3.1 Introduction

Stilbene has been a molecule of interest, as it presents intriguing questions with respect to molecular structure and dynamics of isomerization. The structure of the ground state of stilbene and the dynamics involved in the cis-trans photoisomerization has been the subject of a number of experimental\textsuperscript{1-6} and theoretical\textsuperscript{7-9} studies, over many decades. The cis-isomer is known to be non-planar, with the two phenyl groups adopting an out-of-plane configuration, due to steric interactions. There is, however, considerable debate on whether the structure of the trans-isomer is planar or non-planar. Gas phase electron diffraction\textsuperscript{10} and photoelectron spectroscopic studies\textsuperscript{11} suggest the structure to be non-planar and that the phenyl groups are rotated by \( \sim 30^\circ \) around C-phenyl bond. However, solid state X-ray diffraction studies\textsuperscript{12,13} and gas phase studies in molecular beams\textsuperscript{14} indicate the structure to be planar. In solution and melts, Raman spectroscopy indicates that the trans isomer appears to lose its planarity; a conclusion arrived at due to the observation of a strong Raman feature at 960 cm\(^{-1}\)\textsuperscript{15} and a weaker feature at 760 cm\(^{-1}\).\textsuperscript{16} These features were observed to be weak in crystals, where the structure was shown to be planar. However, apart from these two vibrational features observed in the Raman spectrum, no other vibrational feature has been observed for this non-planar structure.

Theoretical calculations ranging from HF, MP2, MP3 and coupled cluster models have been used in a number of studies on this molecule, but have not led to an unambiguous resolution of this problem. Arenas et al.\textsuperscript{17} have calculated the geometric parameters and the frequencies for trans- and cis-stilbene using a 3-21G basis and showed that the cis-stilbene is non planar with phenyl to ethylene torsional angles (i.e. the 10-1-12-14 and 12-14-16-25
dihedral angles in Fig. 3.1a) of 44.7°, whereas trans-stilbene was shown to have a value of 27.2° for these torsional angles (Fig. 3.1b). This geometry for trans-stilbene agreed fairly well with that observed in the electron diffraction study.\textsuperscript{10} When a 6-31G* basis set was used, Choi and Kertesz\textsuperscript{18} found that HF and MP2 methods showed trans-stilbene to be non-planar, while calculations at the BLYP, B3LYP and BVWN levels, indicated a planar structure for this isomer. Han et al.\textsuperscript{19} concluded from their theoretical analysis that the phenyl groups of trans-stilbene can rotate freely up to about 30°. Kwasniewski et al.\textsuperscript{20} have applied focal point analysis for a comparison of the planar and non-planar trans-stilbene. They estimated an energy difference of 0.46 kcal/mol between the planar and non-planar form, with the latter being lower in energy, at the CCSD(T)/6-31G** level. This difference almost vanished (0.02 kcal/mol) at the CCSD(T)/cc-pVDZ level, while the planar form was indicated to be more stable at the Møller-Plesset levels of theory in conjunction with Dunning’s correlation consistent polarized valence basis sets. They eventually concluded that in the non-relativistic limit and within the frozen core approximation, trans-stilbene in vacuum has, as its minimum energy structure, a strictly planar form. Chowdary et al.\textsuperscript{21} have performed computations on this problem at the MP2/6-31G**, and have shown that the zero-point-vibrational corrections are comparable to the barriers between the planar and non-planar form. Consequently, they argue, that the controversy that exists in experimental studies of the planar/non-planar enigma is as much caused by this “vibrational quasi-planarity”. The above discussion highlights the ambiguity in our understanding of the structure of the ground state of trans-stilbene.

The issue of cis-trans photoisomerizm in stilbene has also been an area of intense study, as this system which leads to cis-trans isomerization through the rotation around the central ethylenic C=C bond, is a model system for the study of photoisomerization process. Orlandi and Siebrand\textsuperscript{7} have reported that the second higher excited singlet state, S\textsubscript{2}, has a potential which has a minimum corresponding to a perpendicular orientation of the two
Fig. 3.1 – Computed structures at the B3LYP/6-31++G** level of (a) cis-stilbene and (b) trans-stilbene, showing the atom numbering.
phenyl groups (i.e. 1-12-14-16 dihedral angle in Fig. 3.1 is 90°); for the same orientation of
the phenyl groups, the $S_1$ state shows a weak maximum, while the ground electronic state, $S_0$,
displays a strong maximum. Waldeck\textsuperscript{1} and later Tavan and Schulten\textsuperscript{8} argued that the $S_1$ state
actually involves a $\pi\rightarrow\pi^*$ state mixed with one or more higher energy doubly excited forms.
From the minimum of the excited state, referred to as the “phantom state”, the molecule
returns to the ground electronic state at its maximum, from where it branches to the trans or
the cis form. The mechanisms have been supported by Wan-Ge Han et al.\textsuperscript{19} who described
that the double excited state is a neutral form and not a zwitterionic species, by using spin
unrestricted density functional theory (VWN Becke-Perdew potential method), including
broken symmetry and spin-projection methods for their simulation. Levine and Martinez\textsuperscript{9}
have emphasized the role of conical intersection and charge transfer for the cis-trans photo
isomerization about carbon double bonds. In a recent publication, Kovalenko\textsuperscript{22} have
experimentally shown the intermediacy of the phantom state in the cis-trans isomerization
reaction, and have deduced, based on spectral shifts in different solvents, that this state is
probably zwitterionic in nature.

The photoisomerization of cis-stilbene is therefore seen to proceed through the
intermediacy of the phantom state and eventually the maximum in the ground state potential.
From this maximum, a branching is observed to occur to the cis and trans forms. If as
reported in some studies, a non-planar trans structure occurs as a weak minimum in the
potential, close to the planar trans isomer, the branching from the maximum in the ground
state potential can be expected to populate, at least to some extent, this weak minimum and
which can likely be trapped in the matrix. Our earlier studies have shown that matrix isolation
spectroscopy can trap weak local minima\textsuperscript{23,24} and it was therefore thought interesting to
examine if a non-planar trans structure can be observed in solid inert gas matrixes. Cis-
stilbene was trapped in different matrixes, $N_2$, Ar, Kr and photoirradiated using a broad band
source and, in some experiments, using the fourth harmonic of a Nd:YAG laser. The photoirradiation was conducted, both during and after deposition of the cis-stilbene in the matrix. The products of photoirradiation were studied using infrared spectroscopy. As a result of this study, we have been able, for the first time, to record the infrared spectrum of the non-planar form of trans-stilbene.

3.2 Experimental details

The experimental procedure followed has already been described in Chapter 2. Three different matrix gases, Ar, N\textsubscript{2} and Kr were used as matrix gases in this study. Trans-stilbene (Sigma Aldrich, 96%), cis-stilbene (Sigma Aldrich, 96%) were used without any further purification. Deposition was done using a double jet nozzle system; through one nozzle, the matrix gas was allowed to effuse out, while through the second nozzle, stilbene was introduced into the vacuum system. Due to the low vapor pressure of trans-stilbene, the sample and the deposition line were heated to temperatures ranging from 303 K to 343 K, while for cis-stilbene, which has a relatively higher vapor pressure, room temperature (~298 K) deposition was employed.

Photoirradiation of the sample was done using a 1000W Xe arc lamp (Hanovia L-5179-000). A few experiments were also done using the fourth harmonic (266 nm) of the Nd-YAG laser (Quantel, Brilliant b) for photoirradiation. Experiments were conducted where photoirradiation was performed both during and after deposition of the sample and matrix gas on the cold substrate.

Infrared spectra of matrix isolated species were recorded by using a BOMEM MB-100 FTIR spectrometer with a spectral resolution 1 cm\textsuperscript{-1}. After recording the IR spectra of the matrix isolated species, the matrix was annealed at various temperatures, and the IR spectra again recorded.
3.3 Computational details

Detailed computations at high levels of theory on the structure of stilbenes exist in the literature; we have, therefore, restricted our work to computing the vibrational features for the various isomers of stilbene, so as to enable us to assign the features in our experiments. *Ab initio* molecular orbital calculations were performed at the B3LYP/6-31++G** level. To compute the vibrational frequencies for cis-stilbene and planar trans-stilbene, the geometries of these isomers were first optimized, without imposing any symmetry constraints, followed by a vibrational frequency calculation, which yielded all-positive frequencies. For the non-planar trans-stilbene, based on the work of Choi and Kertesz,\(^{18}\) we froze the phenyl-ethylene dihedral angle at 30°, and then performed the geometry optimization, without imposing any further constraints. Frequency calculations were performed for this optimized geometry of the non-planar trans-stilbene, which yielded all frequencies to be positive.

3.4 Results

3.4.1 Experimental

Fig. 3.2 shows the infrared spectra of trans-stilbene (trace ‘a’) and cis-stilbene (trace ‘b’), in a N\(_2\) matrix. Trace ‘c’ is the spectra recorded after photoirradiation of cis-stilbene (before annealing), while trace ‘d’ corresponds to the spectra recorded after annealing the photoirradiated matrix at 32 K. The spectra span the region 1000-900 cm\(^{-1}\) (grid A), 800-650 cm\(^{-1}\) (grid B) and 550-510 cm\(^{-1}\) (grid C) which correspond to CH bending, wagging and ring deformation in stilbenes.

Cis-stilbene, which has an absorption maximum at 275 nm,\(^{25}\) is known to undergo photoisomerization to yield trans-stilbene. When the matrix containing cis-stilbene was photoirradiated, not unexpectedly, we observed infrared features of trans-stilbene, in addition to those of cis-stilbene, as shown in Fig. 3.2. In addition to the peaks due to cis- and trans-stilbene, the matrix containing photoirradiated cis-stilbene, showed features at 525, 538, 739,
Fig. 3.2 – IR spectra of stilbenes in N₂ matrix at 12 K. (a) trans-stilbene (sample maintained at 343 K); (b) cis-stilbene (sample maintained at 298 K); (c) cis-stilbene after photoirradiation for 90 minutes; (d) Matrix corresponding to trace ‘c’ annealed at 32 K for 10 minutes.
763, 960 cm\(^{-1}\) which could not be assigned to either of these two isomers, and which we shall refer to as ‘extra features’. On annealing the matrix, these extra features decreased significantly in intensity. A corresponding increase in the intensity of the trans-stilbene features was observed. The increase in the intensity of the trans-stilbene features were confirmed by calculating the ratio of the peak intensity of the trans-stilbene with respect to a feature of cis-stilbene, used as a reference. For example, the ratio of the features at 964 cm\(^{-1}\) (of trans-stilbene) and 927 cm\(^{-1}\) (of cis-stilbene) increased from a value of 2.4 in the pre-annealed matrix to 3.5 in the annealed matrix, thereby implying that during the process of annealing, the trans isomer was being produced.

It must be noted that the features at 538, 739, and 960 cm\(^{-1}\) which are produced during photoirradiation of cis-stilbene are also observed in the spectrum of trans-stilbene (unirradiated) but with a significantly smaller intensity.

The extra features observed in the photoirradiation experiments, may be due, either, to matrix site effects or to new products produced in the photoirradiation process. Experiments were performed in various matrixes to confirm the presence or not, of matrix site effects. Figs. 3.3 and 3.4 represent the experiments performed using Ar and Kr as matrix gases respectively. Traces ‘a’, ‘b’ and ‘c’ in both the figures show the spectra of trans-stilbene, cis-stilbene and photoirradiated cis-stilbene in the corresponding matrixes. The spectra recorded after annealing the matrixes corresponds to spectra in trace ‘c’ are shown in trace ‘d’. The annealing temperature was 35 and 50 K for Ar and Kr matrixes respectively. The spectral regions showed in different grids follows the same trend as in Fig. 3.2. From the Figs. 3.2, 3.3 and 3.4 it can be clearly observed that the extra features occurred in all the matrixes, N\(_2\), Ar and Kr, which makes it highly unlikely that these features are due to matrix site effects. We therefore rule out matrix site effects as a possible cause for the extra features mentioned above.
**Fig. 3.3** – IR spectra of stilbenes in Ar matrix at 12. K (a) trans-stilbene (sample maintained at 343 K); (b) cis-stilbene (sample maintained at 298 K); (c) cis-stilbene after photoirradiation for 90 minutes; (d) Matrix corresponding to trace ‘c’ annealed at 35 K for 10 minutes.
Fig. 3.4 – IR spectra of stilbenes in Kr matrix at 12 K. (a) trans-stilbene (sample maintained at 343 K); (b) cis-stilbene (sample maintained at 298 K); (c) cis-stilbene after photoirradiation for 90 minutes; (d) Matrix corresponding to trace ‘c’ annealed at 50 K for 10 minutes.
We considered the possibility that the extra features may be due to a photodecomposition product of cis-stilbene. A possible product, though minor (~5%), produced during photoirradiation of cis-stilbene is 4a,4b-dihydrophenanthrene. The spectrum of this compound reported by Rodier et al. does not match with the extra features that we observed. Furthermore, the computed vibrational frequencies for this compound by Zhou et al. at the HF/4-21G level and our own at the B3LYP/6-31++G** level, do not agree with the frequencies of the extra features referred above. Dihydrophenanthrene as a candidate responsible for the extra features is therefore ruled out.

We also found that quinoline could be present in commercial cis-stilbene (purity 96%), as an impurity. To rule out possibility that quinoline or photoproducts of quinoline were responsible for the extra features, we recorded the spectrum of quinoline and photoirradiated quinoline, under conditions identical to that employed in the photoirradiation of cis-stilbene. These experiments too, did not yield any of the extra features referred to above. We therefore conclusively ruled out the possibility that any impurity in cis-stilbene was responsible for the extra features referred to above.

The extra features are therefore likely to be due to reaction products produced in the photoirradiation process, and as we will show below, is the result of a photoisomerization reaction.

Since cis-stilbene is known to have a strong $S_0 \rightarrow S_1$ absorption near the 260 nm wavelength, experiments were also performed using the 266 nm output of the Nd:YAG laser. Identical results were obtained with the laser as with the broad band source.

### 3.4.2 Computational

As mentioned earlier, all calculations were done at the B3LYP/6-31++G** level of theory. For the purpose of assigning the experimental features, the computed vibrational frequencies at this level were used, after appropriate scaling. To compute the scaling factor,
the strongest experimental feature of trans-stilbene at 691 cm\(^{-1}\), was correlated to the strongest computed feature for this isomer in this region, which was at 703 cm\(^{-1}\). The factor, 0.9829, that brought this computed feature in agreement with experiment was then used as the scaling factor to scale the computed features for all the isomers of stilbene. The scaled features in combination with experimental results are shown in Table 3.1. Our B3LYP level calculations were generally in agreement with those reported by Choi and Kertesz,\(^\text{18}\) where the level of theory used was BLYP/6-31++G**, with a C\(_2\) symmetry imposed on the geometric framework. It may be noted that the frequencies reported by Choi and Kertesz\(^\text{18}\) are unscaled.

The optimized structures of the cis- and planar trans-stilbene are shown in Fig. 3.1 and some selected geometrical parameters are given in Table 3.2.

### 3.5 Discussion

At the outset, the features in traces ‘a’ and ‘b’ of Fig. 3.2 agree well with the features reported for trans and cis-stilbene respectively.\(^\text{17,18}\) These features also agree well with our computed and scaled infrared features for these isomers at the B3LYP/6-31++G**, shown in Table 3.1. In trace ‘c’, which is the spectrum recorded after photoirradiation of cis-stilbene, extra features were observed in addition to the features of the cis- and trans-stilbene.

Choi and Kertesz\(^\text{18}\) computed the vibrational frequencies, at the BLYP/6-31++G** level theory, for the non-planar trans-stilbene, by freezing the dihedral angles that correspond to the orientation of the phenyl groups with respect to the ethylenic plane (i.e. 10-1-12-14 dihedral) at 30° and imposing a C\(_2\) symmetry on the geometry. They showed that the non-planar trans-stilbene features are slightly red shifted with respect to the planar trans-stilbene features, as does our own computations. Table 3.1 shows the computed frequencies of Choi and Kertesz, together with our own computed frequencies and also the frequencies observed in our matrix isolation experiments. It can be seen that the extra features observed in the
Table 3.1 – Experimental and computed vibrational wavenumbers for the various isomers of stilbene.

<table>
<thead>
<tr>
<th>Isomer</th>
<th>Experimental Wavenumbers (cm⁻¹)</th>
<th>Computed Wavenumbers (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>This workᵃ</td>
</tr>
<tr>
<td></td>
<td>N₂</td>
<td>Ar</td>
</tr>
<tr>
<td>Cis</td>
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</tr>
<tr>
<td></td>
<td>700</td>
<td>697</td>
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<tr>
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<td>786</td>
</tr>
<tr>
<td></td>
<td>927</td>
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<tr>
<td>Planar trans</td>
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</tr>
<tr>
<td></td>
<td>541</td>
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</tr>
<tr>
<td></td>
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<td></td>
<td>766</td>
<td>763</td>
</tr>
<tr>
<td></td>
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<td>960</td>
</tr>
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<td></td>
<td>985</td>
<td>981</td>
</tr>
<tr>
<td>Non-planar trans</td>
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</tr>
<tr>
<td></td>
<td>538</td>
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<td></td>
<td>960</td>
<td>956</td>
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</table>

ᵃComputed using B3LYP/6-31++G** level of theory and scaled by 0.9829.
ᵇRef. 18, computed using BLYP/6-31++G** level of theory; frequencies are unscaled.
ᶜNot discerned in experiments as it occurs between two strong features of cis and trans-stilbene.
ᵈInfrared intensities (km/mol) are shown in parenthesis.
ᵉX=Phenyl ring, Y=Ethyene double bond.
Table 3.2 – Selected structural parameters, bond distances (Å), bond angles (°) and torsional angles⁸ (°) of the various isomers of stilbene.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Cis-stilbene</th>
<th>Planar Trans-stilbene</th>
<th>Non-planar trans-stilbene</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-C12</td>
<td>1.477</td>
<td>1.467</td>
<td>1.470</td>
</tr>
<tr>
<td>C12-C14</td>
<td>1.351</td>
<td>1.350</td>
<td>1.349</td>
</tr>
<tr>
<td>C14-C16</td>
<td>1.477</td>
<td>1.467</td>
<td>1.470</td>
</tr>
<tr>
<td>C1-C12-C14</td>
<td>130.7</td>
<td>127.2</td>
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</tr>
<tr>
<td>C12-C14-C16</td>
<td>130.8</td>
<td>127.1</td>
<td>125.7</td>
</tr>
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<td>C10-C1-C12</td>
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</tr>
<tr>
<td>C14-C16-C25</td>
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<td>123.6</td>
<td>122.4</td>
</tr>
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<td>30.0</td>
</tr>
<tr>
<td>C25-C16-C14-C12</td>
<td>-35.0</td>
<td>0.0</td>
<td>30.0</td>
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</tbody>
</table>

⁸Torsional angles of the fragment ABCD, denotes the angle between ABC and BCD planes.
photoirradiation experiments agree well with the computed features for the non-planar trans-stilbene.

Choi and Kertesz\textsuperscript{18} have assigned their calculated feature at 724 cm\textsuperscript{-1} with the observed Raman band\textsuperscript{17} at 734 cm\textsuperscript{-1} and considered it as a clear evidence for the existence of non-planar trans-stilbene. The same feature was found at 739 cm\textsuperscript{-1} in both our calculation and experiments.

In order to obtain the vibrational spectrum of the non-planar trans-stilbene, the spectra of cis- and trans-stilbene spectra were subtracted from the photoirradiated cis-stilbene spectra, after scaling the intensity of cis- and trans-stilbene spectra, so as to eliminate the features of these isomers. The subtracted spectrum, which represents the spectrum of non-planar trans-stilbene, is shown in Fig. 3.5b. The subtraction process helps in discerning the feature at 696 cm\textsuperscript{-1}, which was merged into the strong features of the cis- and planar-trans form near 700 cm\textsuperscript{-1}. The computed spectrum of non-planar trans-stilbene is also shown in Fig. 3.5a for comparison, which agrees well with the subtracted spectrum shown in Fig. 3.5b. When calculating the spectra for the non-planar trans-stilbene (Fig. 3.5a), computed frequencies scaled by 0.9829 were used.

It can be seen that the features of the planar and non-planar trans-stilbene occur only slightly shifted from each other. In order to resolve the features of these two structures, a curve fitting routine, implemented through Origin 6.1 was used to decompose the spectral features in the regions 985-945, 780-755, 750-725 and 550-515 cm\textsuperscript{-1}. The curves were fitted to Lorentzian profiles and iterated to obtain a minimum in the $\chi^2$ value. The fitted curves were interpolated using B-spline for smoothing. The non-planar trans-stilbene feature which appeared overlapped with those of the planar trans isomer can be clearly discerned in this spectral decomposition procedure, which is shown in Fig. 3.6.
Fig. 3.5 – (a) Computed spectra for non-planar trans-stilbene and (b) Spectra of non-planar trans-stilbene in a N₂ matrix, obtained after subtracting the features of cis- and trans-stilbene from the spectra of photoirradiated cis-stilbene (See text for details).
Fig. 3.6 – Spectral decomposition of the features in the region 985-945, 780-755, 750-725 and 550-515 cm\(^{-1}\) by fitting to Lorentzian profiles. (See text for details).
The features assigned to non-planar trans-stilbene reduced significantly on annealing the matrix at 32 K, with a concomitant increase in the intensity of the features due to planar trans-stilbene. The conversion of the non-planar form to the planar form indicates a very small barrier between these two structures. Furthermore, the conversion of the non-planar form to the planar form also indicates that the planar form is lower in energy than the non-planar form.

To summarize, cis-stilbene on photoirradiation undergoes excitation from $S_0$ to $S_1$ state, where the 1-12-14-16 dihedral angle adopts a perpendicular orientation, following a rotation about the ethylenic C-C bond. Through the intermediacy of the phantom state, the molecule eventually returns, non-radiatively, to the maximum of the ground state potential. From here on, the molecule branches to either cis-, planar trans- or to the shallow non-planar trans orientation of stilbene. Even though, the non-planar form is separated from the planar-trans structure by only a small barrier, the matrix cage helps in trapping the shallow local minimum. The trapped non-planar form relaxes to the planar form on annealing the matrixes.

It must be emphasized that earlier structural determinations of trans-stilbene, performed in the gas phase and in crystals yielded either a non-planar or a planar trans structure. Experiments using melts have shown both forms; however, the identification of the non-planar structure in this experiment rested on the assignment of just one feature at 960 cm$^{-1}$. Our matrix isolation experiments yielded both forms of the trans-stilbene and we have also been able to obtain a detailed vibrational spectrum of the non-planar structure. Clearly, the matrix has had a role to play in trapping both forms of trans-stilbene.

### 3.6 Conclusion

For the first time, we have trapped the non-planar trans-stilbene isomer in inert gas matrixes and recorded its infrared spectra. The non-planar structure was obtained following the photo irradiation of cis-stilbene and trapping the products in solid inert gas matrixes at
temperature near 10 K. Earlier studies had identified only one mode for the non-planar trans-stilbene and the identification of this isomer rested on the observation of just the one mode at 960 cm\(^{-1}\). This work therefore represents the first report of the vibrational spectrum for this structure. The almost quantitative loss of the non-planar trans conformer, on annealing, with a corresponding increase in the intensity features of the planar trans-stilbene indicates the planar trans form to be lower in energy than the non-planar structure.
References


Chapter 3


