it is an inner-centre luminescence. This is in agreement with the results from dielectric loss measurements showing that $Zn(SCN)_2$-Pb excited with the mercury line 365 nm is not photoconducting.

As known for mercury-like activator ions, a correspondence was established [5] between the electron transition energies in the free ion and in the ion embedded in the crystal: The ion incorporation results in a contraction of the term diagram without disturbing the succession of the terms. In the same way the activator term system in β-$Zn(SCN)_2$-Pb could be affected, regardless of the conjecture [3] that Zn-Pb-SCN-complexes are centres in this phosphor. As far as the β-$Zn(SCN)_2$ lattice seems to have moderate symmetry according to preliminary X-ray diffraction data, there is no reason to suppose that the electron transition $^1S_0 \rightarrow {}^3P_0$ which is allowed by monoclinic symmetry occurs in β-$Zn(SCN)_2$-Pb. In that case, the activator absorption in the longwave UV-region (curve 2, A) could be due to the transitions $^1S_0 \rightarrow {}^3P_1^{(1,2,3)}$ when rhombic lattice symmetry is assumed. The fact that the band groups A and B are separated from each other may be connected with the relatively large distance between the terms $^3P_1$ and $^3P_2$ in comparison with the distance between the components arising by their splitting; this is known for Pb^{2+} in alkali halides [6, 7] and can be expected for Pb^{2+} in β-$Zn(SCN)_2$ also. Thus, in the band group B the longwave elementary bands could be ascribed to transitions to three components of the splitted $^3P_2$ term. The bands superposed in the shortwave part of B can be attributed to the $^1P_1$ term components.

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Mean Amplitudes of Vibration and Coriolis Coupling Constants for Methyl Silyl Acetylene

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Mean amplitudes of vibration, Bastiansen-Morino linear shrinkages and the most important first order Coriolis coupling constants have been calculated for the molecule Methyl Silyl Acetylene. The effect of torsional vibration on the non-bonded mean amplitudes has also been investigated.

Introduction

The complete vibrational frequency assignment for the molecule Methyl Silyl Acetylene was first made by Robinson and Reeves [1]. Later Duncan [2], in the vibrational study of a series of Silicon compounds performed a normal coordinate analysis for this molecule and reported a set of F matrix elements and coriolis coupling constants. He also pointed out some errors in the vibrational assignment of Robinson and Reeves. As the spectroscopic determination of the mean amplitudes of vibration and the Bastiansen-Morino linear shrinkages [3] could be of great use to future electron diffraction studies, in this paper an attempt has been made to evaluate the above mentioned quantities. Incidentally a qualitative study has also been made to determine the dependence of mean amplitudes of vibration on torsional vibration. The most important first order coriolis coupling constants have also been determined.

Normal Coordinate Analysis

The molecule $H_3SiCCCH_3$ has a staggered C_{3v} symmetry with the normal modes distributed as $7\,A_1 + 1\,A_2 + 8\,E$, the A_2 mode representing the torsional vibration. The A_2 mode is inactive both in Raman and I.R. spectra. The Wilson's symmetry coordinates used in the present work were the same as those given by Devarajan and Cyvin [4] for Acetonitrile-Borontrifluoride. The F matrix elements given by Duncan [2] were suitably modified for the newly defined set of symmetry coordinates and properly adjusted so that the eigenvalues of the GF product matrix agreed well with experimentally observed frequencies.

The vibrational frequencies used in these calculations were the ones given by Robinson and Reeves [1], with the changes suggested by Duncan [2].

Mean Amplitudes of Vibration

The mean amplitudes of vibration and Bastiansen-Morino linear shrinkages were determined by Cyvin's method [3] and the values are given in Table 1. As in a previous publication [4] the torsional symmetry coordinate was also included in the calculation with the hypothetical frequency values 50 cm^{-1} and 150 cm^{-1}. It was found that only gauche H...H non-bonded mean amplitude was dependent on the torsional mode. The linear shrinkages remained unaffected.

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Table 1. Mean Amplitudes of Vibration (l) and Bastiansen-Morino Linear Shrinkages for SiH_3CCCH_3 in Å.

Atom Pair	l	
	0 °K	298 °K
C—H	0.0782	0.0782
C—C	0.0469	0.0474
C≡C	0.0365	0.0365
Si—C	0.0479	0.0508
Si—H	0.0900	0.0901
C . . . C	0.0503	0.0512
Si . . . C (short)	0.0495	0.0530
Si . . . C (long)	0.0575	0.0626
C . . . H (Methyl) (short)	0.1057	0.1069
C . . . H (Methyl) ((long)	0.1236	0.1336
Si . . . H (Methyl)	0.1358	0.1628
C . . . H (Silyl) (short)	0.1242	0.1274
C . . . H (Silyl) (medium)	0.1380	0.1475
C . . . H (Silyl) (long)	0.1499	0.1732
H . . . H (Methyl)	0.1256	0.1258
H . . . H (Silyl)	0.1501	0.1510
trans-H . . . H	0.1732	0.1828
gauche-H . . . H	0.2250 [a] 0.2123 [b]	0.3682 [a] 0.2726 [b]
δ C . . . C	0.0081	0.0134
δ Si . . . C (short)	0.0083	0.0155
δ Si . . . C (long)	0.0167	0.0376

[a] at torsional frequency 50 cm^{-1}.
[b] at torsional frequency 150 cm^{-1}.

Coriolis Coupling Constants

The most important first order Coriolis coupling constants viz. $\zeta^Z(E_a \times E_b)$ were calculated by the method of MEAL and POLO [5] and they are given in Table 2. The calculated values of Duncan and the experimentally observed values are also given in Table 2 for comparison.

Table 2. Diagonal Elements of $\zeta^Z(E_a \times E_b)$ fgr SiH_3CCCH_3.

$\zeta^Z(E_a \times E_b)$	This work	Ref. [2]	Exptl. (Ref. [1])
ζ_{99}	0.0599	0.06	—
ζ_{1010}	0.0153	0.01	0
ζ_{1111}	−0.3161	−0.29	—
ζ_{1212}	0.4162	0.38	—
ζ_{1313}	−0.2271	−0.21	−0.23
ζ_{1414}	0.3144	0.35	0.34
ζ_{1515}	0.8423	0.83	—
ζ_{1616}	0.9135	0.88	—

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Über die Bildung von Molekülkomplexen bei der Feldionisation organischer Moleküle

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Hetero-dimer ions are observed in the field ionization mass spectra of aniline-nitrobenzene mixtures, and also in mixtures of some other organic substances which yield charge-transfer complexes in solutions. It is shown that the structure of the hetero-dimer ions is different from the sandwich structure of the corresponding CT-complexes in solutions. Arguments are given for assuming hydrogen bonds between the components of the complexes, with an additional weak CT-bond.

JOB und PATTERSON [1] haben vor einigen Jahren in den Feldionisations (FI)-Massenspektren von Mischungen von Nitrobenzol und Anilin (Nb, An) hetero-Dimere der Zusammensetzung $(Nb-An)^+$ gefunden, die sie als „Charge Transfer Complexes" (CT) bezeichneten. In der vorliegenden Arbeit soll untersucht werden, ob diese Beobachtung sich auf andere Molekülpaare mit Donator-Akzeptoreigenschaften übertragen läßt und ob die Struktur der hetero-Dimeren derjenigen von CT-Komplexen in Lösung unter normalen Bedingungen entspricht. BLOCK [2] fand, daß die in Lösung stabilen Donator-Akzeptor-Komplexe Naphthalin—Chinon im FI-Massenspektrum nicht nachweisbar sind. Auch deren metastabile Zerfallsprodukte waren nicht zu beobachten.

Experimentelles

Für die Untersuchungen wurde ein ATLAS-CH4-Massenspektrometer mit einer speziellen Feldionenquelle [3] benutzt. Als Feldanode wurden Wolframdrähte von 10 μm Durchmesser verwandt, die mit Benzonitril aktiviert wurden [4]. Die Feldionisation erfolgte also an halbleitenden, organischen Mikronadeln (bei Feldstärken von größenordnungsmäßig $5 \cdot 10^7$ V/cm). Die Sub-

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