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E-PROPENE-1-THIOL: VIBRATION AND ROTATION SPECTRA AND MOLECULAR CONFORMATION

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ABSTRACT

Analysis of the vibration and rotation spectra together with NMR and mass spectral data for E-propene-1-thiol has shown that the molecule exists in the gas phase in a conformation with the thiol hydrogen atom in a non-planar, near *anti* orientation with respect to the double bond. This result is assessed in the light of ab initio predictions indicating the existence of both a *syn* and *gauche* rotameric form for the molecule.

INTRODUCTION

The first simple unsaturated thiol to be studied in depth using both IR and microwave spectroscopy was ethene thiol, and the information gleaned about the molecular structure, conformation, rotational isomerism and structure relaxation in this compound revealed a number of interesting features [1—4]. These studies were further augmented by ab initio calculations regarding the preferred conformations, and provided a basis for understanding the variation of rotational constants with torsional excitation [5]. The related study of propene-1-thiol was initiated in order to extend our investigations of the nature of the internal rotation about the C—S bond in unsaturated thiols. In particular, we wished to assess the effect of replacing a β-hydrogen atom by a methyl group on the conformational behaviour of the SH group located on the α carbon atom of the ethene bond, and to establish whether or not such a substitution would significantly affect the relative energies of the stable conformations as compared to that found for ethene thiol.

EXPERIMENTAL

The first successful synthesis of propene-1-thiol was by Stacey and Harris in 1963 [6]. They initiated a reaction between hydrogen sulphide and propyne in a 1:1 mixture using X-rays, irradiating at room temperature for

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about 3.5 h. The propene-1-thiol product was found to be a single geometric isomer which readily decomposed at ambient temperatures to give a polymeric oil. More recently, Brandsma [7] prepared propene-1-thiol and related compounds using the classical method of cleaving the S—R bond in propenylethylsulphides with alkali metal in liquid ammonia. Small quantities of propene-1-thiol have also been found recently in the thermal or photochemical decomposition of plant extracts [8, 9].

Our preparation was based on the work of Strausz and co-workers [10], whereupon the addition of hydrogen sulphide to propyne was effected by UV radiation. Strauss' experiments were usually carried out using liquid reactants at 195 K, whereas we carried out the photolytic reaction in the gas phase at pressures considerably below atmospheric, thus reducing the risk of explosion. A possible free radical reaction scheme leading to the formation of propene-1-thiol reproduced from Strausz' work is shown in Fig. 1.

Commercial propyne (supplied by Cambrian Chemicals) and hydrogen sulphide (supplied by B.D.H. Company) were used without further purification. The hydrogen sulphide (approx 25 cm Hg pressure) was frozen into a round bottom quartz flask (500 cm^3) using a liquid nitrogen bath. An approximately equal amount of propyne gas was then transferred into the bulb in a similar way. The gaseous mixture was irradiated for 3 min at room temperature using an unfiltered medium pressure Hanovia mercury lamp (Type 504/4). Extending the period of irradiation or using different relative quantities of reagents increased the formation of unwanted decomposition products. The reaction mixture was then condensed in a cold finger at 77 K. Replacement of the liquid nitrogen bath with an ice—salt mixture allowed the unreacted gases to distil back into the quartz bulb while retaining the products in the cold finger. The whole irradiation-trapping procedure was repeated several times, and the accumulated product transferred to a sample tube at 77 K.

For the purpose of purification and subsequent analysis, the reaction product was dissolved in a small quantity of chlorobenzene (≈ 1 cm^3) and the solution (300 μl samples) injected into a preparative carbowax column (2 m, 6 mm 15% PEG 20 H in 60—72 mesh diatomite C, AW) thermostatted

1. $H_2S + h\nu \rightarrow H + SH$
2. $CH_3C{\equiv}CH + SH \rightarrow CH_3C{=}HSH$
3. $CH_3C{=}CHSH + H_2S \rightarrow CH_3CH{=}CHSH + SH$
4. $CH_3C{=}CHSH + SH \rightarrow CH_3CSH{=}CHSH$
5. $2\,SH \rightarrow H_2S_2$
6. $2CH_3C{=}CHSH \rightarrow (CH_3C{=}CHSH)_2$
7. $H + H_2S \rightarrow H_2 + SH$
8. $H + CH_3C{\equiv}CH \rightarrow CH_3C{=}CH_2$
9. $CH_3C{=}CH_2 + H_2S \rightarrow CH_3CH{=}CH_2 + SH$

Fig. 1. Possible reaction schemes in the photochemical preparation of E-propene-1-thiol [11].

at 30°C in a Pye gas chromatograph. Three main fractions were collected, the first consisted of dissolved propyne, the second was propene-1-thiol, and the third was the chlorobenzene solvent. The retention times of these substances were sufficiently different that purification and collection were easily attained.

NMR AND MASS SPECTRAL DATA

A mass spectrum of the purified propene-1-thiol was obtained using a Finnegan 1020 mass spectrometer. The fragmentation pattern was consistent with that found for the compound by Wiebe et al. [10], and shows a molecular ion at $m/z = 74$ and the strongest peak at $m/z = 41$.

The ^{1}H NMR spectrum (taken with a JEOL JNM-FX60 spectrometer) is shown in Fig. 2. The double doublet at 1.70 δ can be assigned to the methyl group (J_{AM} = 7 Hz, J_{BM} = 1.5 Hz), whereas the doublet at 2.65 δ (J_{BX} = 9 Hz) is due to the SH group. this was confirmed by the effect on the spectrum of shaking the sample with D_2O. The vinylic protons gave a complex signal between 5.40 and 6.15 δ. Decoupling irradiation at 102 Hz (1.7 δ) and 159 Hz (2.65 δ) shows H_A at 5.70 δ (J_{AB} = 9 Hz and J_{AM} = 7 Hz) and H_B at 6.0 δ (J_{AB} = 9 Hz, J_{BX} = 9 Hz and J_{BM} = 1.5 Hz). This data is consistent with the findings of Strausz et al. [11]. where the vinylic proton signals were not resolved.

In the ^{13}C spectrum (Fig. 3), the methyl carbon resonates at 13.45 δ and

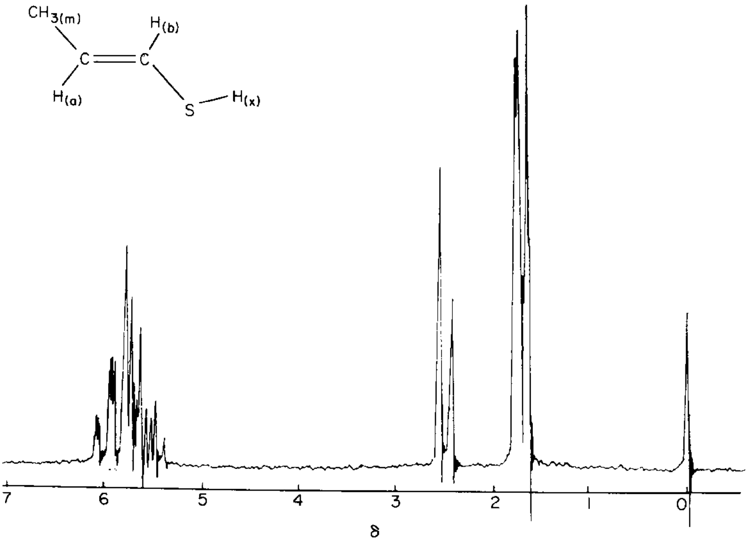

Fig. 2. Proton NMR spectrum of E-propene-1-thiol.

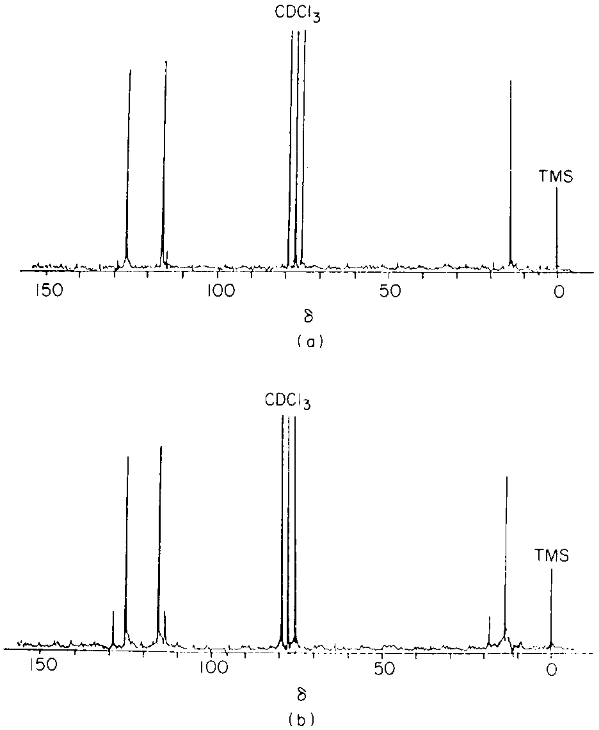

Fig. 3. (a) ^{13}C NMR spectrum of E-propene-1-thiol; (b) After UV irradiation (see text).

the sp^2 carbons at 115.52 and 125.53 δ respectively, thus confirming the presence of only one isomer. Figure 3(b) illustrates the ^{13}C spectrum after irradiating the sample for 3 h at 488 nm with an argon laser. Three new signals appear at 18.45, 114.22 and 128.69 δ, most probably corresponding to another isomer (Z or *cis*). A related experiment irradiating with unfiltered UV light from a mercury lamp led to rapid decomposition of the sample.

MICROWAVE SPECTRUM

The most generally employed method of analysing the rotational spectrum of a compound is to compare the experimentally determined spectral pattern with that predicted for various molecular models. For propene-1-thiol the three different possible geometric structures are shown in Fig. 4. For model calculations, parameters were taken from related compounds such as ethene thiol and 1-chloropropene, and rotational constants, together with the predicted rotational spectrum were computed for each structure. In addition, the orientation of the SH group was allowed to vary, via internal rotation around the C—S bond, between planar *syn* (α = 0°) and planar *anti* (α = 180°), and rotational constants were calculated for nineteen different conformations (representing a 10° variation in torsional angle) for each geometric isomer.

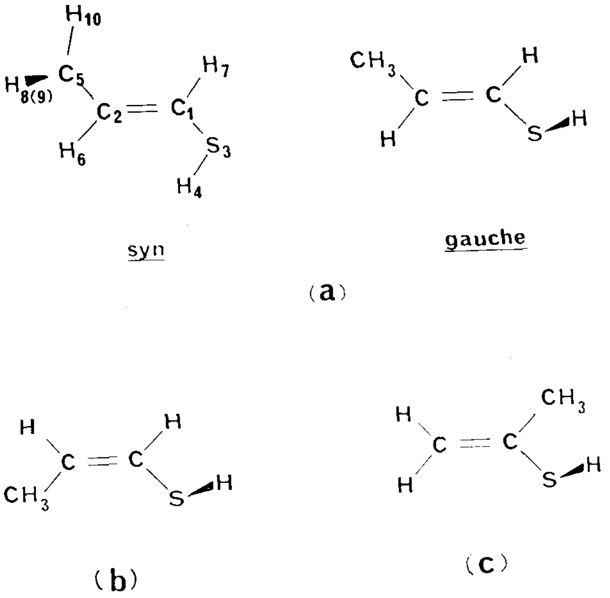

Fig. 4. Possible structures of propene-1-thiol.

The observed rotational spectrum was found to be extremely weak. However the easily recognisable pattern of μ_a-type lines, characteristic of a prolate rotor, was identified and assigned. Each line of the pattern was found to be accompanied by a partner of similar intensity and Stark effect a few MHz to high frequency of the original absorption. The observed line frequencies for both sets of assigned transitions are given in Table 1 together with the relevant rotational constants. The large experimental error associated with the A rotational constants arises mainly through the absence of the μ_b-type transactions from the fit. Attempts to assign μ_b transitions were unsuccessful largely because of the exceptional weakness of the spectrum and lack of identifiable Stark effects on these lines which could be seen. The observed rotational constants are consistent only with E-propene-1-thiol, Fig. 4(a), (see Tables 1 and 2).

The observed doubling of the μ_a-transitions is characteristic of torsional splitting associated with tunnelling of the proton of the SH group through a low, or, at most, modest potential energy barrier. The possibility that this doubling could be attributed to the effects of internal rotation of the methyl group was discounted on the grounds that the observed splitting pattern within a given transition was quite unlike that expected for a methyl group attached to a vinylic framework and, in addition, it would imply a methyl group internal rotation barrier which bears little resemblance to known barriers for vinylic methyl groups either Z-(*cis*) or E-(*trans*) to another substituent. The two sets of μ_a transitions of Table 1 are therefore designated $V = 0$ and $V = 1$ to indicate their association with the two lowest

TABLE 1

Frequencies (MHz) of rotational transitions of propene-1-thiol for the ground and first excited states of the SH torsional mode

Transition	$V = 0$		$V = 1$	
	Observed	Calculated	Observed	Calculated
$4_{04}-3_{03}$	19054.3	19054.1	19067.3	19067.1
$4_{14}-3_{13}$			18860.6	18860.2
$4_{13}-3_{12}$	19272.7	19272.5	19277.7	19277.9
$5_{05}-4_{04}$	23815.7	23815.7	23832.2	23832.0
$5_{14}-4_{13}$	24090.0	24090.2	24097.8	24097.0
$5_{23}-4_{22}$	23825.6	23825.4	23841.4	23841.4
$5_{15}-4_{14}$	23549.2	23549.3	23574.9	23574.8
$5_{24}-4_{23}$			23835.9	23836.4
$6_{06}-5_{05}$	28576.1	28576.1	28595.6	28595.7
$6_{24}-5_{23}$	28592.6	28592.8	28611.4	28611.9
$6_{16}-5_{15}$	28258.8	28258.4		
$7_{07}-6_{06}$			33357.5	33357.8
$7_{17}-6_{16}$	32966.9	32967.2	33003.3	33003.0
Rotational constants (MHz)[a]				
	$V = 0$		$V = 1$	
A	36856 ± 600		36856 ± 600	
B	2436.17 ± 0.04		2435.96 ± 0.18	
C	2328.00 ± 0.05		2331.46 ± 0.17	

[a] Values obtained from a least squares fit of the above frequencies. The constants are associated with the 'A' species lines of transitions split by internal rotation of the methyl group.

torsional states of the SH group. A consequence of the poorly determined A rotational constants is that the inertial defect cannot be used as a guide as to which is the ground state set and which is the excited state set. The labelling of Table 1 is, therefore, arbitrary.

When examined at high resolution some of the lines showed evidence of very slight splitting, e.g. $J = 4 \rightarrow 5$, $K_{-1} = 0$ at 23832 MHz was split by 0.7 MHz, which was attributed to internal rotation of the methyl group. The observed absorption pattern for the upper frequency set of the $J = 4 \rightarrow 5$ transition is shown in Fig. 5(a). Two other absorption patterns have been included for comparison in Figs. 5(b) and (c), where the effect of internal rotation of the methyl group for two different values of the methyl group rotational barrier can be clearly seen. Methyl group internal rotation barriers measured for related molecules [12, 13], are generally close to 8 kJ mol^{-1} but comparison of the $K_{-1} = 0$ splitting for the $J = 4 \rightarrow 5$ transition with predictions using the internal axis method of Woods [14] suggests that in the case of E-propene-1-thiol the barrier may be closer to 4 kJ mol^{-1}. Accurate evaluation of this barrier would require measurement

TABLE 2

Rotational constants (MHz) for the *syn* and *gauche* rotamers of E-propene-1-thiol calculated from the relevant fully optimised 4-21G geometries[a]

	A	B	C
syn (α = 0°)	38102.7	2411.4	2299.7
gauche (α = 120°)	37608.0	2418.8	2327.5

[a]Taken from ref. 5.

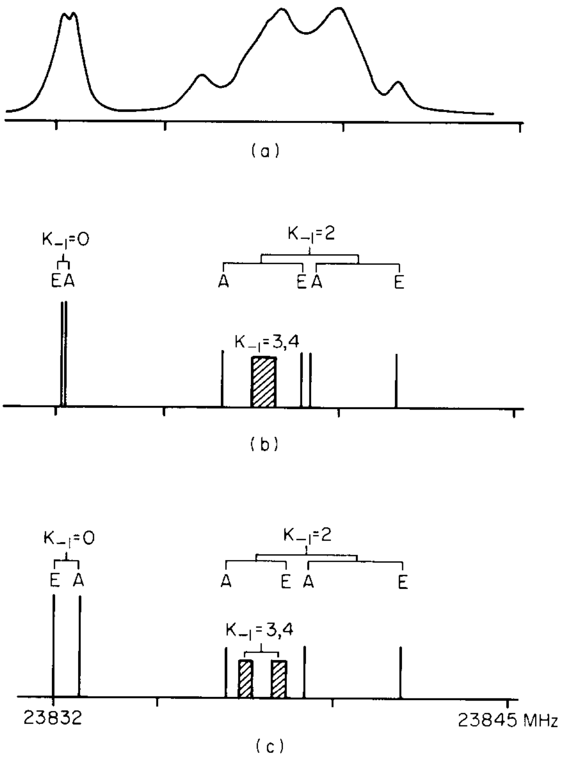

Fig. 5. (a) Part of the V = 1, J = 4 → 5 rotational transition of E-propene-1-thiol. (b) The corresponding pattern calculated with a barrier to internal rotation of the methyl group of 4 kJ mol^{-1}. (c) The predicted pattern with V_3 = 8 kJ mol^{-1} for the methyl group.

of the internal rotation splittings of many more transitions and also of μ_b lines which are sensitive to the barrier height, but owing to the general weakness of the spectrum this proved to be impossible. The transition frequencies and rotational constants of Table 1 are for the 'A' species lines arising from internal rotation of the methyl group insofar as they could be identified.

The above data, although in this instance unusually scant and limited in precision for microwave spectroscopy, imply that the origin of the observed rotational spectrum is a *gauche* rotameric form of E-propene-1-thiol. Furthermore the relative intensities of the set of transitions labelled $V = 0$ and $V = 1$ in Table 1 strongly indicate that the separation between O^+ and O^- states is less than 30 cm^{-1}.

VIBRATIONAL SPECTRUM

Obtaining good IR spectra of E-propene-1-thiol in the gas phase was difficult since some decomposition occurred during the time required to scan from 4000 to 200 cm^{-1}, with products condensing on the cell walls and windows. However, by scanning the region in small sections, a satisfactory spectrum was eventually obtained. Solution phase spectra were recorded using solvents of different polarities (CCl_4 and CH_3CN), and spectra of the solid state at 30—300 K were obtained using a CTI cryodyne refrigeration unit. Matrix isolation spectra, using nitrogen and carbon dioxide as diluent gases, were also recorded at cryogenic temperatures ($\approx$20 K).

A comparison of the spectra taken in the two different solvents showed no evidence of the occurrence of rotational isomerism in E-propene-1-thiol. This conclusion was also found to be consistent with the results of the matrix isolated spectra, and with experiments conducted at different temperatures in order to anneal the amorphous solid first produced by rapidly cooling the vapour.

The fact that E-propene-1-thiol vapour is found to have a rather sparse and relatively weak IR spectrum confirms the conclusions based on microwave data regarding the E-(*trans*) configuration about the double bond. Z-(*cis*) disubstituted ethenes tend to have a richer spectrum with considerably stronger absorption bands. The molecule can execute 24 normal vibrations, and an initial assignment of the main absorptions to these normal modes was facilitated by comparing the spectrum of propene-1-thiol with that of structurally similar species, e.g. propene, 1-chloro-1-propene and ethene thiol. Use was also made of Raman data and of a normal coordinate programme in the assignment of the absorptions seen for the gas phase sample [15]. Since all of the 24 normal modes of propene-1-thiol were not observed, estimated values for the missing vibrations were included in the computational analysis, but these were weighted for the purpose of the normal coordinate calculations in the ratio of 1:6 in comparison to the observed frequencies. For the purpose of tabulating the vibrational data the point group of the molecule is taken to be C_1, since an out-of-plane conformation of the thiol hydrogen atom seems probable from the microwave analysis. Table 3 lists the observed IR absorptions for gas, solution and solid phases, and also includes Raman data for a solution in CCl_4. A summary of the force field used is given in Table 4, and a comparison of observed and calculated data for those absorptions measured for the gas

TABLE 3

Absorption spectral data (cm^{-1}) for E-propene-1-thiol

Infrared		Raman	
Vapour	Solution (CCl_4, CH_3CN)	Solid	Solution (CCl_4)
3050		3049	3050
3030	3025	3022	2020
2938			
2935	2935	2933	2917
2875	2870	2870	2857
2599	2585	2550	2585
1620	1620	1617	1620
1435	1440	1428	1440
1385	1380	1375	1382
1337	1333	1326	1335
		1297	1297
1247	1247	1240	1227
			1213
		1068	
			960
926	938	945	935
914	916	909	915
737		730	737
672	666	674	
		534	535
			413

TABLE 4

Normal coordinate force field data for propene-1-thiol[a]

Localised vibration	Force constant[b]	Localised vibration	Force constant[b]
1 C=C stretch	7.586	16 C—C—H_9 bend	0.589
2 C—S stretch	3.871	17 C—C—H_{10} bend	0.589
3 C—H_6 stretch	5.032	18 H_8—C—H_9 bend	0.504
4 C—C stretch	4.395	19 H_8—C—H_{10} bend	0.504
5 C—H_7 stretch	5.000	20 H_9—C—H_{10} bend	0.508
6 S—H stretch	3.888	21 "Out of plane" C—H_7 wag	0.222
7 C—H_8 stretch	4.646	22 "Out of plane" C—H_7 wag	0.140
8 C—H_9 stretch	4.635	23 C—S torsion	0.005
9 C—H_{10} stretch	4.635	24 C—C torsion	0.021
10 C=C—S bend	0.926	25 C=C torsion	0.653
11 C—S—H bend	0.781	26 Interaction between (13) and (14)	0.260
12 C=C—H_7 bend	0.900	27 Interaction between (25) and (21)	0.161
13 C=C—C bend	0.585	28 Interaction between (1) and (12)	0.228
14 C=C—H_6 bend	0.992	29 Interaction between (1) and (14)	0.228
15 C—C—H_8 bend	0.411	30 Interaction between (1) and (13)	0.001

[a] Numbering system for atoms as in Fig. 4. [b] Units: stretching, mdyn A^{-1}, bending, mdyn Å rad^{-2}; stretch/bend interactions, mdyn rad^{-1}.

phase is shown in Table 5. Attempts to improve the latter by increasing the number of measured absorption bands beyond 15 by including data from spectra of the other phases and from Raman data were unsuccessful; consequently the final force field should be accorded only limited significance for this molecule. An account of the vibrational assignments is given in Table 6.

DISCUSSION

The main product generated by reacting hydrogen sulphide and acetylene photolytically in the gas phase has been shown to be E-propene-1-thiol. It is well known that E—Z (*trans—cis*) olefin isomerisation occurs photolytically and, indeed, we found that UV irradiation induced conversion from the E to Z isomers in this system to some extent. The spectroscopic data presented here are consistent with a non-planar *gauche* conformation of the thiol group with the thiol hydrogen atom located at a torsional angle close to 120° from the *syn* conformation. These conclusions and the inferences, necessarily limited, concerning the potential function for internal rotation around the CS bond are in accord with the results of ab initio predictions for E-propene-1-thiol [5].

The 4-21G internal rotation potential function is reproduced in Fig. 6 for reference. Also shown are the energy levels for the SH torsional mode computed from the 4-21G structure [5] using the particular simple Hamiltonian for the vibration

TABLE 5

Comparison of observed (gas phase) and calculated vibrational frequencies for E-propene-1-thiol

	Observed (cm^{-1})	Calculated (cm^{-1})	Approximate description
1	3050	3047	H—C stretch
2	3030	3028	H—C stretch
3	2938	2931	CH_3 antisymmetric and symmetric stretch
4	2935	2949	
5	2875	2846	
6	2599	2599	S—H stretch
7	1620	1620	C=C stretch
8	1435	1435	CH_3 antisymmetric and symmetric deformation
9	1385	1385	
10	1337	1337	H—C bending
11	1247	1247	CH_3 rocking
12	926	927	H—C bending
13	914	914	C—S—H bending
14	737	737	C—S stretch
15	672	672	H—C—C bending

TABLE 6

Vibrational assignments for E-propene-1-thiol[a]

Frequency ($\mathrm{cm^{-1}}$)	Assignment
3050, 3030	Vinylic hydrogen stretching modes
2935, 2875	Antisymmetric and symmetric stretching modes of the CH_3 group
2599	Stretching of the S—H bond, characteristically weak in the gas phase but much stronger in the condensed phases
1620	C=C stretching mode, very strong in the Raman spectrum
1435, 1385	Antisymmetric and symmetric bending modes of the CH_3 group
1337, 1297	"In-plane" bending (Raman only)
1247	Possible CH_3 rocking mode (observed in Raman)
926	"Out-of-plane" bending of the vinylic C—H bonds; the position of this absorption is quite sensitive to the nature of the substituent attached to the C=C group
914	Appears as a shoulder on the 926 $\mathrm{cm^{-1}}$ absorption in the spectrum of the vapour, but it is well resolved in the liquid and solid states; it is assigned to the C—S—H bending vibration
737	C—S stretching mode; appears much stronger in the Raman, which tends to be characteristic of such groups
672	This is the strongest absorption in the spectrum of propene thiol vapour and it is assigned to the "out-of-plane" bending of the vinylic C—H bonds (corresponding absorption in ethene thiol is at 576 $\mathrm{cm^{-1}}$)

[a] Weak absorptions are also observed at 535 and 413 $\mathrm{cm^{-1}}$ in the condensed phase spectra, and they are assigned to skeletal bending modes (C—C—S and C—C—C bending respectively). The C—CH_3 and C—S torsional modes expected between 400 and 50 $\mathrm{cm^{-1}}$ were not detected.

$$H = -F\frac{\partial^2}{\partial\alpha^2} + V(\alpha)$$

$$V(\alpha) = \Sigma\,\frac{V_n}{2}(1 - \cos n\alpha)$$

where $V(\alpha)$ is the potential energy and α is the torsional angle. The reduced rotational constant $F = 10.05\ \mathrm{cm^{-1}}$, assumed to be invariant with torsional angle, was calculated from the fully optimised 4-21G geometry for the *gauche* rotamer [5]. The torsional equation was set up using the free rotor basis set.

While there is little doubt that the main features of the observed spectra and the observed rotational constants are consistent with the *gauche* conformation of E-propene-1-thiol (see Tables 1 and 2) the potential function of Fig. 6 clearly implies the existence of a *syn* conformation with the ground torsional state some 130 $\mathrm{cm^{-1}}$ above that of the *gauche* rotamer. In favourable circumstances the population of such a state would be quite adequate for detecting the microwave spectrum of the *syn* rotamer. However, in this

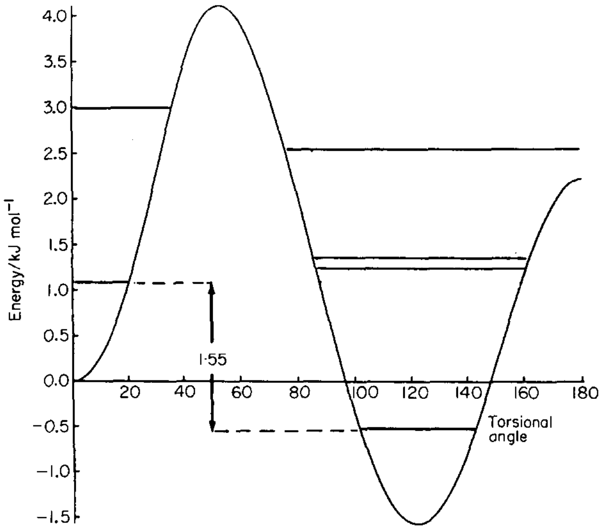

Fig. 6. The fully optimized 4-21G internal rotation potential function for the S—H torsional vibration [5].

instance, a search of the regions of the spectrum in which transitions associated with the *syn* rotamer are expected to fall yielded no unambiguous assignment of lines to that rotamer.

The predictive ability of ab initio calculations with regard to relative rotamer stability for simple cases such as propene-1-thiol is, on the whole, good. Even when account is taken of the basis set dependence of the details of the potential function of Fig. 6, including the predicted barrier heights and vibrational energy level separations, it seems unlikely that the existence of the very definite minimum at the *syn* conformation is an artifact of the calculations. A more likely explanation for the failure to detect the *syn* rotamer lies in the possibility that an unfavourable dipole moment is responsible for the inherent weakness of the spectrum and, for the *syn* rotamer, that this is exacerbated by population reduction resulting from the relative instability of the rotamer. The contention that the μ_a dipole component is small is certainly compatible with the weakness of the assigned microwave spectrum of the *gauche* rotamer. Futher support is indicated by consideration of the bond moments of the propene fragment and the CSH fragment. In propene itself the dipole moment is 0.36 D [8] and is directed almost parallel to the a-inertial axis. In E-propene-1-thiol the a-axis passes close to the carbon atom of the methyl group and almost through the sulphur nucleus as shown in Fig. 7. The moment for the CSH group is less easily defined. The magnitude and direction depend crucially on the polarity of the CS bond which is difficult to judge. If, for E-propene-1-thiol the polarity is C^-S^+, the CSH moment will be directed as shown in Fig. 7(b) and will tend to reduce the μ_a component from that associated with the propene

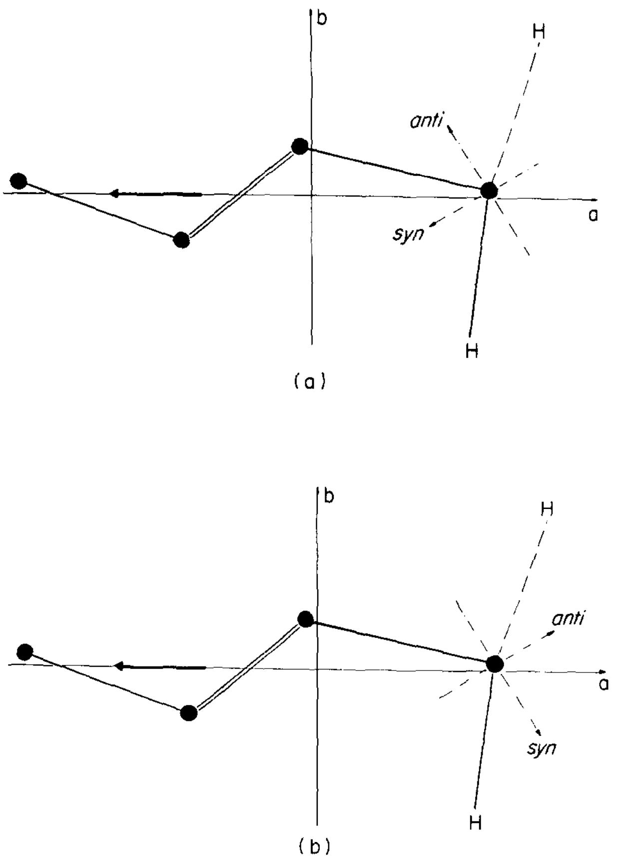

Fig. 7. Bond moments in E-propene-1-thiol. The chained arrows show the CSH bond moment directions for the *syn* and *anti* conformations.

fragment. Rotation to the *anti* rotamer would not alter this situation. The alternative choice of C^+S^- would give rise to a CSH bond moment directed close to the bisector of the CSH angle (Fig. 7(a)) and with a tendency to enhance the propene μ_a contribution in both *syn* and *anti* conformations. The absence of identifiable Stark effects in the microwave spectrum eliminates any chance of making a definite choice between these alternatives but on the basis of the limited data available, the former case (case (b) of Fig. 7) would appear to fit the overall picture most satisfactorily.

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