Studies of Chain Conformational Kinetics in Poly(di-*n*-alkylsilanes) by Spectroscopic Methods. 4. Piezochromism in Symmetrical Poly(di-*n*-alkylsilanes)

Kigook Song,† Robert D. Miller, Gregory M. Wallraff, and John F. Rabolt*

IBM Research Division, Almaden Research Center, 650 Harry Road,
San Jose, California 95120-6099

Received November 5, 1990; Revised Manuscript Received February 4, 1991

ABSTRACT: The effect of elevated pressure on backbone conformation in a series of symmetrically substituted poly(di-*n*-alkylsilanes) has been investigated using UV–vis, Raman, and FTIR spectroscopy. Initially at low pressures, lateral compression occurs, which gives rise to gross changes in conformation, e.g., a change from a helical to a planar zigzag structure. This is manifested by a dramatic red shift of UV absorption bands by as much as 50 nm. At high pressures axial compression occurs, which leads to a geometrical distortion of the σ-conjugated backbone, which in turn causes a reversible continuous blue shift of UV absorption bands. Raman measurements at ambient and elevated pressures support these results.

I. Introduction

Polysilanes[1] represent an interesting class of radiation-sensitive polymers for which new applications have been discovered in microlithography and nonlinear optics. Even though the polymer backbone is composed only of silicon–silicon single bonds, all high molecular weight polysilanes absorb strongly in the UV.[1–11] Many of the alkyl[2–8] and aryl-substituted[9] polysilane derivatives exhibit an order–disorder phase transition with temperature, which is manifested by a shift in the UV absorption. This thermochromic behavior has been studied extensively by using NMR,[4,5,7] IR,[2,8] Raman,[3] and FT-Raman[11] spectroscopies, X-ray diffraction,[4,5] and thermal analysis.[2,8] For the symmetrically substituted poly(alkylsilanes), three different regimes of backbone conformational order have been observed depending on the side-chain length. The di-*n*-pentyl and di-*n*-butyl derivatives exhibit a 7/3 helical structure,[6,7] di-*n*-hexyl, di-*n*-heptyl, and di-*n*-octyl substituents favor a planar zigzag backbone,[3,8] and poly(di-*n*-tetradecylsilane)[10] appears to have a TGTG′ backbone conformation. It is thus of interest that such a small change in the polymer side chains causes a substantial difference in the conformation of the polymer backbone.

The 7/3 helical polymers of poly(di-*n*-butylsilane) (PDBS)[7] and poly(di-*n*-pentylsilane) (PDPS)[6] have a UV absorption band at 315 nm at room temperature. Although a first-order phase transition is observed at 76 and 74 °C for PDBS[7] and PDPS,[6] respectively, the position of the UV absorption band at 315 nm remains unchanged, but there is a broadening of the band observed with temperature. It is known[6,7] that above the solid-state phase transition the 7/3 helical conformation is disordered while the interchain packing is preserved. In contrast to the helical polysilanes, planar zigzag poly(di-*n*-hexylsilane) (PDHS), poly(di-*n*-heptylsilane) (PDHepS), and poly(di-*n*-octylsilane) (PDOS) exhibit a dramatic change in their UV absorption above the phase-transition temperature.[3,8] For PDHS a thermochromic shift of the UV absorption from 370 nm at room temperature to 315 nm above 42 °C occurs. At this temperature, PDHS has been shown[3] to undergo a reversible transformation from a planar zigzag backbone to one that appears to be a disordered helix. Poly(di-*n*-tetradecylsilane) (PDTS), which has a TGTG′ conformation, also exhibits thermochromic behavior with a 25-nm red shift in its UV absorption maximum above the transition temperature.[10]

Recently the effect of high pressure on the UV absorption spectrum of polysilanes has been investigated. A preliminary study[12] on this piezochromism in PDHS using FTIR and Raman spectroscopy indicated that while external pressure initially causes a conformational ordering through lateral compression at low pressures, a conformational disordering occurs at high pressures due to axial compression along the chain. Similar piezochromic behavior has also been observed in polygermanes.[13] The nature of the piezochromic effect in poly(di-*n*-alkylsilanes) in the low-pressure regime (<2.5 kbar) has been studied extensively by X-ray diffraction and NMR spectroscopy.[14,15] In the present study, the piezochromic behavior of a series of poly(di-*n*-alkylsilanes) has been investigated up to 25 kbar, and they were found to exhibit different piezochromic behavior depending on the length of the side chain.

II. Experimental Section

Sample Preparation. Samples of poly(di-*n*-alkylsilanes) were synthesized as previously described.[16,17] The high molecular weight fractions ($M_w > 1 \times 10^6$) were isolated by slow precipitation from hexane by using isopropyl alcohol. These samples were used in the subsequent spectroscopic studies. For the measurements of all high-pressure spectra, a diamond anvil cell[18] was used. A detailed description of this cell and the pressure calibration procedure was given elsewhere.[19] Thin films of UV–vis absorption measurements were obtained by casting a dilute solution of polymer in hexane onto a 0.01-in.-thick metal gasket with a 0.03-in. hole at the center supported on a diamond anvil. After drying overnight in a vacuum, a small piece of powdered ruby was enclosed within the hole for the calibration of the pressure and a drop of ethanol/methanol (4:1) mixture was placed in the gasket hole as a pressure transmitting fluid. The other diamond anvil was then quickly replaced and sealed. For the Raman measurement, the polymer sample was enclosed directly within the metal gasket on the diamond anvil. The diamond anvil cell was then placed into the Raman spectrometer using a 180° back-scattering geometry.

Characterization. UV–vis spectra were obtained by using a Hewlett-Packard photodiode array spectrometer fitted with a neutral density and a cutoff filter to eliminate photodegradation of the polysilanes during the measurement. Raman spectra were recorded with a Jobin-Yvon HG-2S double monochromator equipped with concave holographic gratings and a spatial filter to enhance stray light rejection. The source of excitation was

---

† Present address: Hoechst Celanese Research Division, Summit, NJ 07901.

0024-9297/91/2224-4084$02.50/0

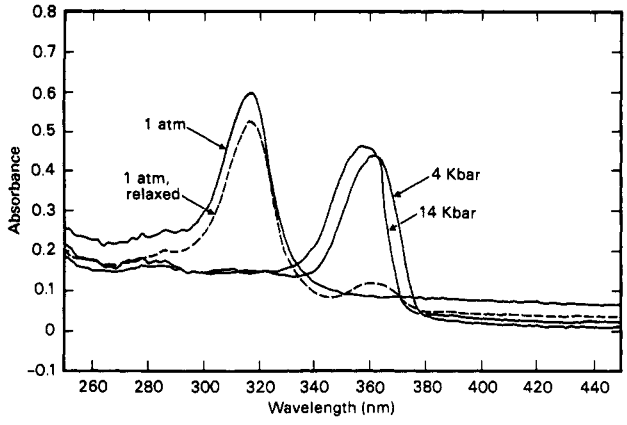

Figure 1. UV spectrum of poly(di-*n*-pentylsilane) as a function of pressure.

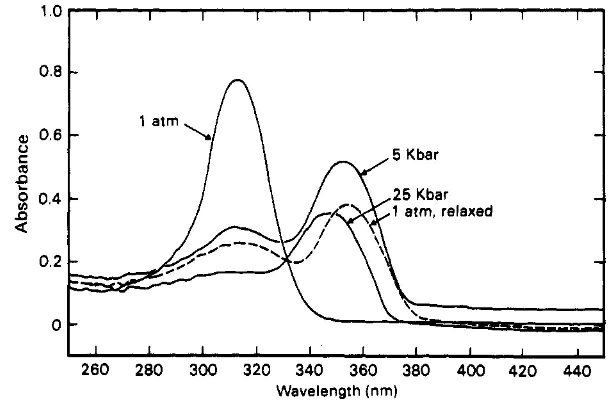

Figure 2. UV spectrum of poly(di-*n*-butylsilane) as a function of pressure.

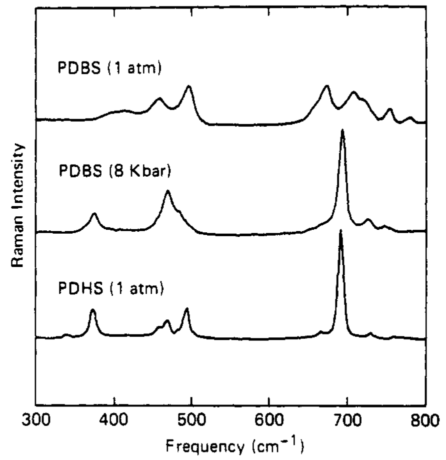

Figure 3. Raman spectra of poly(di-*n*-butylsilane) at 1 atm and 8 kbar; poly(di-*n*-hexylsilane) at 1 atm.

provided by a Spectra Physics 2020 argon ion laser operating at 514.5 nm with 400 mW of power incident on the sample. The scattered light was focused onto a cooled RCA 31034A-02 photomultiplier tube and the signal processed by using standard photon-counting electronics. All data were collected digitally by a Nicolet 1180 data system. Typical spectra were recorded at 6-cm^{-1} resolution with the coaddition of 5–10 scans.

III. Results and Discussion

A. Poly(di-*n*-butylsilane) and Poly(di-*n*-pentylsilane). Although the UV spectra of PDPS and PDBS in the solid state show little change in position of the absorption maximum with temperature,[6,7] their spectral behavior with pressure is quite dramatic, as seen in Figures 1 and 2. At atmospheric pressure PDPS has a 7/3 helical backbone conformation[6] and exhibits a UV absorption band at 315 nm whose position remains virtually unchanged at elevated temperature. However, as shown in Figure 1, at a pressure of 4 kbar the 315-nm band is completely replaced by a red-shifted band at 360 nm. A further increase in pressure brings about a small continuous blue shift of the 360-nm band. When the pressure is released, the spectrum immediately returns to the original spectrum except for a small band, which remains at 360 nm. This observation suggests the PDPS has been completely transformed into a new conformation above 4 kbar, with a small amount of this pressure-induced conformation being stable upon return to ambient conditions.

PDBS, which also has a 7/3 helical structure,[7] shows similar piezochromic behavior (Figure 2). With increasing pressure the 315-nm band observed at ambient pressure decreases its intensity and a new absorption band develops at 355 nm. At 25 kbar the 315-nm band almost completely disappears while the red-shifted absorption band at 355 nm exhibits a blue shift to 350 nm. As will be discussed later, this is a result of two sequential events. In the low-pressure regime the 315-nm band is replaced by the band at 355 nm while in the high-pressure regime this band shows a continuous blue shift of 5 nm. It is worth noting that upon release of the pressure the 350-nm band shifts back to 355 nm and maintains significant intensity while the 315-nm band reappears with reduced intensity. In this way the behavior differs from that of PDPS where only a small amount of the 355-nm form exists upon return to ambient pressure.

Raman studies have provided insight into the solid-state phase transition, which is observed in PDBS with pressure. As seen in Figure 3, the Raman spectrum of PDBS at 8 kbar is completely different from that of PDBS obtained at ambient conditions. The high-pressure spectrum of PDBS is similar to that of PDHS, which has a planar zigzag backbone at room temperature and ambient pressure. Most of the bands shown in Figure 3 are attributable to vibrations[3] of the silicon backbone. A particularly obvious change in the spectrum of PDBS with pressure is the presence of a very intense band at 689 cm^{-1}, which has been used as an indicator of the presence of a planar zigzag backbone conformation. This band has previously been assigned[3] to a Si–C symmetric stretching vibration in the planar zigzag conformation by using an isotopically substituted PDHS sample. Its asymmetric counterpart is observed at 727 cm^{-1} and is considerably weaker in intensity. There are also significant differences in the Si–Si stretch region (350–500 cm^{-1}) between the Raman spectra of PDBS obtained at 1 atm and that obtained at 8 kbar. The bands at 375 and 470 cm^{-1} in the high-pressure spectrum of PDBS are also found in the spectrum of PDHS. These two bands can be attributed to the symmetric and the asymmetric Si–Si stretching vibrations of a planar zigzag silicon backbone, respectively. It is thus evident that by the application of pressure PDBS undergoes a conformational transition from a 7/3 helix to a planar zigzag structure.

In addition to the assignments of the Raman bands characteristic of the planar zigzag silicon backbone, the bands belonging to the 7/3 helical conformation can be identified by comparing the spectra of PDBS and PDHS in Figure 3. The origin of a medium-intensity band at 495 cm^{-1} and weak bands at 670 and 460 cm^{-1} observed in the

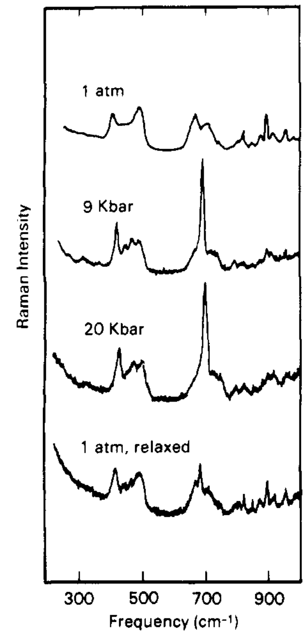

Figure 4. Raman spectrum of poly(di-*n*-pentylsilane) as a function of pressure.

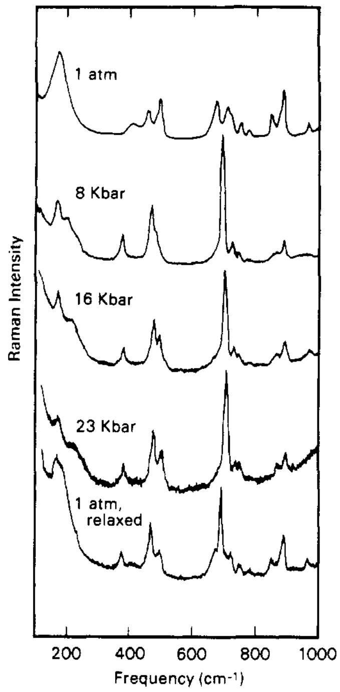

Figure 5. Raman spectrum of poly(di-*n*-butylsilane) as a function of pressure.

PDHS spectrum may result from the presence of a second non-trans conformer, which has been shown to exist as a disordered helical structure by UV[2] and X-ray studies.[3,4] These Raman bands are not found in the spectrum of PDBS at 8 kbar, as expected for a planar structure, but are observed in the 1-atm spectrum of PDBS as prominent bands. Interestingly, other helical polysilanes, such as PDPS (Figure 4) and poly(*n*-pentyl-*n*-hexylsilane),[20] also show clear Raman bands around 710, 675, 495, and 410 cm^{-1} at ambient conditions, and these Raman bands disappear when their conformations transform into a planar zigzag structure. This suggests that these four Raman bands can be assigned to the vibrations of helical silicon backbone sequences occurring in either ordered or disordered chains. Therefore, the strong Raman band at 675 cm^{-1} shown in the 1-atm spectrum of PDBS is assigned to the symmetric Si–C stretching vibration while the weak band near 710 cm^{-1} can be attributed to the asymmetric Si–C stretch. The strong band found at 495 cm^{-1} and the broad band around 410 cm^{-1} are assigned to the asymmetric and symmetric Si–Si backbone stretching vibrations of a helical backbone, respectively. The origin of the 460-cm^{-1} Raman band is unclear at the present time.

A change in structure of PDPS with pressure can be observed in the Raman spectra shown in Figure 4. As for the case of PDBS, the high-pressure Raman spectrum of PDPS is completely different from its spectrum obtained at ambient pressure. The presence of the intense 689-cm^{-1} band in the spectrum obtained at 9 kbar indicates that the application of pressure causes a change in backbone conformation from a 7/3 helix to a planar zigzag structure. This finding is consistent with the observation in the UV spectra shown in Figure 1. In the low-pressure regime the UV absorption band at 315 nm found at ambient pressure is replaced by an absorption band located at longer wavelength (360 nm) because the effective σ-conjugated length along the silicon backbone increases in planar zigzag structure. Recently, Schilling et al.[15] have found the same pressure-induced conformational changes for PDBS and PDPS samples subjected to pressure using X-ray diffraction and solid-state NMR spectroscopy.

As the pressure is further increased, that is, in the high-pressure regime, the 360-nm absorption band exhibits a continuous blue shift in both PDBS and PDPS. As seen in Figure 5 the Raman bands in the 450–500-cm^{-1} region of PDBS due to Si–Si asymmetric stretching vibrations change as a function of pressure. After the conformation of PDBS converts to the planar zigzag structure at 8 kbar, the Raman band at 470 cm^{-1} characteristic of the planar silicon backbone appears with a shoulder near 490 cm^{-1}. As the pressure is further increased, the shoulder near 490 cm^{-1} characteristic of a nonplanar silicon backbone becomes a definite Raman band and then increases its intensity relative to those characteristic of the planar structure. Although other Raman bands characteristic of the nonplanar silicon backbone are present, the only noticeable change found in the Raman spectra in the high-pressure regime is the appearance of the 490-cm^{-1} band. Interestingly, for the disordered PDHS the 495-cm^{-1} band has the strongest intensity among the Raman bands characteristic of the nonplanar backbone (Figure 3). Hence, these observations in the Raman and UV spectra in the high-pressure regime suggest that a distortion of the silicon backbone occurs, perturbing the σ-conjugation and resulting in a blue shift in the UV absorption band. Similar observations of a blue shift in the UV absorption have been reported previously by Harrah and Ziegler[21] on films of unsymmetrically substituted atactic poly(*n*-alkylsilanes) subjected to elevated pressures or low temperatures.

Thus, it becomes apparent that, as pressure is applied, two sequential events occur. In the low-pressure regime a conversion of a helical into a planar zigzag structure brings about a replacement of the 315-nm UV absorption band with a red-shifted band at 360 nm while in the high-pressure regime conformational distortion results in a continuous reversible shift of this band to lower wavelength. This represents the difference between lateral compression at low pressures compared with chain compression at elevated pressures. The volume of the crystalline region is initially reduced through the lateral compression, which causes a full extension of the silicon backbone through a collapse of the helix. In the high-pressure regime, however, the lateral compression has

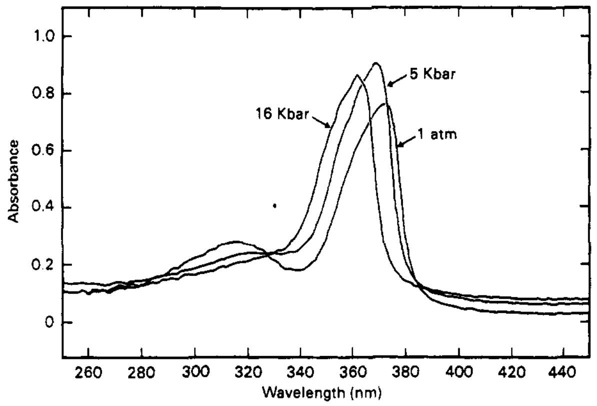

Figure 6. UV spectrum of poly(di-*n*-hexylsilane) as a function of pressure.

reached its maximum and a further reduction in the sample volume can be achieved only by compression along the chain axis, resulting in geometrical distortions of planar zigzag backbone through changes in Si–Si bond lengths, Si–Si–Si bond angles, and Si–Si–Si–Si dihedral angles. This in turn gives rise to a reversible blue shift of the 360-nm band.

Upon release of pressure the UV spectrum of PDPS (Figure 1) exhibits the small pressure-induced absorption band at 360 nm while returning the 315-nm absorption band almost to its original intensity. The same change is observed in the pressure-released Raman spectrum in Figure 4 where the intense 689-cm^{-1} band disappears with the reappearance of the Raman bands characteristic of a 7/3 helix. For PDBS, the Raman spectrum obtained after releasing pressure (see the bottom spectrum in Figure 5) shows that the intensities of the bands characteristic of the planar structure are still more intense than those characteristic of the 7/3 helix. This is also in agreement with that found in the UV spectrum (Figure 2) where the intensity of the residual 355-nm absorption band is stronger than that of the 315-nm band upon release of pressure. This implies that the pressure-induced structure of PDBS is more stable than that of PDPS at ambient conditions.

B. Poly(di-*n*-hexylsilane), Poly(di-*n*-heptylsilane), and Poly(di-*n*-octylsilane). The response of the intermediate length side chain symmetrically substituted poly(alkylsilanes) to pressure is somewhat different. PDHS, PDHepS, and PDOS have a planar zigzag structure together with a small amount of a disordered component at ambient conditions. This is manifested by a strong UV absorption at 370 nm and a weak absorption at 315 nm, respectively,[8] as shown in Figure 6 for PDHS. A shift of the 315-nm absorption band to 370-nm and a continuous blue shift of this band with pressure have been observed for PDHS, PDHepS, and PDOS. A detailed interpretation using FTIR and Raman spectroscopy of this piezochromic behavior in PDHS has been given in a preliminary report.[12] The effect of pressure is similar to that found for PDBS and PDPS at high pressures except that the UV absorption characteristic of the planar structure is found at 370 nm (instead of 355 nm) and its shift toward the blue begins to occur at a lower pressure than that for PDBS and PDPS. At 20 kbar the 370-nm absorption band in PDHS shows a blue shift of 15 nm, which is much larger than the shift observed in PDBS. This may be attributed to a difference in the extent of planar zigzag sequences found for both the PDHS and PDBS since PDHS already has an extended planar structure at ambient pressure as indicated by the UV absorption maximum at 370 nm.

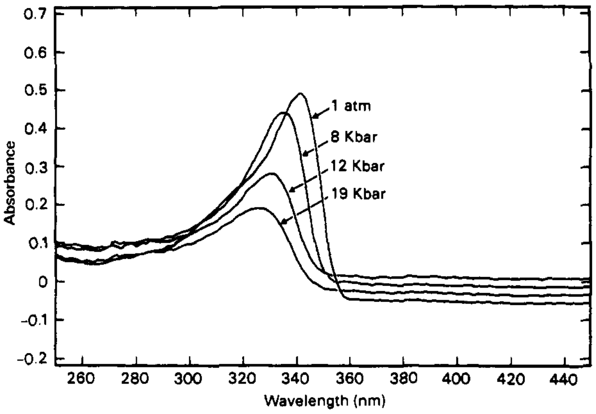

Figure 7. UV spectrum of poly(di-*n*-tetradecylsilane) as a function of pressure.

The effect illustrated in Figure 6 most likely occurs due to lateral compression at low pressures causing a reduction in intensity of the 315-nm band as reported previously by Schilling et al.[15] followed by axial compression causing a geometrical distortion of the backbone. This results in a distortion of the backbone electronic structure, resulting in a blue shift of the 370-nm band.

C. Poly(di-*n*-tetradecylsilane). The last symmetrically substituted poly(alkylsilane) investigated in this study is PDTS, which has a TGTG′ backbone conformation according to recent X-ray diffraction measurements on oriented fibers.[10] As shown in Figure 7, PDTS exhibits a reversible continuous blue shift of its 345-nm UV absorption band with pressure. It is surprising to see that PDTS does not show a sudden red shift of the UV absorption band with pressure as seen in other symmetrically substituted poly(alkylsilanes). This observation indicates that a conformational transition with pressure from a TGTG′ to a planar zigzag structure does not occur in PDTS. This is understandable upon consideration of the bond rotations required to transform a TGTG′ structure into its trans planar analogue. It is sterically impossible solely by lateral compression to transform this conformation into a trans planar backbone. Further support for this premise can be obtained from Raman spectroscopy where no bands characteristic of a planar silicon backbone are found in the high-pressure spectrum.

It is interesting to note that there is precedent for such an observation. Poly(vinylidene fluoride) (PVF$_2$) exhibits both a TGTG′ (form II) and a planar (form I) structure depending on the sample processing history.[22] In this case also the application of pressure alone cannot transform form II into a planar conformation.

Further insight into this observation can be obtained by considering that the long side chains ($C_{14}H_{29}$) of PDTS hamper the lateral compression of a silicon backbone by reducing their volumes easily with pressure. Hence, the interchain separation changes only slightly with pressure. The continuous blue shift of the UV absorption band to 325 nm at 19 kbar would then suggest that the backbone conformation of PDTS becomes distorted with increasing pressure due to changes in Si–Si bonds and Si–Si–Si angles. This behavior is similar to that observed for PDHS shown in Figure 6.

IV. Conclusions

Piezochromism in a series of symmetrically substituted poly(alkylsilanes) has been investigated by UV and Raman spectroscopy. PDBS and PDPS exhibit a UV absorption band at 315 nm, which is replaced by a red-shifted absorption band at 360 nm at low pressures while higher pressures bring about a continuous blue shift of this absorption band. This is a result of two sequential event that occur with increasing pressure. The volume of the sample is initially reduced through the lateral compression, which causes a conformational transition from a 7/3 helix to a planar zigzag structure. This conformational change results in the red shift of the UV absorption band because the effective σ-conjugated length along the silicon backbone is increased in the planar zigzag structure. In the high-pressure regime, the lateral compression has reached its maximum and a further reduction in the sample volume can be achieved by compression along the chain axis, giving rise to distortions of the planar zigzag silicon backbone. This is reflected in the UV spectrum as a continuous blue shift of the 360-nm absorption band since the geometrically distorted backbone perturbs the σ-conjugation along the silicon backbone.

PDHS, PDHepS, and PDOS, which have a planar zigzag structure at ambient conditions, exhibit similar piezochromic behavior as PDBS and PDPS. However, trans planar polysilanes begin to experience the chain axis compression at lower pressure and show much larger blue shift of their 370-nm UV absorption band. PDTS, which has a TGTG′ conformation, exhibits a continuous blue shift of the UV absorption band at 345 nm. It is interesting that PDTS does not show a red shift of the UV band with pressure, implying that pressure cannot induce a transition to the planar zigzag conformation.

Acknowledgment. We acknowledge the financial support and technical motivation of L. Siperko and D. Barr of the IBM Endicott Laboratories.

References and Notes

(1) West, R. *J. Org. Met. Chem.* **1986**, *300*, 327.
(2) Miller, R. D.; Hofer, D.; Rabolt, J. F.; Fickes, G. N. *J. Am. Chem. Soc.* **1985**, *107*, 2172.
(3) Kuzmany, H.; Rabolt, J. F.; Farmer, B. L.; Miller, R. D. *J. Chem. Phys.* **1986**, *85*, 7413.
(4) Lovinger, A. J.; Schilling, F. C.; Bovey, F. A.; Ziegler, J. M. *Macromolecules* **1986**, *19*, 2657.
(5) Schilling, F. C.; Bovey, F. A.; Lovinger, A. J.; Ziegler, J. M. *Macromolecules* **1986**, *19*, 2660.
(6) Miller, R. D.; Farmer, B. L.; Fleming, W.; Sooriyakumaran, R.; Rabolt, J. F. *J. Am. Chem. Soc.* **1987**, *109*, 2509.
(7) Schilling, F. C.; Lovinger, A. J.; Zeigler, J. M.; Davis, D. D.; Bovey, F. A. *Macromolecules* **1989**, *22*, 3055.
(8) Rabolt, J. F.; Hofer, D.; Miller, R. D.; Fickes, G. N. *Macromolecules* **1986**, *19*, 611.
(9) Miller, R. D.; Sooriyakumaran, R. *Macromolecules* **1988**, *21*, 3120.
(10) Farmer, B. L.; Miller, R. D.; Rabolt, J. F.; Fleming, W. W.; Fickes, G. N. *Bull. Am. Phys. Soc.* **1988**, *33*, 657.
(11) Hallmark, V. M.; Sooriyakumaran, R.; Miller, R. D.; Rabolt, J. F. *J. Chem. Phys.* **1989**, *90*, 2486.
(12) (a) Kuzmany, H.; Rabolt, J. F.; Miller, R. D. Proceeding of the International Conference on Macromolecules, Merseburg, GDR, 1987. (b) Song, K.; Kuzmany, H.; Wallraff, G. M.; Miller, R. D.; Rabolt, J. F. *Macromolecules* **1990**, *23*, 3870.
(13) Song, K.; Rabolt, J. F.; Wallraff, G. M.; Miller, R. D. *Bull. Am. Phys. Soc.* **1990**, *35*, 744.
(14) Walsh, C. A.; Schilling, F. C.; Macgregor, R. B., Jr.; Lovinger, A. J.; Davis, D. D.; Bovey, F. A.; Zeigler, J. M. *Synth. Met.* **1989**, *28*, C559.
(15) Schilling, F. C.; Bovey, F. A.; Davis, D. D.; Lovinger, A. J.; Macgregor, R. B., Jr.; Walsh, C. A.; Zeigler, J. M. *Macromolecules* **1989**, *22*, 4645.
(16) Miller, R. D.; Hofer, D., McKean, D. R.; Wilson, C. G.; West, R.; Trefonas, P. T. In *Materials for Microlithography*; Thompson, L. F.; Wilson, C. G.; Frechet, J. M., Eds.; ACS Symposium Series 266; Americal Chemial Society: Washington, DC, 1984; Chapter 14.
(17) Trefonas, P. T.; Djurovich, P. L.; Zhang, X. H.; West, R.; Miller, R. D.; Hofer, D. *J. Polym. Sci., Polym. Lett. Ed.* **1983**, *26*, 819.
(18) Ferraro, J. F. *Vibrational Spectroscopy at High External Pressure*; Academic Press: New York, 1984.
(19) Rabolt, J. F.; Piermarini, G.; Block, S. *J. Chem. Phys.* **1978**, *69*, 2872.
(20) Song, K.; Miller, R. D.; Wallraff, G. M.; Rabolt, J. F. submitted for publication in *J. Chem. Phys.*
(21) Harrah, L.; Ziegler, J. *ACS Symp. Ser.* **1987**, *358*, 452.
(22) Hasegawa, R.; Takahashi, Y.; Chatani, Y.; Tadokoro, H. *Polym. J.* **1972**, *3*, 600.

Registry No. PDPS (homopolymer), 97036-66-3; PDPS (SRU), 96228-24-9; PDBS (homopolymer), 97036-65-2; PDBS (SRU), 95999-72-7; PDHS (homopolymer), 97036-67-4; PDHS (SRU), 97036-67-4; PDHepS (homopolymer), 100044-91-5; PDHepS (SRU), 100044-92-6; PDOS (homopolymer), 97036-68-5; PDOS (SRU), 98865-30-6; PDTS (homopolymer), 117652-56-9; PDTS (SRU), 107999-70-2.