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IBRATIONAL SPECTRA OF HEXAMETHYLCYCLODISILAZANE

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ummary

The geometry of hexamethylcyclodisilazane has been investigated by infra-ed and Raman spectroscopy. The assignment of the bands can be very satisfac-orily made by assuming D_{2h} symmetry for the molecule.

Recent X-ray diffraction investigations have revealed the interesting molec-lar structure of some phenylcyclodisilazanes [1—3]. The full-methylated deriva-ive, however, is liquid in room temperature, and so an X-ray diffraction experi-nent is difficult. Since the geometry of four-membered ring compounds de-ends strongly on the nature of substituents [4] the plane structure of the four-nembered ring cannot be assumed without experimental proof.

We have now investigated the structure of hexamethylcyclodisilazane by neans of IR and Raman spectrophotometry.

xperimental

The IR spectrum was recorded on a Nicolet 7000 instrument using KBr lates. The range 400—50 cm^{-1} was studied on a Grub Parson FIR instrument. he Raman spectrum was recorded on a Ramanor HG-2S instrument using 14.3 nm light from an argon ion laser.

esults

If D_{2h} symmetry is assumed the molecule must contain a symmetry centre. ccording to the exclusion rule the vibrations appear alternately in the Raman nd IR spectra. Neglecting the H-atoms the molecular skeletal vibrations can be haracterised by 24 normal modes (Table 1).

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TABLE 1

NORMAL MODES OF THE MOLECULAR SKELETAL AT D_{2h} SYMMETRY

Species	Vibration	Activity
a_g	skel, skel, ν(NC), $\nu_s(SiC_2)$, $\beta_s(SiC_2)$	R
a_u	$\tau(SiC_2)$	inactive
b_{1g}	$\nu_{as}(SiC_2)$, $\beta_{as}(SiC_2)$	R
b_{1u}	skel, ν(NC), $\gamma(SiC_2)$	IR
b_{2g}	γ(NC), $\tau(SiC_2)$	R
b_{2u}	skel, β(NC), $\nu_s(SiC_2)$, $\beta_s(SiC_2)$	IR
b_{3g}	skel, β(NC), $\gamma_s(SiC_2)$	R
b_{3u}	skel, γ(NC), $\nu_{as}(SiC_2)$, $\beta_{as}(SiC_2)$	IR

The experimental frequencies and the assignments are shown in Table 2. The assignments can be very satisfactorily made by assuming D_{2h} symmetry. Two skeletal vibrations (in plane deformation and ring puckering) which are probably situated at very low frequency [5], could not be found. The vibration γ(NC) (b_{3u}) is probably very weak and close to the vibration β_{as}(SiC) (b_{3u}) at 240 cm^{-1}.

Some vibrations clearly show the operation of the exclusion rule, e.g. the skeletal vibration at 595 cm^{-1} in the infrared spectrum or the totally symmetric "breathing" mode at 552 cm^{-1} and the in-plane deformation vibration at 421 cm^{-1} in Raman spectrum.

TABLE 2

IR AND RAMAN VIBRATIONS AND ASSIGNMENTS FOR THE HEXAMETHYLCYCLODISILAZANE SKELETON (cm^{-1})

Raman			IR		Assignment
Wave number (cm^{-1})	Relative intensity	Depolarised	Wave number (cm^{-1})	Relative intensity	
1259	3	0.19			a_g ν_s(NC)
			1195	vs	b_{1u} ν_{as}(NC)
871	2	0.71			b_{3g} skel.
			860	vs	b_{1u} skel.
			785	s	b_{3u} $\nu_{as}(SiC_2)$
769	5	0.75			b_{1g} $\nu_{as}(SiC_2)$
725	11	0.34			a_g $\nu_s(SiC_2)$
			680	w	b_{2u} $\nu_s(SiC_2)$
676	5	0.75			b_{3g} β(NC)
			630	vw	b_{2u} β(NC)
			595	w	b_{2u} skel.
552	100	0.01			a_g skel.
421	76	0.01			a_g $\beta_s(SiC_2)$
			383	m	b_{2u} $\beta_s(SiC_2)$
292	3	0.75			b_{2g} γ(NC)
245	8	0.72			b_{1g} $\beta_{as}(SiC_2)$
			240	m	b_{3u} β_{as}(SiC)
203	22	0.59			b_{3g} $\gamma_s(SiC_2)$
			190	w	b_{1u} $\gamma_s(SiC_2)$
177	13	0.75			b_{2g} $\tau(SiC_2)$

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