
					27-25;25-23	11 174.680			
13	5	8 -12	6	7	29-27;23-21	11 183.266	11 183.296	AA	11 185.927
					27-25;25-23	11 183.326			
					29-27;23-21	11 183.380	11 183.410	EE	
					27-25;25-23	11 183.439			
					29-27;23-21	11 107.811	11 107.842	EA*	
					27-25;25-23	11 107.871			
					29-27;23-21	11 107.871	11 107.904	EE*	
					27-25;25-23	11 107.935			
					29-27;23-21	–	11 108.124	AE*	
					27-25;25-23	11 108.155			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
14	5	9 -13	6	8	31-29;25-23	22 712.431	22 712.456	AA	22 715.004
					29-27;27-25	22 712.498			
					31-29;25-23	22 712.498	22 712.533	EE	
					29-27;27-25	22 712.558			
					31-29;25-23	22 728.866	22 728.891	EA	
					29-27;27-25	–			
					31-29;25-23	22 728.998	22 729.024	EE	
					29-27;27-25	22 729.049			
					31-29;25-23	22 729.208	22 729.233	AE	
					29-27;27-25	–			
					31-29;25-23	22 538.660	22 538.685	EA*	
					29-27;27-25	–			
					31-29;25-23	22 538.759	22 538.790	EE*	
					29-27;27-25	22 538.820			
						22 539.036	22 539.036	AE*	
14	5	10 -13	6	7	31-29;25-23	22 520.725	22 520.750	AA	22 523.299
					29-27;27-25	22 520.785			
					31-29;25-23	22 520.785	22 520.820	EE	
					29-27;27-25	22 520.845			
					31-29;25-23	22 511.579	22 511.604	AE	
					29-27;27-25	–			
					31-29;25-23	22 511.714	22 511.742	EE	
					29-27;27-25	22 511.769			
					31-29;25-23	–	22 511.961	EA	
					29-27;27-25	22 511.936			
					31-29;25-23	22 701.852	22 701.877	AE*	
					29-27;27-25	–			
					31-29;25-23	22 701.944	22 701.967	EE*	
					29-27;27-25	22 701.990			
						22 702.182	22 702.182	EA*	
15	6	10 -14	7	7	33-31;27-25	8 979.941	8 979.967	AA, EE	8 982.822
					31-29;29-27	8 979.993			
					33-31;27-25	8 993.520	8 993.548	EE*	
					31-29;29-27	8 993.575			
					33-31;27-25	8 993.575	8 993.606	AE*	
					31-29;29-27	8 993.636			
					33-31;27-25	8 993.636	8 993.661	EA*	
					31-29;29-27	8 993.689			
15	6	9 -14	7	8	33-31;27-25	8 996.650	8 996.681	AA	8 999.514
					31-29;29-27	8 996.712			
					33-31;27-25	–	8 996.857	EE	
					31-29;29-27	8 996.892			
					33-31;27-25	8 991.435	8 991.463	EE*	
					31-29;29-27	8 991.488			
					33-31;27-25	8 991.488	8 991.518	EA*	
					31-29;29-27	8 991.548			
					33-31;27-25	8 991.548	8 991.573	AE*	
					31-29;29-27	8 991.601			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
16	6	10	-15	7	9	20 421.011	20 421.011	AA	20 423.796
						20 421.167	20 421.167	EE	
						20 442.637	20 442.637	EA	
						20 442.905	20 442.905	EE	
						20 443.134	20 443.134	AE	
						20 398.988	20 398.988	EE*,EA*	
						20 399.176	20 399.176	AE*	
16	6	11	-15	7	8	20 384.687	20 384.687	AA,EE	20 387.436
						20 370.790	20 370.790	AE	
						20 371.030	20 371.030	EE	
						20 371.267	20 371.267	EA	
						20 414.837	20 414.837	EE*,AE*	
						20 415.020	20 415.020	EA*	
18	7	11	-17	8	10	39-37;33-31 18 249.125	18 249.149	AA	18 252.009
						37-35;35-33 18 249.172			
						39-37;33-31 -	18 249.336	EE	
						37-35;35-33 18 249.357			
						39-37;33-31 18 250.661	18 250.682	EE*	
						37-35;35-33 18 250.719			
						39-37;33-31 18 250.719	18 250.753	AE*,EA*	
						37-35;35-33 18 250.775			
18	7	12	-17	8	9	18 242.636	18 242.636	AA	18 245.523
						18 248.989	18 248.989	EE*	
						39-37;33-31 18 249.545	18 249.567	EE*	
						37-35;35-33 18 249.603			
						39-37;33-31 18 249.603	18 249.638	AE*,EA*	
						37-35,35-33 18 249.661			
20	8	12	-19	9	11	16 130.605	16 130.605	AA	16 133.473
						16 134.831	16 134.831	EE*	
20	8	13	-19	9	10	16 129.521	16 129.521	AA	16 132.382
						16 133.813	16 133.813	EE*	
22	9	13	-21	10	12	14 049.609	14 049.609	AA	14 052.367
						14 049.473	14 049.473	EE*	
						14 053.722	14 053.722	EE*	
22	9	14	-21	10	11	14 049.379	14 049.379	AA	14 052.174
						14 049.609	14 049.609	EE*	
						14 053.489	14 053.489	EE*	
23	9	14	-22	10	13	49-47;43-41 25 397.710	25 397.729	AA	25 400.426
						47-45;45-43 25 397.748			
						49-47;43-41 25 397.850	25 397.871	EE	
						47-45;45-43 25 397.891			
						49-47;43-41 25 397.488	25 397.510	EE*	
						47-45;45-43 25 397.531			
						49-47;43-41 25 401.626	25 401.647	EE*,AE*	
						47-45;45-43 25 401.668			
						49-47;43-41 25 401.668	25 401.690	EA*	
						47-45;45-43 25 401.712			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
23	9	15	-22	10	12	49-47;43-41 25 397.333	25 397.354	AA,EE	25 400.036
						47-45;45-43 25 397.375			
						49-47;43-41 25 397.710	25 397.729	EE*	
						47-45;45-43 25 397.748			
						49-47;43-41 25 401.369	25 401.390	EE*	
						47-45;45-43 25 401.410			
						49-47;43-41 25 401.410	25 401.433	EA*	
						47-45;45-43 25 401.456			
24	10	14	-23	11	13	12 002.319	12 002.319	AA	12 004.910
						12 005.892	12 005.892	EE*	
24	10	15	-23	11	12	12 002.319	12 002.319	AA	12 004.899
						12 006.423	12 006.423	EE*	
25	10	15	-24	11	14	23 315.160	23 315.160	AA	23 317.673
						23 318.660	23 318.660	EE*	
25	10	16	-24	11	13	23 315.160	23 315.160	AA	23 317.649
						23 319.100	23 319.100	EE*	
26	11	15	-25	12	14	9 988.601	9 988.601	AA	9 990.949
						9 991.508	9 991.508	EE*	
26	11	16	-25	12	13	9 988.601	9 988.601	AA	9 990.949
						9 992.676	9 992.676	EE*	
27	11	16	-26	12	15	21 269.417	21 269.417	AA	21 271.673
						21 272.245	21 272.245	EE*	
27	11	17	-26	12	14	21 269.417	21 269.417	AA	21 271.677
						21 273.304	21 273.304	EE*	
29	12	17	-28	13	16	19 260.141	19 260.141	AA	19 262.121
						19 262.323	19 262.323	EE*	
29	12	18	-28	13	15	19 260.141	19 260.141	AA	19 262.121
						19 263.844	19 263.844	EE*	
31	13	18	-30	14	17	17 288.147	17 288.147	AA	17 289.824
						17 288.703	17 288.703	EE*	
31	13	19	-30	14	16	17 288.147	17 288.147	AA	17 289.824
						17 291.573	17 291.573	EE*	
33	14	19	-32	15	18	15 354.861	15 354.861	AA	15 356.223
						15 355.851	15 355.851	EE*	
33	14	20	-32	15	17	15 354.861	15 354.861	AA	15 356.223
						15 357.913	15 357.913	EE*	
35	15	20	-34	16	19	13 462.028	13 462.028	AA	13 463.083
						13 462.515	13 462.515	EE*	
35	15	21	-34	16	18	13 462.028	13 462.028	AA	13 463.083
						13 464.660	13 464.660	EE*	

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F'-2F$	ν_{obs}	$\nu_{hfs,\,unsplit}$	Γ	$\nu_{unsplit}$
37	16	21	-36	17	20	11 611.611	11 611.611	AA	11 612.399
						11 613.817	11 613.817	EE*	
37	16	22	-36	17	19	11 611.611	11 611.611	AA	11 612.399
						11 611.737	11 611.737	EE*	
39	17	22	-38	18	21	9 805.750	9 805.750	AA	9 806.291
						9 807.529	9 807.529	EE*	
39	17	23	-38	18	20	9 805.750	9 805.750	AA	9 806.291
						9 805.555	9 805.555	EE*	

1b.2.3. P-branch :

7	5	3	- 8	4	4	15-17;13-15	20 639.590	20 639.669	EE	20 637.427
						17-19;11-13	-			
						15-17;13-15	20 639.789	20 639.869	AA	
						17-19;11-13	20 639.945			
						15-17;13-15	20 662.887	20 662.966	AE*	
						17-19;11-13	20 663.063			
						15-17;13-15	20 663.063	20 663.159	EE*,EA*	
						17-19;11-13	20 663.234			
							20 676.500	20 676.500	EE*	
7	5	2	- 8	4	5	15-17;13-15	20 676.776	20 676.858	AA,EE	20 674.391
						17-19;11-13	20 676.937			
						15-17;13-15	-	20 640.108	EE*	
						17-19;11-13	20 640.184			
						15-17;13-15	20 646.110	20 646.189	EA*	
						17-19;11-13	20 646.294			
						15-17;13-15	20 646.294	20 646.387	EE*,AE*	
						17-19;11-13	20 646.463			
8	5	4	- 9	4	5	17-19;15-17	9 378.015	9 378.073	EE	9 375.794
						19-21;13-15	9 378.140			
						17-19;15-17	9 378.140	9 378.199	AA	
						19-21;13-15	9 378.255			
						17-19;15-17	9 457.926	9 457.984	AE*	
						19-21;13-15	-			
						17-19;15-17	9 458.146	9 458.204	EE*	
						19-21;13-15	9 458.246			
						17-19;15-17	9 458.246	9 458.280	EA*	
						19-21;13-15	9 458.336			
8	5	3	- 9	4	6	17-19;15-17	9 473.623	9 473.679	AA,EE	9 471.284
						19-21;13-15	9 473.735			
						17-19;15-17	9 386.360	9 386.416	EA*	
						19-21;13-15	9 386.472			
						17-19;15-17	9 386.540	9 386.597	EE*	
						19-21;13-15	9 386.641			
						17-19;15-17	9 386.641	9 386.682	AE*	
						19-21;13-15	9 386.738			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F'-2F$	ν_{obs}	$\nu_{hfs,\,unsplit}$	Γ	$\nu_{unsplit}$
9	6	4	-10	5	5	19-21;17-19	22 753.563	22 753.623	EE	22 751.089
						21-23;15-17	-			
						19-21;17-19	22 753.825	22 753.885	AA	
						21-23;15-17	22 753.973			
						19-21;17-19	22 751.479	22 751.539	AE*,EA*	
						21-23;15-17	22 751.580			
						19-21;17-19	22 751.580	21 751.631	EE*	
						21-23;15-17	22 751.691			
						19-21;17-19	22 759.998	22 760.058	EE*	
						21-23;15-17	-			
9	6	3	-10	5	6	19-21;17-19	22 760.283	22 760.343	AA	22 757.549
						21-23;15-17	22 760.407			
						19-21;17-19	22 760.407	22 760.462	EE	
						21-23;15-17	22 760.524			
						19-21;17-19	22 753.973	22 754.034	EE*	
						21-23;15-17	22 754.107			
						19-21;17-19	22 754.200	22 754.260	AE*,EA*	
						21-23;15-17	22 754.317			
						19-21;17-19	22 754.317	22 754.378	EE*	
						21-23;15-17	22 754.439			
10	6	5	-11	5	6	21-23;19-21	11 526.632	11 526.665	EE	11 524.155
						23-25;17-19	11 526.698			
						21-23;19-21	11 526.853	11 526.897	AA	
						23-25;17-19	11 526.940			
						21-23;19-21	11 532.114	11 532.161	AE*	
						23-25;17-19	11 532.209			
						21-23;19-21	11 532.209	11 532.257	EA*	
						23-25;17-19	11 532.249			
						21-23;19-21	11 532.249	11 532.299	EE*	
						23-25;17-19	11 532.346			
10	6	4	-11	5	7	21-23;19-21	11 543.983	11 544.030	AA	11 541.280
						23-25;17-19	11 544.067			
						21-23;19-21	11 544.067	11 544.091	EE	
						23-25;17-19	11 544.138			
						21-23;19-21	11 530.382	11 530.429	EA*	
						23-25;17-19	11 530.480			
						21-23;19-21	11 530.480	11 530.528	AE*	
						23-25;17-19	-			
						21-23;19-21	11 530.516	11 530.560	EE*	
						23-25;17-19	11 530.607			
11	7	5	-12	6	6		24 832.927	24 832.927	AA	24 829.888
						23-25;21-23	24 827.519	24 827.568	AE*,EA*	
						25-27;19-21	24 827.601			
						23-25;21-23	24 827.601	24 827.653	EE*	
						25-27;19-21	24 827.691			
						23-25;21-23	24 833.733	24 833.778	EE*	
						25-27;19-21	24 833.838			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
11	7	4 −12	6	7	23-25;21-23	24 833.906	24 833.964	AA	24 830.933
					25-27;19-21	24 834.014			
					23-25;21-23	24 830.162	24 830.211	AE*,EA*	
					25-27;19-21	24 830.250			
					23-25;21-23	24 830.250	24 830.292	EE*	
					25-27;19-21	24 830.342			
					23-25;21-23	24 832.927	24 832.974	EE*	
					25-27;19-21	24 833.022			
12	7	6 −13	6	7	25-27;23-25	13 619.063	13 619.104	AA	13 616.141
					27-29;21-23	13 619.145			
					25-27;23-25	13 621.742	13 621.779	EE*	
					27-29;21-23	13 621.815			
					25-27;23-25	13 614.792	13 614.832	AE*,EA*	
					27-29;21-23	13 614.872			
					25-27;23-25	13 614.872	13 614.912	EE*	
					27-29;21-23	13 614.952			
12	7	5 −13	6	8	25-27;23-25	13 619.145	13 619.199	EE*	13 619.036
					27-29;21-23	13 619.239			
					25-27;23-25	13 621.982	13 622.020	AA	
					27-29;21-23	13 622.057			
					25-27;23-25	13 617.333	13 617.373	AE*,EA*	
					27-29;21-23	13 617.412			
					25-27;23-25	13 617.412	13 617.449	EE*	
					27-29;21-23	13 617.489			
14	8	7 −15	7	8	29-31;27-29	15 681.948	15 681.976	AA	15 678.855
					31-33;25-27	15 682.004			
					29-31;27-29	15 682.184	15 682.235	EE*	
					31-33;25-27	15 682.272			
					29-31;27-29	15 676.604	15 676.644	AE*,EA*	
					31-33;25-27	15 676.688			
					29-31;27-29	15 676.688	15 676.727	EE*	
					31-33;25-27	15 676.768			
14	8	6 −15	7	9	29-31;27-29	15 682.380	15 682.416	AA	15 679.309
					31-33;25-27	15 682.452			
					29-31;27-29	15 681.948	15 681.976	EE*	
					31-33;25-27	15 682.004			
					29-31;27-29	15 678.376	15 678.411	AE*,EA*	
					31-33;25-27	15 678.454			
					29-31;27-29	15 678.454	15 678.491	EE*	
					31-33;25-27	15 678.526			
16	9	8 −17	8	9	33-35;31-33	17 718.998	17 719.029	AA,EE*	17 715.920
					35-37;29-31	17 719.059			
					33-35;31-33	17 713.928	17 713.959	AE*,EA*	
					35-37;29-31	17 714.001			
					33-35;31-33	17 714.001	17 714.032	EE*	
					35-37;29-31	17 714.063			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
16	9	7 −17	8	10	33-35;31-33	17 718.941	17 718.970	EE*	17 715.964
					35-37;29-31	17 718.998			
					33-35;31-33	17 719.059	17 719.090	AA	
					35-37;29-31	17 719.121			
					33-35;31-33	17 714.740	17 714.771	AE*	
					35-37;29-31	17 714.787			
					33-35;31-33	17 714.787	17 714.823	EA*	
					35-37;29-31	17 714.859			
					33-35;31-33	17 714.859	17 714.879	EE*	
					35-37;29-31	17 714.910			
18	10	9 −19	9	10	37-39;35-37	19 729.181	19 729.224	AA	19 726.189
					39-41;33-35	19 729.252			
						19 724.705	19 724.705	EE*	
18	10	8 −19	9	11	37-39;35-37	19 729.113	19 729.139	EE*	19 726.182
					39-41;33-35	19 729.181			
					37-39;35-37	19 729.181	19 729.224	AA	
					39-41;33-35	19 729.252			
						19 724.705	19 724.705	EE*	
19	10	10 −20	9	11	39-41;37-39	8 509.827	8 509.861	AA,EE*	8 506.890
					41-43;35-37	8 509.894			
					39-41;37-39	8 505.327	8 505.359	EA*	
					41-43;35-37	8 505.390			
					39-41;37-39	8 505.365	8 505.399	AE*	
					41-43;35-37	8 505.432			
					39-41;37-39	8 505.432	8 505.443	EE*	
					41-43;35-37	8 505.476			
19	10	9 −20	9	12	39-41;37-39	8 509.770	8 509.799	EE*	8 506.939
					41-43;35-37	8 509.827			
					39-41;37-39	8 509.871	8 509.898	AA	
					41-43;35-37	8 509.914			
					39-41;37-39	8 505.432	8 505.456	AE*	
					41-43;35-37	8 505.484			
					39-41;37-39	8 505.484	8 505.503	EA*	
					41-43;35-37	8 505.521			
					39-41;37-39	8 505.521	8 505.547	EE*	
					41-43;35-37	8 505.572			
20	11	10 −21	10	11	41-43;39-41	21 710.243	21 710.272	AA,EE*	21 707.423
					43-45;37-39	21 710.300			
					41-43;39-41	21 706.360	21 706.385	EA*	
					43-45;37-39	21 706.425			
					41-43;39-41	21 706.425	21 706.460	EE*,AE*	
					43-45;37-39	21 706.485			
20	11	9 −21	10	12	41-43;39-41	21 710.181	21 710.206	EE*	21 707.423
					43-45;37-39	21 710.243			
					41-43;39-41	21 710.243	21 710.272	AA	
					43-45;37-39	21 710.300			
					41-43;39-41	21 705.531	21 705.556	AE*	
					43-45;37-39	21 705.602			
					41-43;39-41	21 705.602	21 705.634	EE*,EA*	
					43-45;37-39	21 705.659			

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
21	11	11	-22	10	12	43-45;41-43	10 507.235	10 507.262	AA, EE*	10 504.490
						45-47;39-41	10 507.282			
						43-45;41-43	10 503.429	10 503.454	EA*	
						45-47;39-41	10 503.479			
						43-45;41-43	10 503.479	10 503.512	EE*, AE*	
						45-47;39-41	10 503.545			
21	11	10	-22	10	13	43-45;41-43	10 507.168	10 507.202	EE*	10 504.490
						45-47;39-41	10 507.235			
						43-45;41-43	10 507.235	10 507.262	AA	
						45-47;39-41	10 507.282			
						43-45;41-43	10 502.684	10 502.712	AE*	
						45-47;39-41	10 502.740			
						43-45;41-43	10 502.740	10 502.778	EA*, EE*	
						45-47;39-41	10 502.815			
22	12	11	-23	11	12	45-47;43-45	23 659.696	23 659.721	AA, EE*	23 657.121
						47-49;41-43	23 659.745			
						45-47;43-45	23 656.541	23 656.567	EA*	
						47-49;41-43	23 656.593			
						45-47;43-45	23 656.593	23 656.618	EE*, AE*	
						47-49;41-43	23 656.643			
22	12	10	-23	11	13	45-47;43-45	23 659.640	23 659.668	EE*	23 657.121
						47-49;41-43	23 659.696			
						45-47;43-45	23 659.696	23 659.721	AA	
						47-49;41-43	23 659.745			
						45-47;43-45	23 655.018	23 655.043	AE*	
						47-49;41-43	23 655.068			
						45-47;43-45	23 655.068	23 655.093	EE*, EA*	
						47-49;41-43	23 655.117			
23	12	12	-24	11	13		12 473.457	12 473.457	AA	12 470.942
							12 470.404	12 470.404	EE*	
23	12	11	-24	11	14		12 473.457	12 473.457	AA	12 470.942
							12 469.012	12 469.012	EE*	
24	13	12	-25	12	13		25 574.974	25 574.974	AA	25 572.674
							25 572.591	25 572.591	EE*	
24	13	11	-25	12	14		25 574.974	25 574.974	AA	25 572.674
							25 570.494	25 570.494	EE*	
25	13	13	-26	12	14		14 406.101	14 406.101	AA	14 403.889
							14 403.785	14 403.785	EE*	
25	13	12	-26	12	15		14 406.101	14 406.101	AA	14 403.889
							14 401.832	14 401.832	EE*	
27	14	14	-28	13	15		16 302.719	16 302.719	AA	16 300.832
							16 301.079	16 301.079	EE*	

Table 1 b (continued)

J'	K'_-	$K'_+ - J$	K_-	K_+	$2F' - 2F$	ν_{obs}	$\nu_{hfs,\ unsplit}$	Γ	$\nu_{unsplit}$
27	14	13	-28	13	16	16 302.719	16 302.719	AA	16 300.832
						16 298.737	16 298.737	EE*	
32	16	17	-33	15	18	8 849.448	8 849.448	AA	8 848.303
						8 849.026	8 849.026	EE*	
32	16	16	-33	15	19	8 849.448	8 849.448	AA	8 848.303
						8 846.470	8 846.470	EE*	
34	17	18	-35	16	19	10 646.082	10 646.082	AA	10 645.236
						10 643.569	10 643.569	EE*	
34	17	17	-35	16	20	10 646.082	10 646.082	AA, EE*	10 645.236
36	18	19	-37	17	20	12 397.406	12 397.406	AA	12 396.848
						12 395.363	12 395.363	EE*	
36	18	18	-37	17	21	12 397.406	12 397.406	AA	12 396.848
						12 397.790	12 397.790	EE*	
38	19	20	-39	18	21	14 101.004	14 101.004	AA	14 100.674
						14 099.405	14 099.405	EE*	
38	19	19	-39	18	22	14 101.004	14 101.004	AA	14 100.674
						14 101.621	14 101.621	EE*	

Table 2a. ^{11}B-quadrupole coupling constants of $CH_3PH_2BD_3$. Standard deviations in brackets in units of the last digit. σ: standard deviation of the fit, $\overline{\Delta\nu}$: mean experimental hfs-splitting.

χ_+	$= \chi_{bb} + \chi_{cc} = -1.085(10)$ MHz
χ_-	$= \chi_{bb} - \chi_{cc} = 0.775(11)$ MHz
χ_{aa}	$= 1.085(10)$ MHz
χ_{bb}	$= -0.155(11)$ MHz
χ_{cc}	$= -0.930(11)$ MHz
σ	$= 6$ kHz
$\overline{\Delta\nu}$	$= 88$ kHz

correlation coefficient: $|(\chi_+, \chi_-)| = 0.05$

$\measuredangle$ (BP, a)	$= 28.6(10)°$
χ_{xx}	$= -0.688(79)$ MHz
χ_{yy}	$= -0.930(11)$ MHz
χ_{zz}	$= 1.618(78)$ MHz

Table 2b. ^{11}B-quadrupole coupling constants of $CH_3PH_2BH_3$. See also Table 2a.

χ_+	$= \chi_{bb} + \chi_{cc} = -0.975(11)$ MHz
χ_-	$= \chi_{bb} - \chi_{cc} = 0.768(13)$ MHz
χ_{aa}	$= 0.975(11)$ MHz
χ_{bb}	$= -0.104(12)$ MHz
χ_{cc}	$= -0.872(12)$ MHz
σ	$= 9$ kHz
$\overline{\Delta\nu}$	$= 88$ kHz

correlation coefficient: $|(\chi_+, \chi_-)| = 0.07$

$\measuredangle$ (BP, a)	$= 31.2(10)°$
χ_{xx}	$= -0.729(97)$ MHz
χ_{yy}	$= -0.872(12)$ MHz
χ_{zz}	$= 1.600(96)$ MHz

The dipole forbidden transitions EE*, EA* and AE* connected with the regular μ_b-type transitions AA, EE, EA and AE belong to selection rules, which are equal to those of μ_c-type transitions (ee−oe, oo−eo). Therefore the forbidden and regular transitions show a different centrifugal distortion effect. Consequently the program (AC3IAM) was modified to include centrifugal distortion up to fourth order (Watsons A-reduction is used [9]).

Because the differences between observed and calculated torsional splittings increase with J, the internal rotation constants were fitted with frequencies of lines with $J \leqq 20$.

The presumable reason for these differences is an approximation made by Woods to reduce the computational effort. The matrix elements of the Hamiltonian, see eq. (1), in the principal axis system are:

$$
\begin{aligned}
&\langle J K_2 M v_2^{(1)} \sigma^{(1)} v_2^{(2)} \sigma^{(2)}(z') \,|\, H \,|\, J K_1 M v_1^{(1)} \sigma^{(1)} v_1^{(2)} \sigma^{(2)}(z')\rangle \\
&\quad = \langle K_2 v_2^{(1)} \sigma^{(1)} \,|\, K_1 v_1^{(1)} \sigma^{(1)}\rangle \cdot \langle K_2 v_2^{(2)} \sigma^{(2)} \,|\, K_1 v_1^{(2)} \sigma^{(2)}\rangle \cdot \langle J K_2 M(z') \,|\, H_R \,|\, J K_1 M(z')\rangle \\
&\qquad + \langle K_2 v_2^{(2)} \sigma^{(2)} \,|\, K_1 v_1^{(2)} \sigma^{(2)}\rangle \left\{ \sum_K \langle J K_2 M(z') \,|\, J K M(z^{(1)})\rangle \cdot \langle J K M(z^{(1)}) \,|\, J K_1 M(z')\rangle \right. \\
&\qquad\qquad \left. \cdot \sum_{v^{(1)}} \langle K_2 v_2^{(1)} \sigma^{(1)} \,|\, K v^{(1)} \sigma^{(1)}\rangle \cdot E^{(1)}_{K v^{(1)} \sigma^{(1)}} \cdot \langle K v^{(1)} \sigma^{(1)} \,|\, K_1 v_1^{(1)} \sigma^{(1)}\rangle \right\} \\
&\qquad + \langle K_2 v_2^{(1)} \sigma^{(1)} \,|\, K_1 v_1^{(1)} \sigma^{(1)}\rangle \left\{ \sum_K \langle J K_2 M(z') \,|\, J K M(z^{(2)})\rangle \cdot \langle J K M(z^{(2)}) \,|\, J K_1 M(z')\rangle \right. \\
&\qquad \left. \cdot \sum_{v^{(2)}} \langle K_2 v_2^{(2)} \sigma^{(2)} \,|\, K v^{(2)} \sigma^{(2)}\rangle \cdot E^{(2)}_{K v^{(2)} \sigma^{(2)}} \cdot \langle K v^{(2)} \sigma^{(2)} \,|\, K_1 v_1^{(2)} \sigma^{(2)}\rangle \right\} \qquad (4)
\end{aligned}
$$

where z' is parallel to a principal axis and $z^{(l)}$ $(l = 1, 2)$ to the $\varrho^{(l)}$-axes, respectively.

Woods simplifies this equation using the following approximation:

$$\langle K_{1,2} v_{1,2}^{(l)} \sigma^{(l)} \,|\, K v^{(l)} \sigma^{(l)}\rangle = \delta_{v^{(l)} v_{1,2}^{(l)}}; \quad l = 1, 2. \qquad (5)$$

To estimate the error we compared a spectrum prediction (program FC3IAM) using the approximation of (5) with a spectrum prediction made by van Eijck using a program, that takes into account the elements off diagonal in v by a van Vleck transformation. Because the contribution of the van Vleck transformation increases with J, the agreement of the splittings is better than 0.3% for $J \leqq 20$ but only ca. 5% for $J = 40$. There are some other assumptions in Woods program, so we believe an error of max. 0.3% for $J = 20$ is acceptable.

Table 3a. Internal rotation parameters of $CH_3PH_2BD_3$. $w_1(s)$: Fourier coefficient, s: reduced barrier height, I_α: moment of inertia of the CH_3 and BD_3 group, respectively, $\sphericalangle(g, i)$: angle between the inertia axis $g = a, b, c$ and the internal rotation axis i, F: reduced internal rotational constant of the internal rotation, V_3: barrier to internal rotation, σ: standard deviation of the fit, $\Delta\nu$: mean experimental methyl torsion splitting. Assumptions in square brackets. Standard errors in units of the last digit in brackets.

CH_3 top		BD_3 top
$w_1(s)$	$= -0.44780(63) \cdot 10^{-4}$	–
I_α	= 3.1996(58) amu Å^2	[8.676 amu Å^2]
$\sphericalangle(a, i)$	= 38.990(66)°	[32.7°]
$\sphericalangle(b, i)$	= 51.010(66)°	[57.3°]
[$\sphericalangle(c, i)$	= 90.00°]	[90.0°]
F	= 173.37(33) GHz	[75.11 GHz]
s	= 51.834(11)	
V_3	= 1.9332(40) kcal/mol	
	= 8.092(17) kJ/mol	
σ	= 14 kHz	
$\Delta\nu$	= 18.57 MHz	

correlation coefficient matrix:

$\sphericalangle w_1(s)$	1.00		
I_α	−0.86	1.00	
$\sphericalangle(a, i)$	−0.96	0.84	1.00

Table 3b. Internal rotation parameters of $CH_3PH_2BH_3$. See also Table 3a.

CH_3 top		BH_3 top
$w_1(s)$	$= -0.47907(42) \cdot 10^{-4}$	$-0.783(19) \cdot 10^{-6}$
I_α	= 3.1992(24) amu Å^2	4.338(42) amu Å^2
$\sphericalangle(a, i)$	= 36.380(38)°	35.3(13)°
$\sphericalangle(b, i)$	= 53.620(38)°	54.7(13)°
[$\sphericalangle(c, i)$	= 90.00°]	[90.0°]
F	= 174.91(14) GHz	133.7(17) GHz
s	= 51.4818(65)	89.22(25)
V_3	= 1.9318(18) kcal/mol	2.559(39) kcal/mol
	= 8.086(8) kJ/mol	10.71(16) kJ/mol
σ	= 18 kHz	
$\Delta\nu$	= 33.377 MHz	

correlation coefficient matrix:

$w_1(s)$	(CH_3)	1.00				
$w_1(s)$	(BH_3)	−0.11	1.00			
I_α	(CH_3)	−0.90	0.00	1.00		
I_α	(BH_3)	0.08	−0.60	−0.04	1.00	
$\sphericalangle(a, i)$	(CH_3)	−0.89	0.02	0.84	−0.03	1.00
$\sphericalangle(a, i)$	(BH_3)	0.23	−0.78	−0.08	0.41	−0.08	1.00

The results for the torsional analyses are given in Table 3a and 3b for $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$, respectively. The internal rotation constants were used to calculate the deviations from the rigid rotor lines (program FC3IAM). These deviations were added to the frequencies $\nu_{\text{hfs, unsplit}}$. The hypothetical unsplit lines ν_{unsplit} were then calculated as a mean value.

The frequencies ν_{unsplit} were used in least squares analyses to fit the constants in the following Hamiltonian (Watsons A-reduction is used, program ZFAP6 [10, 11]):

$$
\begin{aligned}
H = {} & 1/2\,(B + C)\,P^2 + [A - 1/2\,(B + C)]\,P_z^2 \\
& + 1/2\,(B - C)\,(P_x^2 - P_y^2) \\
& - \Delta_J P^4 - \Delta_{JK} P^2 P_z^2 - \Delta_K P_z^4 - 2\,\delta_J P^2 (P_x^2 - P_y^2) \\
& - \delta_K [P_z^2 (P_x^2 - P_y^2) + (P_x^2 - P_y^2)\,P_z^2] \\
& + \Phi_J P^6 + \Phi_{JK} P^4 P_z^2 + \Phi_{KJ} P^2 P_z^4 + \Phi_K P_z^6 \\
& + 2\,\varphi_J P^4 (P_x^2 - P_y^2) + \varphi_{JK} P^2 [P_z^2 (P_x^2 - P_y^2) \\
& + (P_x^2 - P_y^2)\,P_z^2] + \varphi_K [P_z^4 (P_x^2 - P_y^2) \\
& + (P_x^2 - P_y^2)\,P_z^4]\,. \qquad (6)
\end{aligned}
$$

The results for the centrifugal distortion analyses are given in Table 4a and 4b for $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$, respectively.

All fitting procedures were repeated until no further changes in the derived parameters were observed.

IV. Results and Discussion

The determination of the methyl barrier of $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$ gives $V_3 = 1933(4)$ and 1932(2) cal/mol, respectively. These results are in a good agreement with the potential $V_3 = 1958(14)$ cal/mol found for methylphosphine, CH_3PH_2, by Kojima [12], but are in a disagreement with the value $V_3 = 2.49(6)$ kcal/mol determined by Durig [2] from the first excited torsion state of the methyl group of $CH_3PH_2BH_3$. Similar the determination of the borane barrier of $CH_3PH_2BH_3$ $V_3 = 2559(39)$ cal/mol is consistent with the potential $V_3 = 2467(50)$ cal/mol found for phosphine-borane by Durig [13], but furthermore in disagreement with the value $V_3 = 1.57(6)$ kcal/mol determined by Durig [2] from the rotational spectra in the first excited torsion state of the borane group.

Because it is not possible to assign the ground state splittings measured in this work with the values given in [2] and since it is possible to assign the torsional fine structure of the first excited states given in [2] with the internal rotation constants determined in this work, we believe our assignment is correct.

Table 4a. Rotational and centrifugal distortion constants of $CH_3PH_2BD_3$. Watsons A-reduction is used. Conversion factor: 505 376 MHz amu Å^2, σ: standard deviation of the fit. Standard errors in units of the last digit in brackets.

A	=	15 039.2527(21) MHz
B	=	5 178.27049(78) MHz
C	=	4 385.67270(66) MHz
Δ_J	=	4.714(16) kHz
Δ_{JK}	=	−28.80(10) kHz
Δ_K	=	130.308(13)kHz
δ_J	=	1.3646(21) kHz
δ_K	=	3.38(11) kHz
Φ_J	=	0.041(24) Hz
Φ_{JK}	=	0.38(40) Hz
Φ_{KJ}	=	−0.38(52) Hz
Φ_K	=	3.89(33) Hz
φ_J	=	0.0090(54) Hz
φ_{JK}	=	0.26(20) Hz
φ_K	=	−1.5(19) Hz
$\varkappa$	=	−0.851205
I_a	=	33.6037974(47) amu Å^2
I_b	=	97.595520(15) amu Å^2
I_c	=	115.233405(18) amu Å^2
σ	=	7 kHz

highest correlation: $|(\Phi_{JK}, \varphi_J)| = 0.991$

Table 4b. Rotational and centrifugal constants of $CH_3PH_2BH_3$. See also Table 4a.

A	=	17 588.8397(19) MHz
B	=	5 973.13681(67) MHz
C	=	4 977.46097(56) MHz
Δ_J	=	6.4256(88) kHz
Δ_{JK}	=	−46.041(67) kHz
Δ_K	=	226.6411(76) kHz
δ_J	=	1.9772(12) kHz
δ_K	=	7.847(47) kHz
Φ_J	=	−0.011(10) Hz
Φ_{JK}	=	0.38(16) Hz
Φ_{KJ}	=	−4.10(41) Hz
Φ_K	=	10.70(29) Hz
φ_J	=	0.0106(21) Hz
φ_{JK}	=	−0.63(14) Hz
φ_K	=	9.1(16) Hz
$\varkappa$	=	−0.842099
I_a	=	28.732765(3) amu Å^2
I_b	=	84.608141(9) amu Å^2
I_c	=	101.532891(11) amu Å^2
σ	=	11 kHz

highest correlation: $|(\Delta_J, \Delta_{JK})| = 0.976$

Next we give a comparison between the moments of inertia of the methyl and borane group determined in this work and the values calculated from the structure given in [1]:

	from structure [1]	from IAM-analysis
$CH_3PH_2BH_3$: $I_z(CH_3)$	3.2035 amu Å^2	3.1992(24) amu Å^2
$I_z(BH_3)$	4.334 amu Å^2	4.338(42) amu Å^2
$CH_3PH_2BD_3$: $I_z(CH_3)$	3.2035 amu Å^2	3.1996(58) amu Å^2

The differences are about 0.004 amu Å^2. We believe this is a good agreement and verifies our assignment.

Furthermore it was an important point of this study to determine the position of the internal rotation axes with respect to the inertia axes. Bryan and Kuczkowski [1] have observed that the methyl and borane group are tilted toward each other. A short time ago Bestmann [14] found a similar effect in propane. So we determined the angle between the internal axes of the methyl and borane group $\measuredangle(i, i) = 108.3(13)°$ in comparison with the angle $\measuredangle$(BPC) = 115.7(4)° [1]. This result verifies in good agreement the observed tilt in [1].

V. Interpretation of the Nuclear Quadrupole Coupling Constants

For $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$ only the measured coupling constants for the axes perpendicular to the molecular symmetry planes are principal axes constants of the nuclear coupling tensors ($\chi_{yy} = \chi_{cc}$). To obtain estimates of the principal constants of the nuclear coupling tensors, we have made the usual transformation with the assumption that the B−P bond will be a principal axis (z-axis) of the coupling tensor. The necessary angles of rotation for this transformation, $\measuredangle$(BP, a), are calculated in the principal axis system of $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$, respectively, using the structure given in Table 13 of [1] and yield the χ_{xx} and χ_{zz} values listed for $CH_3PH_2BD_3$ and $CH_3PH_2BH_3$ in Table 2a and 2b, respectively.

To calculate the standard errors of χ_{xx} and χ_{zz} we use an error of 1° for the angle $\measuredangle$(BP, a).

The difference between the values of χ_{xx} and χ_{yy} is consistent with the proposal that the classical σ dative bond can be supplemented by $d\pi - p\pi$ bonding involving the phosphorus d orbitals and the borane group. This "back donation" description was suggested some time ago by Graham and Stone [15] to account for the unexpected stability of BH_3 adducts with very weak bases.

Next we interpret the quadrupole coupling constants in terms of the bond order following Townes and Dailey [16] and Gordy [17]. For details see [18].

The following equation is used:

$$\chi_{gg} = -(U_p)_g \cdot \frac{e\,Q\,q_{210}}{1 + (n_p + n_{H_s} + 2\,n_{H_a} - 3)\cdot\varepsilon}; \quad g = x, y, z \quad (7)$$

with χ_{gg} the experimental boron principal quadrupole coupling constants, $eQq_{210} = -5.39$ MHz [19] the ^{11}B quadrupole coupling constant induced by a $2p_z$ electron, $\varepsilon = 0.5$ [20] the shielding constant of boron, n_p the number of electrons donated by the phosphorus to the boron, n_{H_s} and n_{H_a} the mean number of electrons occupying the orbitals to hydrogen in the symmetry plane H_s and out of the symmetry plane H_a, and $(Up)_g$ the number of "unbalanced" p-electrons in g-direction $(g = x, y, z)$. $(Up)_g$ may be calculated from:

$$\begin{aligned}(Up)_g = &-1/2\,(3\cos^2(g, \mathrm{BP}) - 1)\cdot n_p \cdot a_p^2(\psi_p)\\ &-1/2\,(3\cos^2(g, \mathrm{BH_s}) - 1)\cdot n_{H_s}\cdot a_p^2(\psi_{H_s})\\ &-(3\cos^2(g, \mathrm{BH_a}) - 1)\cdot n_{H_a}\cdot a_p^2(\psi_{H_a})\,. \qquad (8)\end{aligned}$$

with $a_p^2(\psi_i)$ $(i = \mathrm{P}, \mathrm{H_s}, \mathrm{H_a})$ the p-electron fraction of the boron orbital directed to phosphorus and hydrogen in and out of the symmetry plane, respectively.

Assuming hybridization mixing of s and p functions:

$$\psi_i = s_i + \lambda(i)\cdot p_i \qquad (9)$$

(see [21], $i = \mathrm{P}, \mathrm{H_s}, \mathrm{H_a}$) one gets

$$a_p^2(\psi_i) = \frac{\lambda(i)^2}{1+\lambda(i)^2} \qquad (10)$$

with

$$\begin{aligned}\lambda(\mathrm{H_a})^2 &= -(\cos(\sphericalangle\,\mathrm{H_aBH_a}))^{-1},\\ \lambda(\mathrm{H_s})^2 &= (\lambda(\mathrm{H_a})\cdot\cos(\sphericalangle\,\mathrm{H_aBH_s}))^{-2},\\ \lambda(\mathrm{P})^2 &= (\lambda(\mathrm{H_a})\cdot\cos(\sphericalangle\,\mathrm{H_aBP}))^{-2}. \qquad (11)\end{aligned}$$

Because of the relation $\sum_g \chi_{gg} = 0$ $(g = x, y, z)$ the three equations (7) are not linear independent. So we need a further relationship to determine the three numbers of electrons occupying the boron orbitals: n_i $(i = \mathrm{P}, \mathrm{H_s}, \mathrm{H_a})$.

We use the approximation

$$1 - i_\sigma = \tfrac{1}{3}(n_{H_s} + 2n_{H_a})\,, \qquad (12)$$

where $i_\sigma = \frac{1}{2}\cdot|\mathrm{EN(H)} - \mathrm{EN(B)}|$ is the ionic character of the B–H bond calculated from the electronegativities EN(H) = 2.15 and EN(B) = 2.0 [22].

Because the structure is known [1], the information is sufficient to determine the bond order for methylphosphine-borane:

$$n_P = 0.54(2)\,;\quad n_{H_s} = 0.90(2)\,;\quad n_{H_a} = 0.93(1)$$

and for methylphosphine-trideuteroborane:

$$n_P = 0.54(2)\,;\quad n_{H_s} = 0.89(3)\,;\quad n_{H_a} = 0.94(1)\,.$$

It is interesting, that the bond order to hydrogen in the symmetry plane is lower than to hydrogen out of the symmetry plane $(n_{H_s} < n_{H_a})$. This is consistent with the result that the bond distance $r(\mathrm{B-H_a}) = 1.229$ Å is shorter than $r(\mathrm{B-H_s}) = 1.234$ Å [1].

A further comparison shows that the B–P bond order in methylphosphine-borane $n_p = 0.54$ is lower than in trifluorophospine-borane: $n_p = 0.57$ previously determined [23]. This is in agreement with the result, that the B–P bond length in trifluorophosphine-borane $r(\mathrm{B-P}) = 1.836$ Å [24] is shorter than in methylphosphine-borane $r(\mathrm{B-P}) = 1.906$ Å [1].

Moreover it is interesting to determine the difference of electrons in x- and y-direction.

Following Gordy [25] we use:

$$n_x - n_y = \tfrac{2}{3}\cdot\frac{\chi_{xx} - \chi_{yy}}{eQq_{210}} \qquad (13)$$

and yield for $CH_3PH_2BH_3$: $n_x - n_y = -0.02$ and for $CH_3PH_2BD_3$: $n_x - n_y = -0.03$.

There is a electron surplus perpendicular to the symmetry plane for both molecules.

Therefore a $p\pi - d\pi$ bond to phosphorus is possible.

This is in agreement with the "back-donation" and "hyperconjugation" description by Graham and Stone [15].

VI. Acknowledgements

We thank Dr. van Eijck for a calculation. W. Kasten acknowledges a scholarship of the Fonds der Chemie, R. L. Kuczkowski of a travel grant to Kiel from the Rackham Graduate School, University of Michigan. We thank the Deutsche Forschungsgemeinschaft and Fonds der Chemie for funds. The calculations were made at the Computer Center of the University of Kiel.

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. **11,** 553 (1972).
[2] J. R. Durig, V. F. Kalasinsky, Y. S. Li, and J. D. Odom, J. Chem. Phys. **79,** 468 (1975).
[3] G. Bestmann, H. Dreizler, H. Mäder, and U. Andresen, Z. Naturforsch. **35a,** 392 (1980).
[4] G. Bestmann and H. Dreizler, Z. Naturforsch. **37a,** 58 (1982).
[5] W. Stahl, G. Bestmann, H. Dreizler, K. Andresen, and R. Schwarz, Rev. Sci. Instrum. **56,** 1759 (1985).
[6] E. Fliege and H. Dreizler, Z. Naturforsch. **39a,** 630 (1984).
[7] R. C. Woods, J. Mol. Spectr. **21,** 4 (1966).
[8] R. C. Woods, J. Mol. Spectr. **22,** 49 (1967).
[9] J. K. G. Watson, J. Chem. Phys. **46,** 1935 (1967).
[10] V. Typke, J. Mol. Spectr. **63,** 170 (1976).
[11] J. K. G. Watson, "Aspects of Quartic and Sextic Centrifugal Effects on Rotational Energy Levels", in Vibrational Spectra and Structure, J. R. Durig, Ed. Vol. 6, Marcel Dekker, New York 1977.
[12] T. Kojima, E. L. Breig, and C. C. Lin, J. Chem. Phys. **35,** 2139 (1961).
[13] J. R. Durig, Y. S. Li, L. A. Carreira, and J. D. Odom, J. Amer. Chem. Soc. **95,** 2491 (1973).
[14] G. Bestmann, W. Lalowski, and H. Dreizler, Z. Naturforsch. **40a,** 271 (1985).
[15] W. A. G. Graham and F. G. A. Stone, J. Inorg. Nucl. Chem. **3,** 164 (1959).
[16] C. H. Townes and A. L. Schawlow, Microwave Spectroscopy, McGraw Hill, London 1955, Chapter 9.
[17] W. Gordy and R. L. Cook, Microwave Molecular Spectra, J. Wiley, New York 1984, Chapter XIV.
[18] W. Kasten, Thesis Kiel (1985).
[19] L. c. [17], Table 14.2.
[20] L. c. [17], Table 14.3.
[21] C. A. Coulson, Die Chemische Bindung, Hirzel, Stuttgart 1969, p. 162, Eq. (1) to (3).
[22] L. c. [17], Equation (14.93) and Appendix G.
[23] W. Kasten, H. Dreizler, and R. L. Kuczkowski, Z. Naturforsch. **40a,** 920 (1985).
[24] R. L. Kuczkowski and D. R. Lide, J. Chem. Phys. **46,** 357 (1967).
[25] L. c. [17], Equation (14.110).