The Rotational Spectrum of 2,2-Dimethylthiirane

H. Hartwig and H. Dreizler

Abteilung Chemische Physik, Institut für Physikalische Chemie der Universität Kiel, Kiel, Germany

Z. Naturforsch. **48a**, 1102–1106 (1993); received August 19, 1993

The rotational spectrum of 2,2-dimethylthiirane (isobutylene sulfide) has been assigned for the ground and torsionally excited states. The rotational and centrifugal distortion constants, as well as the potential parameters V_3 and V_{12}' are determined. The ground state spectra of the ^{13}C and ^{34}S isotopomers were assigned in natural abundance and heavy atom structure parameters are given.

Introduction

The torsional fine structure in the microwave spectra of molecules with two equivalent internal rotors has attracted the interest of our group for several years. In preceding publications we reported on investigations of dimethyloxiranes [1, 2]. We now focus our interest on the analogous dimethylthiiranes to compare the effects on structure and potential parameters when oxygen is replaced by sulphur in the three membered ring.

2,2-Dimethylthiirane, $(CH_3)_2H_2C_2S$, (DMT) has C_s symmetry. The potential barrier hindering the internal rotation of the two equivalent methyl groups can be evaluated for this molecule only from the torsionally excited states.

Experimental

The substance was prepared from 2,2-dimethyloxirane and KSCN by the method of Snyder, Stewart, and Ziegler [3]. The measurements were performed using different types of microwave spectrometers: The assignments of the normal, the ^{13}C and ^{34}S isotopomers in natural abundance were done using a scanning molecular beam cavity Fourier transform microwave spectrometer (MB FTMW) [4, 5]. A mixture of 1 Vol% DMT in argon with a backing pressure of 0.5 bar was used. No internal rotation splitting was observed in the ground state transitions.

Waveguide Fourier transform microwave spectrometers (WG FTMW) in the frequency range from 4.5–8.0 GHz and 8.0–15.0 GHz [6, 7] were used to measure the torsionally excited states. The pressure was about 0.05 Pa, the cell was cooled to 220 K. The polarization power was about 25 dBm with pulses of 200 ns duration. The narrowest torsional fine structure splitting resolved was 39 kHz at 10.5 GHz as shown in Figure 1. The Doppler width in this region is about 6 kHz HWHH. The frequencies of the recorded time domain signals were obtained from a least squares fit, because the splittings yielded by a Fourier transformation are erroneously when linewidth and splittings are of the same magnitude [8, 9].

Reprint requests to Prof. Dr. H. Dreizler, Institut für Physikalische Chemie, Olshausenstr. 40, D-24098 Kiel.

Ground State

The internal rotation of the methyl groups does not affect measurably the rotational spectrum of DMT in the torsional ground state, because the hindering potential is relatively high. The rotational and centrifugal distortion constants of DMT and its isotopomers were determined in the I^r representation using Watson's A reduction [10]. DMT has dipole moment components along the a and c axes. The measurements are given in Tables 1–3 for all isotopomers. The rotational and centrifugal distortion constants are compiled in Table 5. The centrifugal distortion constants of the ^{34}S and ^{32}S isotopomers are in good agreement. The rotational constants of the ^{13}C species were determined with the centrifugal distortion constants fixed to the values of the normal isotopomer.

Torsionally Excited States

The use of the scanning version of the WG FTMW spectrometers [7] facilitated the measurement and assignment. The measurements are given in Table 4. The

0932-0784 / 93 / 1100-1102 $ 01.30/0. – Please order a reprint rather than making your own copy.

Dieses Werk wurde im Jahr 2013 vom Verlag Zeitschrift für Naturforschung in Zusammenarbeit mit der Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. digitalisiert und unter folgender Lizenz veröffentlicht: Creative Commons Namensnennung-Keine Bearbeitung 3.0 Deutschland Lizenz.

This work has been digitalized and published in 2013 by Verlag Zeitschrift für Naturforschung in cooperation with the Max Planck Society for the Advancement of Science under a Creative Commons Attribution-NoDerivs 3.0 Germany License.

Zum 01.01.2015 ist eine Anpassung der Lizenzbedingungen (Entfall der Creative Commons Lizenzbedingung „Keine Bearbeitung") beabsichtigt, um eine Nachnutzung auch im Rahmen zukünftiger wissenschaftlicher Nutzungsformen zu ermöglichen.

On 01.01.2015 it is planned to change the License Conditions (the removal of the Creative Commons License condition "no derivative works"). This is to allow reuse in the area of future scientific usage.

Table 1. Rotational transitions of 2,2-dimethylthiirane in the ground state in MHz. $\delta\nu = \nu(\text{obs.}) - \nu(\text{calc.})$ in kHz, standard deviation $\sigma = 1.6$ kHz.

J'	K'_-	K'_+	$-J$	K_-	K_+	ν(obs.)	$\delta\nu$
1	0	1 −	0	0	0	6 486.330	−0.9
1	1	0 −	0	0	0	8 997.559	−3.0
2	0	2 −	1	0	1	12 898.850	−0.4
2	1	1 −	1	1	0	13 447.551	−1.4
2	1	2 −	1	1	1	12 497.734	−0.7
2	1	1 −	1	0	1	15 958.783	−0.6
2	2	1 −	2	0	2	9 168.880	1.2
2	2	0 −	2	1	2	7 607.472	2.0
2	2	1 −	2	1	1	6 108.946	0.4
3	0	3 −	2	1	1	16 114.907	1.2
3	2	2 −	3	0	3	9 452.956	1.2
3	2	2 −	3	1	2	5 446.875	0.1
3	3	1 −	3	1	2	16 858.701	0.4
4	0	4 −	3	2	1	15 483.507	0.6
4	1	4 −	3	2	2	16 578.030	0.2
4	2	3 −	4	0	4	10 046.013	1.0
4	3	2 −	4	2	2	10 589.718	0.1
4	3	1 −	4	2	3	11 648.022	0.0
5	1	4 −	4	3	1	16 958.416	−2.1
5	1	5 −	4	3	2	10 080.291	1.9
5	3	3 −	4	4	1	16 815.314	3.5
5	2	4 −	5	0	5	11 011.834	−2.0
5	1	4 −	5	1	5	6 928.325	2.4
5	2	3 −	5	1	5	12 722.461	1.6
5	3	3 −	5	2	3	9 815.211	−4.1
6	2	4 −	5	4	1	14 619.632	−2.1
6	2	5 −	6	0	6	12 334.851	−1.8
7	2	6 −	7	0	7	13 950.632	−1.3
7	2	5 −	7	2	6	5 862.207	2.1
7	3	5 −	7	2	5	7 457.828	0.0
7	4	4 −	7	3	4	14 593.951	−0.1
8	3	6 −	8	2	6	6 035.081	0.5
8	4	5 −	8	3	5	13 597.229	1.3
10	3	7 −	10	3	8	6 529.969	1.1
12	4	9 −	12	3	9	6 862.619	−0.4
13	4	9 −	13	4	10	6 824.779	0.4
13	4	10 −	13	3	10	5 067.698	0.6
14	5	10 −	14	4	10	11 790.360	1.1
16	5	11 −	16	5	12	6 832.260	−0.2
16	5	12 −	16	4	12	7 245.194	0.1
19	6	13 −	19	6	14	6 622.364	−0.9
20	6	15 −	20	5	15	7 289.889	−0.9
22	7	15 −	22	7	16	6 255.603	0.3

Table 2. Rotational transitions of 2,2-dimethylthiirane ^{34}S isotopomer, ground state. Frequencies in MHz, errors $\delta\nu = \nu(\text{obs.}) - \nu(\text{calc.})$ in kHz, standard deviation $\sigma = 1.0$ kHz.

J'	K'_-	K'_+	$-J$	K_-	K_+	ν(obs.)	$\delta\nu$
1	0	1 −	0	0	0	6 354.904	−0.5
1	1	0 −	0	0	0	8 901.030	0.3
2	0	2 −	1	0	1	12 644.833	−0.1
2	1	2 −	1	1	1	12 259.849	−0.5
2	1	1 −	1	1	0	13 159.733	0.7
2	2	0 −	2	1	2	7 703.318	1.6
3	2	1 −	3	1	3	8 667.588	−1.1
3	3	1 −	3	2	1	11 327.433	−0.2
4	1	4 −	3	2	2	16 054.291	0.0
4	2	2 −	4	1	4	10 211.872	−0.1
4	3	1 −	4	2	3	11 849.553	−0.5
4	3	2 −	4	2	2	10 910.990	0.1
4	4	0 −	4	3	2	16 147.048	−0.1
4	4	1 −	4	3	1	16 105.546	−0.2
5	3	2 −	5	2	4	12 280.833	0.4
5	3	3 −	5	2	3	10 203.624	−0.4
5	4	1 −	5	3	3	16 126.666	−0.7
5	4	2 −	5	3	2	15 962.396	1.2

rotational transitions of the torsionally excited states could not be detected using the molecular beam spectrometer. If the two methyl tops are regarded to be independent two degenerate first torsionally excited states exist ($v_1 = 0$, $v_2 = 1$ and $v_1 = 1$, $v_2 = 0$). This degeneracy is lifted by torsion–torsion interaction, resulting in two observed torsionally excited states labeled $q = 1$ and $q = 2$. The rotational transitions of these states showed a torsional fine structure, which appears as a symmetric narrow triplet. It was resolvable only with values of $J \geq 7$. For the same rotational transition the $q = 2$ state showed a 26% wider splitting compared to the $q = 1$ state. If the molecule is considered under configurational symmetry the two states are classified by the a' and a'' species of the group C_s [11] and designated by $v_{18} = 1$ and $v_{33} = 1$.

$J'K'_-K'_+ - JK_-K_+$	$^{13}C_{rm}$		$^{13}C_{rh}$		$^{13}C_m$	
	ν(obs.)	$\delta\nu$	ν(obs.)	$\delta\nu$	ν(obs.)	$\delta\nu$
1 0 1 − 0 0 0	6 443.382	0.2	6 475.526	−0.2	6 388.643	−0.4
1 1 0 − 0 0 0	8 869.878	−0.2	8 991.189	0.0	8 861.966	−0.6
2 0 2 − 1 0 1	12 821.873	0.6	12 877.978	0.3	12 696.747	0.4
2 1 2 − 1 1 1	12 448.195	−0.4	12 477.969	−0.2	12 286.010	0.0
2 1 1 − 1 1 0	13 325.295	−0.4	13 424.099	−0.1	13 268.525	−0.4
2 1 1 − 1 0 1	15 751.792	0.2	15 939.762	0.1	15 741.850	0.5
2 0 2 − 1 1 0	–	–	10 362.315	0.1	–	–

Table 3. Rotational transitions of 2,2-dimethylthiirane ^{13}C isotopomers, ground state. Frequencies in MHz, errors $\delta\nu = \nu(\text{obs.}) - \nu(\text{calc.})$ in kHz, standard deviation $\sigma = 1.6$ kHz. C_{rh} = ring C atom adjacent to H's, C_{rm} = ring C atom adjacent to methyl tops, C_m = methyl top C atom.

Table 4. Rotational transitions of 2,2-dimethylthiirane in the torsionally excited states. If no symmetry label Γ is given, the torsional splitting was not resolved. $\delta\nu = \nu(\text{obs.}) - \nu(\text{calc.})$. $\delta\Delta\nu = \Delta\nu(\text{obs.}) - \Delta\nu(\text{calc.})$ with $\Delta\nu = \nu_{AA} - \nu_{\Gamma}$. The $\delta\nu$ values are given for the unsplit and AA transitions, the $\delta\Delta\nu$ values for the EA, AE, EE symmetry species. Frequencies in MHz, differences in kHz.

$J'K'_-K'_+ - JK_-K_+$	Γ	$v_{33}=1$ $(q=1)$		$v_{18}=1$ $(q=2)$	
		ν(obs.)	$\delta\nu$, $\delta\Delta\nu$	ν(obs.)	$\delta\nu$, $\delta\Delta\nu$
1 0 1 – 0 0 0	–	6 480.773	−1.9	6 481.009	2.2
1 1 0 – 0 0 0	–	8 990.795	1.9	8 987.482	−2.2
2 0 2 – 1 0 1	–	12 887.504	−5.2	12 886.983	4.1
2 1 1 – 1 1 0	–	13 436.995	6.8	13 440.173	0.6
2 1 2 – 1 1 1	–	12 486.054	−1.5	12 483.806	−4.7
2 2 0 – 2 1 2	–	7 604.055	4.4	7 594.436	7.6
2 2 1 – 2 1 1	–	6 103.630	−4.1	6 084.863	−5.5
3 3 0 – 3 2 2	–	11 411.801	3.9	11 388.044	15.0
3 3 1 – 3 2 1	–	11 045.573	−3.3	11 016.954	−12.4
4 3 2 – 4 2 2	–	10 580.201	2.4	10 546.304	−5.2
7 1 6 – 7 1 7	AA	12 025.698	−5.9	12 077.672	−2.2
	EE	12 025.765	−14.6	12 077.747	−4.5
	AE, EA	12 025.811	−8.2	12 077.81	−6.4
8 2 6 – 8 2 7	AA	8 372.899	−0.5	8 441.864	−0.9
	EE	8 372.959	−4.6	8 441.938	0.9
	AE, EA	8 373.013	−2.5	8 442.012	1.8
9 2 7 – 9 2 8	AA	11 150.623	−1.4	11 231.911	3.8
	EE	11 150.694	−3.6	11 231.997	5.1
	AE, EA	11 150.768	−9.3	11 232.093	0.2
10 2 8 – 10 2 9	AA	14 056.693	7.1	14 145.302	0.5
	EE	14 056.767	2.8	14 145.405	0.6
	AE, EA	14 056.842	5.2	14 145.506	3.2
10 4 7 – 10 3 7	AA	10 563.334	−0.4	10 468.850	1.0
	EE	10 563.295	3.4	10 468.799	0.1
	AE, EA	10 563.256	3.4	10 468.751	−2.0
11 3 8 – 11 3 9	AA	9 281.448	1.4	9 389.958	−2.1
	EE	9 281.860	−3.0	9 390.064	1.4
	AE, EA	9 281.939	−1.1	9 390.170	2.3
11 4 8 – 11 3 8	AA	8 725.561	−1.7	8 623.069	0.2
	EE	8 725.516	1.6	8 623.009	−1.8
	AE, EA	8 725.470	0.4	8 622.947	−0.1
12 3 9 – 12 3 10	AA	12 337.384	−6.8	12 462.455	0.0
	EE	12 337.484	−6.1	12 462.582	0.6
	AE, EA	12 337.575	−1.2	12 462.709	0.6
13 5 9 – 13 4 9	AA	13 942.980	−1.5	13 804.223	0.0
	EE	13 942.920	5.2	13 804.146	−2.0
	AE, EA	13 942.863	2.3	13 804.069	−1.5
14 4 10 – 14 4 11	AA	–	–	9 918.325	−2.7
	EE	–	–	9 918.467	0.0
	AE, EA	–	–	9 918.608	0.1
14 5 10 – 14 4 10	AA	11 752.991	−0.7	11 600.791	0.6
	EE	11 752.923	1.9	11 600.697	−0.7
	AE, EA	11 752.856	−2.6	11 600.602	2.4
15 4 11 – 15 4 12	AA	13 067.117	3.8	13 242.671	0.6
	EE	13 067.239	0.5	13 242.835	3.4
	AE, EA	13 067.363	2.1	13 243.001	3.6
15 5 11 – 15 4 11	AA	9 453.682	2.4	9 296.236	−0.9
	EE	9 453.606	3.0	9 296.131	0.9
	AE, EA	9 453.531	−0.1	9 296.031	0.0
17 5 12 – 17 5 13	AA	9 901.490	−1.4	10 099.760	1.1
	EE	9 901.620	1.7	10 099.934	2.6
	AE, EA	9 901.747	3.8	10 100.109	1.8

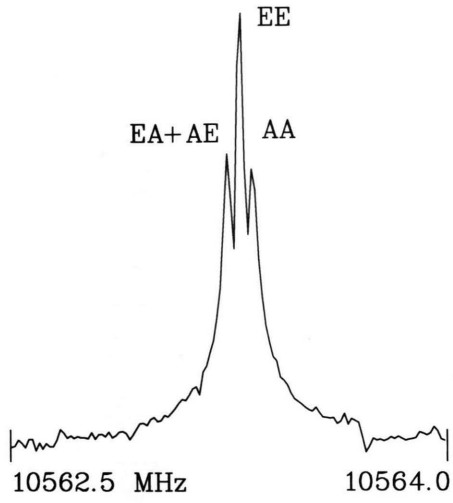

Fig. 1. Wave guide FTMW measured of 2,2-dimethylthiirane. Transition $J'K'_-K'_+ - JK_-K_+ = 10\,4\,7 - 10\,3\,7$ of the torsionally excited state $v_{33}=1$. 4096 data points recorded with a sampling interval of 10 ns, 10 million cycles averaged, polarizing frequency 10 563 MHz, temperature 220 K, polarizing time 200 ns with 25 dBm power.

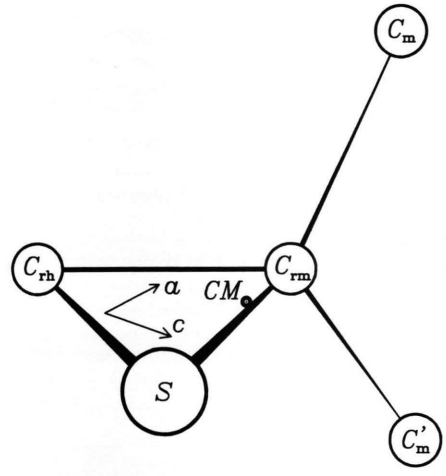

Fig. 2. Heavy atom frame of 2,2-dimethylthiirane. The H atoms are not drawn.

The symmetric $v_{18}=1$ niveau is considered to be the higher $(q=2)$ and the antisymmetric $v_{33}=1$ niveau as the lower $(q=1)$ one analogous to dimethylamine [12].

For the analysis of the spectra we used the procedure given in [13]. The basic Hamiltonian is:

$$H = B_x P_x^2 + B_y P_y^2 + B_z P_z^2 + D_{xy}(P_x P_y + P_y P_x) - 2Q_x P_x(p_1+p_2) - 2Q_y P_y(p_1+p_2) - 2Q_z P_z(p_1-p_2) + F p_1^2 + F p_2^2 + F'(p_1 p_2 + p_2 p_1) + V(\alpha_1, \alpha_2). \quad (1)$$

Table 5. Rotational and centrifugal distortion constants (Watson's A reduction, I^r representation, in MHz) of 2,2-dimethylthiirane calculated from unsplit lines and AA components. σ: single standard deviation, n: number of transitions. Centrifugal distortion constants of ^{13}C isotopomers fixed to values of normal isotopomer.

		Normal isotopomer			^{34}S isotopomer
		$v=0$	$v_{33}=1$ $(q=1)$	$v_{18}=1$ $(q=2)$	$v=0$
A	MHz	5516.94431(22)	5512.6755(23)	5507.8927(31)	5498.60897(25)
B	MHz	3480.62199(17)	3478.1236(22)	3479.5963(30)	3402.42468(22)
C	MHz	3005.71152(17)	3002.6555(22)	3001.4139(30)	2952.48245(22)
Δ_J	kHz	0.6613(40)	1.052(293)	0.826(400)	0.6526(72)
Δ_{JK}	kHz	0.5849(34)	0.633(12)	0.571(17)	0.631(18)
Δ_K	kHz	0.8036(99)	0.774(70)	0.780(94)	0.796(16)
δ_j	kHz	0.09577(25)	0.0960(8)	0.0952(10)	0.0950(47)
δ_k	kHz	−0.3717(44)	−0.326(16)	−0.383(21)	−0.553(47)
n	–	43	23	24	18
σ	kHz	1.7	4.7	6.3	0.9
		Ground state $v=0$			
		$^{13}C_{rh}$	$^{13}C_{rm}$	$^{13}C_m$	
A	MHz	5428.91445(63)	5516.8956(16)	5422.01820(73)	
B	MHz	3440.96802(22)	3474.29769(63)	3439.95252(26)	
C	MHz	3002.41643(22)	3001.23114(64)	2948.69308(25)	
n	–	6	7	6	
σ	kHz	0.7	0.3	0.8	

Table 6. Internal rotational parameters of 2,2-dimethylthiirane calculated from the splitting of the excited torsional states (program TTWF1). $\angle(a, i)$ is calculated from $\angle(b, i)$ and $\angle(c, i)$. Angles between principal axes and internal rotation axes calculated from the r_s structure are given additionally (assumed value in brackets).

		TTWF1	r_s
V_3	kJ/mol	15.172(36)	
	kcal/mol	3.624(9)	
V_{cc}	kJ/mol	−1.258(12)	
	kcal/mol	−0.300(3)	
$\angle(a, i)$	°	59.42(53)	59.38
$\angle(b, i)$	°	33.29(50)	32.80
$\angle(c, i)$	°	78.12(127)	79.39
I_α	uÅ²	[3.165]	
F	GHz	163.78	
F'	GHz	−0.933	
s		103.3(25)	
n		54	
σ	kHz	3.9	

Table 7. Heavy atom r_s coordinates of 2,2-dimethylthiirane in Å. The sign is choosen from the r_0 structure. See text for the magnitude of the errors.

Atom	a	b	c
C_{rh}	−0.4290 ( )	[0.0000]	1.2258 ( )
C_{rm}	0.5092 ( )	[0.0000]	−0.0845(2)
C_m	1.2826 ( )	±1.2763( )	0.1950 ( )
S	−1.2438 ( )	[0.0000]	−0.4035 ( )

Table 8. Structure parameters of 2,2-dimethylthiirane derived from cartesian coordinates. ( ): the parameter is more precisely calculated than the number of digits given. Bond length in Å, angles in degree.

		r_s	r_0
Dist.	$C_{rh}-C_{rm}$	1.478 ( )	1.513(10)
	$C_{rh}-S$	1.822 ( )	1.821(7)
	$C_{rm}-S$	1.820 ( )	1.838(2)
	$C_{rm}-C_m$	1.518 ( )	1.509(4)
Angle	$C_{rh}-C_{rm}-C_m$	117.8 ( )	116.8(5)
	$C_m-C_{rm}-C'_m$	114.4 ( )	116.3(5)
	$S-C_{rm}-C_m$	116.2 ( )	116.0(4)
	$S-C_{rh}-C_{rm}$	66.0 ( )	66.2(4)
	$S-C_{rm}-C_{rh}$	66.1 ( )	65.0(3)

The potential function is:

$$V(\alpha_1, \alpha_2) = \frac{V_3}{2}(2 - \cos(3\alpha_1) - \cos(3\alpha_2)) + V_{12}(\cos(3\alpha_1)\cos(3\alpha_2) - 1) + V'_{12}\sin(3\alpha_1)\sin(3\alpha_2)\ldots, \quad (2)$$

P_g, $g = x, y, z$ components of overall angular momentum,

p_i, $i = 1, 2$ internal angular momentum of the methyl top i. (3)

The Hamiltonian is invariant under the group $C_3^- \times C_{3v}^+$ [14]. The interaction between the torsionally excited

states represented by the parameters F' and V'_{12}. The results of the modified principal axis method are given in Table 6. The moment of inertia of the methyl group was fixed to the value of 2,3-dimethyloxirane [1] as it is highly correlated to the potential parameter V_3. The parameters evaluated are V_3, V'_{12}, $\angle(i, b)$, and $\angle(i, c)$. The standard deviation is of the order of the magnitude of the measuring error. It should be mentioned that the barrier V_3 is considerably higher than the barrier of 2,2-dimethyloxirane ($V_3 = 11.3$ kJ/mol) [2].

Structure

The set of rotational constants of all heavy atoms allowed to determine the partial r_s structure of the frame [15] under assumption of the C_s symmetry. The positions of the atoms are given in Table 7, the designation refers to Figure 2. The calculated errors of the r_s coordinates do not reflect the methodological errors, they originate only from the errors of the rotational constants. It should be stressed that the c coordinate of C_{rm} is very small which gives rise to an error ten times larger compared with the uncertainty of the other coordinates. In all other cases the errors are less then the number of digits given. The sign of the r_s coordinates are chosen to correspond with a r_0 structure calculation. This r_0 structure was performed by fitting the same set of rotational constants with fixed positions of the H atoms. The angles of the H atoms attached to the ring were taken from [16], the C_{rh}–H distance was assumed to 1.08 Å. The methyl group was considered to be tetrahedral with C_m–H bond lengths of 1.09 Å.

A compilation of the derived distances and angles is given in Table 8. The resulting $C_{rm}SC_{rh}$ angle of 47.9° agrees reasonably with that determined for thiirane [16].

Acknowledgements

We thank all the members of our group for help and discussions, the Deutsche Forschungsgemeinschaft, the Fonds der Chemie and the Land Schleswig-Holstein for funds. The calculations were performed partially at the computer center of the University Kiel.

[1] H. Hartwig and H. Dreizler, Z. Naturforsch. **47a,** 1051 (1992).
[2] H. Hartwig and H. Dreizler, Z. Naturforsch. **47a,** 1063 (1992).
[3] H. R. Snyder, J. M. Stewart, and J. B. Ziegler, J. Amer. Chem. Soc. **69,** 2672 (1947).
[4] U. Andresen, H. Dreizler, J.-U. Grabow, and W. Stahl, Rev. Sci. Instrum. **61,** 3694 (1990).
[5] J.-U. Grabow and W. Stahl, Z. Naturforsch. **45a,** 1043 (1990).
[6] M. Krüger and H. Dreizler, Z. Naturforsch. **45a,** 724 (1990).
[7] M. Krüger, H. Harder, C. Gerke, and H. Dreizler, Z. Naturforsch. **48a,** 737 (1990).
[8] I. Merke and H. Dreizler, Z. Naturforsch. **43a,** 196 (1988).
[9] J. Haekel and H. Mäder, Z. Naturforsch. **43a,** 203 (1988).
[10] J. K. G. Watson, in: Vibrational Spectra and Structure, Vol. 6, (J. R. Durig, ed.), Elsevier, Amsterdam 1977, p. 39.
[11] G. Herzberg, Molecular Spectra and Molecular Structure, p. 105f., van Nostrand, Princeton, New Jersey 1945.
[12] D. Consalvo, J. W. I. van Bladel, R. Engeln, and J. Reuss, Chem. Phys. **171,** 221 (1993).
[13] M. Meyer and H. Dreizler, J. Mol. Spectrosc. **148,** 310 (1991).
[14] H. Dreizler, Z. Naturforsch. **16a,** 1354 (1961).
[15] W. Gordy and R. L. Cook, Microwave Molecular Spectra, John Wiley, New York 1984, Chapt. 13.
[16] K. Okiye, C. Hirose, D. G. Lister, and J. Sheridan, Chem. Phys. Lett. **24,** 111 (1974).