Conformational mobility and intramolecular rearrangements of bis(3-thioxo-1-phenylpropenyl) sulfide

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Possible intramolecular transformations of bis(3-thioxo-1-phenylpropenyl) sulfide were studied by the quantum-chemical semiempirical AM1 method. A group of the most stable, potentially spectroscopically discernible rotamers was distinguished. A possibility of intramolecular rearrangements giving thiirane structures was considered. The ability of bis(3-thioxo-1-phenylpropenyl) sulfide for spontaneous trimerization was evaluated.

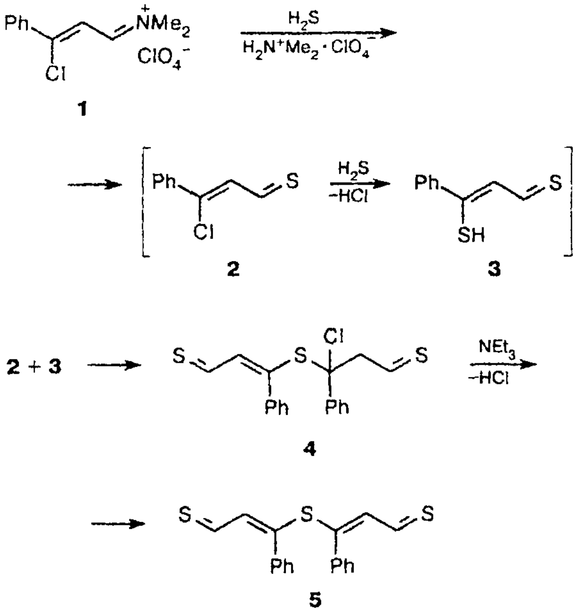
Key words: quantum-chemical AM1 method, conformation, bis(3-thioxo-1-phenylpropenyl) sulfide, cyclization, trimerization, rearrangement, thiirane, solvation.

Bis-imonio-substituted symmetric and asymmetric α,β-unsaturated sulfides of the propene, cyclohexene, and indene series have been synthesized in the reactions of enaminothioketones with halo-substituted imonium salts.[1] It was assumed[2] that these compounds can be ancestors of 1,7-dithials, 1,7-thialthiones, and 1,7-dithiones which have not been synthesized yet. The preparation of these compounds was stimulated by the successful use of the method for preparation of mesomerically stabilized α,β-unsaturated thioketones (X—C=C—C=S, X = AlkO, AlkS, Cl) *via* hydrothiolysis of imonium salts.[3] α,β-Unsaturated thioaldehydes have previously been prepared by this method.[4]

The study of the reaction of dimethyl(3-phenyl-3-chloro-2-propenylidene)ammonium (**1**) with H_2S in anhydrous DMF showed that an S-nucleophile attacks only the $C=N^+$ group rather than the C—Cl bond, as assumed previously.[5] This results in the formation of 3-phenyl-3-chloro-2-propenethial (**2**), which was not isolated in a stable form (monomeric or oligomeric), most likely due to the fact[4] that the primarily formed chloropropenethial **2** reacts rapidly with H_2S at the C—Cl bond to give mercaptopropenethial **3**. Thiol **3** reacts with chlorothial **2** to give sulfide **4**, which is transformed by triethylamine into 1,7-dithial, bis(3-thioxo-1-phenylpropenyl) sulfide (**5**) (Scheme 1).

Thials **2**, **3**, and **5** are very promising starting reagents due to their ability for intramolecular conformational and isomeric transformations that can afford new substances, in particular, those of the heterocyclic series, as well as a tendency of these compounds to form macrocyclic systems *via* dimerization, trimerization, or oligomerization. These compounds contain bulky phenyl substituents capable of steric screening of various reaction centers depending on the conformational state of the molecule, which can exert a decisive effect on the pathways of chemical reactions.

Scheme 1



Therefore, in this work, we theoretically studied the main stationary states of bis(3-thioxo-1-phenylpropenyl) sulfide (**5**) and estimated their lability in chemical processes, which is necessary for predicting the probabilities of reaction channels.

Calculation procedure

Taking into account a variety of reaction channels and possible pathways of intramolecular rearrangements (Scheme 2)

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Scheme 2

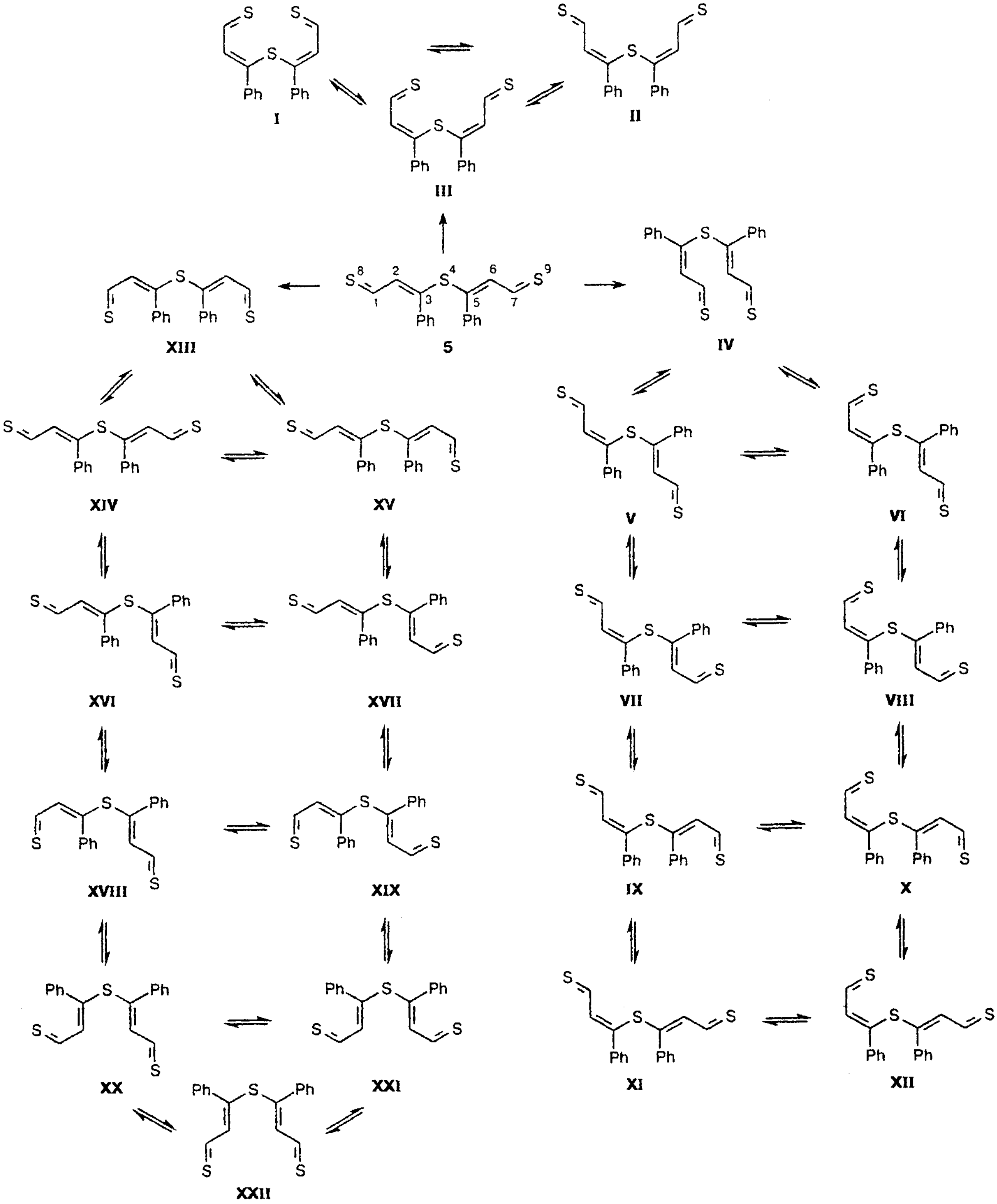
I
II
III
IV
V
VI
VII
VIII
IX
X
XI
XII
XIII
XIV
XV
XVI
XVII
XVIII
XIX
XX
XXI
XXII
5
S
Ph
1
2
3
4
5
6
7
8
9

Table 1. Relative energies (ΔE/kcal mol^{-1}) and main geometric parameters* of rotamers **I—III** of compound **5** with *cis*-arrangement of ordinary bonds in chains 1—4 and 4—7

Form	ΔE	R_{ij}/Å								φ_{ijk}							$\vartheta_{ijk/\text{Ph}}$	
		1—2	2—3	3—4	4—5	5—6	6—7	1—8	7—9	deg							deg	
										123	234	345	456	567	218	679	234/Ph	456/Ph
I	0	1.412	1.383	1.688	1.688	1.383	1.412	1.572	1.572	121.4	116.0	116.0	116.0	121.4	119.8	119.8	87.0	87.0
II	18.0	1.446	1.355	1.703	1.703	1.355	1.446	1.530	1.530	124.6	118.3	110.6	118.3	124.6	125.5	125.5	44.4	44.4
III	6.4	1.392	1.401	1.637	1.724	1.349	1.449	1.611	1.530	119.4	114.3	114.1	121.1	124.4	119.3	125.1	55.1	42.5

* For numeration of atoms, see Scheme 2; *R* are interatomic distances, φ are bond angles, and θ are dihedral angles.

on the potential energy surface (PES), it would be reasonable to use semiempirical approximation. We chose the AM1 method,[6,7] because our calculations for the related compound 3-methylthio-3-phenyl-2-propenethial gave rather good results.[8] In the search for the transition states (TS) in the gas phase, the saddle points on the PES were identified from the presence of a single negative eigenvalue of the matrix of the second derivatives by geometric parameters. Solvent effects were taken into account according to a procedure previously described in detail.[9—11] It uses two parameters that determine the properties of a solvent: the dielectric constant ε and the *c* constant independent of the sort of atoms.

Results and Discussion

Preliminary examination of the stationary states found, which are potentially capable of retaining their individual character in the reaction medium, showed a great variety of possible combinations of directed attacks of various fragments of compound **5**. As a whole, the rotational forms obtained can be divided into three groups. The specificity of each group is that which of its representatives are predominantly formed during the synthesis depends on the configuration of compounds **2** and **3** and the mechanism of their interaction. The probability of transition of the rotamers from one group to another is low, because this is related to rotation about the double bond, and the activation energy of this process for structures **I—XXII** lies in an interval of 60—130 kcal mol^{-1}.

Rotamers with *cis*-arrangement of both the C(1)—C(2) and C(3)—S(4) bonds and the S(4)—C(5) and C(6)—C(7) bonds are attributed to the first group, containing the lowest number of stationary states. Three energy minima, corresponding to forms **I**, **II**, and **III**, were found on the PES (see Scheme 2). In closed structure **I**, the phenyl rings are almost orthogonal to the basic skeleton. The skeleton remains almost planar, and the maximum shift of the atoms from the plane does not exceed 0.02 Å.

As a whole, structure **I** represents two 1,2-dithiolane fragments coordinated to the central S atom (R(S(9)—S(4)) = R(S(8)—S(4)) = 2.31 Å), in which planar forms are present instead of skewed forms due to a higher interatomic S—S distance than that in classical 1,2-dithiolanes.[12] Electron transfer from the central S atom to the C and terminal S atoms, which are valence-bound with the central S atom, increases sharply as compared to that in **II** (the charges of atoms $\rho_{S(4)}$, $\rho_{C(3)}$, and $\rho_{S(8)}$ for forms **II** and **I** are equal to +0.37, −0.20, and 0.06 au and +0.78, −0.38, and −0.01 au, respectively). The high stability of the closed structure **I** is due to the presence of the conjugated pseudo-cyclic system enabling internal donor-acceptor stabilization. The double-bond character for the C=C and C=S fragments in this system is much lower than that in the open fragments of structures **II** and **III** and increases noticeably for the C—C and C—S bonds (see Table 1).

A similar stabilizing character of the structural changes is also observed in the closed fragment of rotamer **III** (see Table 1). In the 1,2-dithiolane moiety, the S(4)—S(8) bond is further shortened (to 2.18 Å), resulting in an increase in the torsion strain due to repulsion between lone electron pairs of the S atoms.[12] As a result, a skewed structure with the C(1)—S(8)—S(4)—C(3) dihedral angle equal to 18° takes place in the stationary state. The donating ability of the S(4) atom in rotamer **III** is only slightly lower than that in form **I** ($\rho_{S(4)}$ = 0.70, $\rho_{S(8)}$ = −0.05, $\rho_{C(3)}$ = −0.22, $\rho_{C(5)}$ = −0.35 au), but the bond lengths are closer to each other. As a result, the central fragment of rotamer **III** gains a pronounced resemblance to ylide structures, which, as known,[13] possess higher possibilities of intramolecular rearrangements (see below). The open fragment of structure **III** is nonplanar, and the shift of the C(6), C(7), and S(9) atoms from the C(3)S(4)C(5) plane amounts to 0.95, 2.1, and 3.2 Å, respectively.

The spatial configuration of rotamer **II** is also nonplanar, and the α and β* angles of the lateral fragments are equal to 165° and 27°, respectively. The activation barriers of transitions **II** → **III** and **III** → **I** are equal to 2.8 and 1.7 kcal mol^{-1}. Due to this and a sufficient difference in the stability of structures **I**, **III**, and **II**, it is improbable to observe open forms of the **II** type in apolar media. In the case of the conrotary pathway, the potentially competitive one-stage transition **II** → **I** has an activation barrier of 6.5 kcal mol^{-1}.

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* Hereinafter in the discussion of the relative spatial structure, two parameters are attributed to the notion of "orientation of lateral fragments": "convolution" S(4)ABC angle (points A, B, and C lie in the middles of the C(2)...C(6), C(2)...C(3), and C(5)...C(6) lines) (α) and "incline" C(2)—C(3)—C(5)—C(6) angle (β).

In the corresponding transition state (TS), the central skeleton is nonplanar, although the C(1)C(2)C(3)S(4) and C(7)C(6)C(5)S(4) fragments remain planar within 0.15 Å. The α angle decreases to 154°. The disrotary pathway of rearrangement is virtually not related to the α-plane distortions (α ≈ 180°). At the same time, the β-deformations are great (in the saddle point β = 43°). The activation energy of the **II** → **I** transition *via* this pathway is only 0.8 kcal mol^{-1} higher than that *via* the conrotary pathway.

The polarity of structures **I**—**III** changes in the following order: **II** > **III** > **I** (the dipole moment μ = 4.7, 4.6, and 3.4 D, respectively). Taking into account the influence of the solvate environment (c = 1.2, ε = 30) results in the inversion of the relative stability of structures **III** and **I**. The half-closed form **III** becomes most stable, being more stable than rotamer **I** by 1.1 kcal mol^{-1}. The difference in stability of the compounds in the whole series is reduced from 18.0 to 13.6 kcal mol^{-1}, and the probability of observation of structures of the **II** type increases. For transitions **I** → **III**, **II** → **III**, and **II** → **I**, the saddle point corresponding to disrotary transformation **II** → **I** corresponds to the most polar state. When the solvation effects are taken into account in simulation, the barrier for disrotary transition **II** → **I** decreases to 4.1 kcal mol^{-1} and that for the conrotary transition increases to 6.9 kcal mol^{-1}. Taking into account that the barriers of one-stage transformations **II** → **III** and **I** → **III** in a polar medium also increase to 4.3 and 4.9 kcal mol^{-1}, respectively, the disrotary mechanism of rearrangement becomes competitive.

The second (more numerous) group of stationary states of compound **5** (see Scheme 2) with the *cis*-C(1)—S(4) and *trans*-S(4)—C(7) chains can conditionally be divided into two subgroups. The first subgroup of rotamers, although most stable but more sensitive to external agents, contains forms **VI**, **VIII**, **X**, and **XII**. The representatives of this subgroup, as well as form **III**, are characterized by a closed fragment with a potentially active structure. However, in this case, transition to a more stable and less active form of the **I** type is improbable because of higher activation barriers (ΔE > 60 kcal mol^{-1}).

Either the interaction with an external reagent and the transition (using this reagent) to a more stable state or spontaneous intramolecular cyclization are possible for forms **VI**, **VIII**, **X**, and **XII**. As a whole, the central skeletons of the structures in this subgroup are planar within 0.1 Å (the α and β angles differ from 180° and 0° by no more than 5°). The phenyl cycles are orthogonal to the skeleton with an accuracy of ±10°. The charge on the central S atom is lower by 0.30—0.34 au than that in the open structures and amounts to 0.71—0.75 au, and that on the carbon center increases from 0.20—0.22 to 0.32—0.35 au. Intramolecular rearrangements **XII** → **VI**, **X** → **XII**, and **VIII** → **VI** are characterized by activation barriers of 8.4, 3.9, and 1.3 kcal mol^{-1}, respectively, *i.e.*, only rotamers **XII** and **VI** are spectroscopically discernible and can be identified experimentally.

The most stable structures in this subgroup (**VI** and **XII**, Table 2) are characterized by the greatest difference

Table 2. Relative energies (ΔE/kcal mol^{-1}) and main geometric parameters* of spectroscopically discernible rotamers of compound **5** with *cis*- and *trans*-configurations of the C(1)—S(4) and S(4)—C(7) bonds, respectively

Form	ΔE	R_{ij}/Å								φ_{ijk}							$\vartheta_{ijk/\mathrm{Ph}}$	
		1—2	2—3	3—4	4—5	5—6	6—7	1—8	7—9	deg							deg	
										123	234	345	456	567	218	679	234/Ph	456/Ph
IV	19.7	1.444	1.352	1.696	1.692	1.350	1.445	1.531	1.533	126.5	130.3	111.0	126.7	124.5	125.0	125.1	57.2	104.1
VI	4.7	1.396	1.398	1.637	1.707	1.347	1.448	1.604	1.534	118.7	114.9	119.1	128.1	124.5	119.9	125.0	88.7	83.0
X	11.6	1.393	1.403	1.634	1.723	1.352	1.445	1.612	1.532	119.7	113.5	123.2	111.4	129.5	119.0	131.5	89.7	90.0
XII	7.2	1.393	1.401	1.635	1.714	1.353	1.447	1.610	1.533	120.1	113.1	121.4	113.3	124.9	119.2	125.1	88.9	86.3

* See Footnote in Table 1.

Table 3. Relative energies (ΔE/kcal mol^{-1}) and main geometric parameters* of spectroscopically discernible rotamers of compounds **5** with *trans*-configuration of the C(1)—S(4) and S(4)—C(7) bonds

Form	ΔE	R_{ij}/Å								φ_{ijk}							$\vartheta_{ijk/\mathrm{Ph}}$	
		1—2	2—3	3—4	4—5	5—6	6—7	1—8	7—9	deg							deg	
										123	234	345	456	567	218	679	234/Ph	456/Ph
XIV	28.3	1.442	1.359	1.694	1.694	1.359	1.442	1.534	1.534	124.3	111.1	119.0	111.1	124.3	124.9	124.9	90.0	90.0
XVI	23.9	1.442	1.358	1.696	1.691	1.348	1.343	1.535	1.534	124.5	112.3	115.9	130.0	128.5	125.0	131.8	86.0	90.0
XXII	22.5	1.446	1.349	1.687	1.687	1.349	1.446	1.534	1.534	124.4	129.0	113.0	129.0	124.4	125.4	125.4	76.2	76.2

* See Footnote in Table 1.

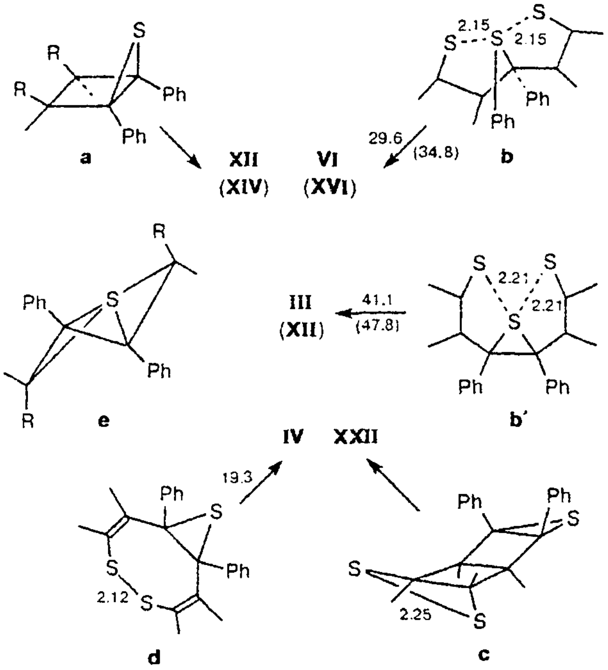
in polarity (μ = 1.9 and 5.4 D, respectively). This results in inverted relative stabilities (form **XII** is more stable, ΔE = 2.1 kcal mol^{-1}) when the effect of the solvent environment is taken into account (c = 1.2, ε = 30), and the probability of observing structures of the **XII** type in polar media increases.

It is most likely that the representatives of the second subgroup, rotamers **V**, **VII**, **IX**, and **XI**, are rather rapidly transformed into the corresponding more stable rotation forms (**V** → **VI**, **VII** → **VIII** → **VI**, **IX** → **X**, **X** → **XII**, and **XI** → **XII**) due to low activation barriers ($\leq$2.5 kcal mol^{-1}). Probably, only the highly polar (μ = 5.0 D) structure **IV** ($E_{\rm act}$ (**IV** → **VI**) = 6.2 kcal mol^{-1}) can be detected spectrally.

The third group of rotamers (forms **XIII**—**XXII**) differs from the most stable representatives of the first two groups by a relatively low stability. The fragments of these rotamers are sufficiently open and incapable of stabilizing due to intramolecular donor-acceptor interactions. In this group, only the most stable structures **XIV**, **XVI**, and **XXII** are spectroscopically discernible (Table 3). The barriers of internal transitions **XVI** → **XXII** and **XIV** → **XVI** are equal to 8.7 and 6.1 kcal mol^{-1}, respectively. The other forms are poorly stable and easily transformed into more stable systems (**XIII** → **XIV**, **XV** → **XIV**, **XVII** → **XVI**, **XVIII** → **XVI**, **XIX** → (**XVII**, **XVIII**) → **XVI**) with activation barriers of at most 2.7 kcal mol^{-1}. Structure **XXII**, which is the most stable in this group, is also the most polar (μ = 5.9 D) and has a nonplanar central skeleton (unlike forms **XIV** and **XVI**). Structures **XIV** and **XVI** are slightly skewed (α = 11° (**XIV**) and 19° (**XVI**)), whereas in form **XXII** the α angle is increased to 44°, and the β angle is decreased to 168°. In a polar medium with ε = 30, the difference in relative stability increases from 1.4 to 4.7 kcal mol^{-1} in favor of structure **XXII** as compared to the closest in stability system **XVI**.

Thus, depending on the conformational state of the starting reagents **2** and **3** and the mechanism of their interaction, the set of possible rotamers of compound **5** is most likely restricted to structures **I**, **III**, **IV**, **VI**, **XII**, **XIV**, **XVI**, and **XXII**. As mentioned above, the properties of thiocarbonylylide groups are pronounced for rotamers **III**, **VI**, and **XII**. Similar compounds, being very active species, readily transform into stable thiirane in the absence of the corresponding scavengers.[14—17] However, in the case of these rotamers, the formation of the thiirane cycle in the central fragment of molecule **5** does not result in complete stabilization of the obtained structure, because its terminal fragment gains a thioketene character, and the stabilization of this fragment requires either its local deprotonation (intramolecular prototropic migration) or the formation of new intramolecular coordination or valent bonds. The most stable cyclic states on the PES appeared for compound **5** due to conformational transformations whose main driving force is the formation of the thiirane cycle in the central part of the skeleton, presented in Scheme 3. The most probable initial rotamers are indicated by arrows, the determined activation barriers (kcal mol^{-1}) of the *cyclic structure* → *rotamers* transitions are designated by figures above the arrows, and the S...S (Å) interatomic distances are also given.

Scheme 3



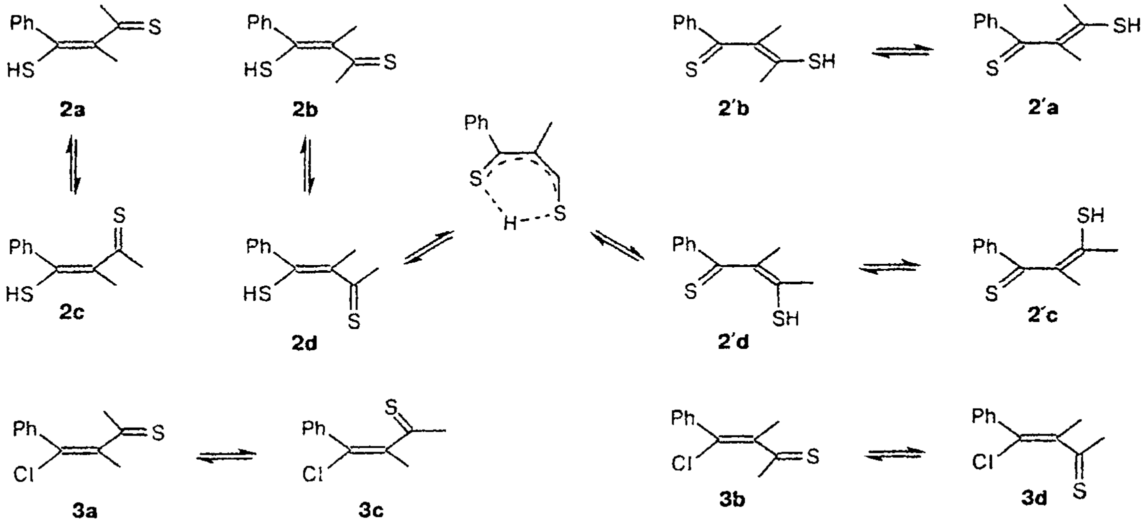
R = H—C=S

Only the minimum on the PES corresponds to system **e**, for which preferable rotational forms were not found. Structures **b** and **b′** are the most stable among the found stationary cyclic forms (Table 4) and can be "rather easily" (from the viewpoint of energy expenditures) obtained by the conrotary mechanism from rotamers **VI**, **XVI** or **III**, **XII**, respectively.

Although structure **d** is ~25 kcal mol^{-1} less stable than structure **b**, its stability is comparable with that of its model "parent," compound **IV**. It is most likely that structure **d** can be distinguished experimentally, because the activation barrier $E_{\rm act}$ for transition **IV** → **d** is 23.6 kcal mol^{-1}. It is rather difficult to observe cyclic forms of the **a**, **c**, and **e** types in the reaction mixture because of their strong strain. Nevertheless, compounds similar to structure **a** have been synthesized by photochemical reactions where an analog of system **5**, bis(1-phenylvinyl) sulfide S(CH=CHPh)$_2$, was used as the starting reagent.[18] These data suggest the photochemical synthesis of structure **a** if the concentrations of the starting rotamers of the **XII** and **XIV** types are high.

The probability of formation of different rotational forms in the reaction under study (see Scheme 2) depends on several factors. The conformational state of the starting compounds **2** and **3** can act as one of these factors (Scheme 4).

Scheme 4



The relative energies (ΔE/kcal mol^{-1}) of rotational forms **a**—**d** of compounds **2**, **2'**, and **3** are presented below.

Compound	ΔE	Compound	ΔE	Compound	ΔE
2a	4.2	**2'a**	4.0	**3a**	0.6
2b	5.0	**2'b**	4.1	**3b**	0
2c	8.4	**2'c**	8.8	**3c**	4.5
2d	0	**2'd**	0.2	**3d**	2.8

Structures **b** and **d** are preferential for mercaptothial **2** and **d** is that for chlorothial **3**, which suggests that compounds **I** and **III** should be initiated with a higher probability from the reactions (see Scheme 1). In structure **2d**, the intramolecular 1,5-prototropic shift (E_{act} = 1.3 kcal mol^{-1}; l(S(1)...H) = 1.654 Å and l(S(5)...H) = 1.614 Å for the saddle point) is quite real from the viewpoint of energy expenditures and should finally result in 1,7-dithials with phenyl substituents in the 1,5-positions. However, these products were not observed in the real reaction mixture. This in no way indicates that rearrangements **2** → **2'** are impossible but reflects only a high stereospecificity of the interaction of compounds **2** and **3**. The obtained series of the relative stability of rotational forms **2**, **2'**, and **3** in the model approximation slightly depends on solvent polarity, *i.e.*, the sequence found is violated in none of the cases.

As is known,[8,19] structures containing S=C—C=CPh—S—R chains are capable of sufficiently fast trimerization. For open rotamers of compound **5**, the probability of whose appearance in the reaction mixture is non-zero, spontaneous trimerization can be a competing route with respect to the channel of formation of thiirane forms. The trimer presented in Fig. 1 is

Table 4. Relative energies (ΔE^*/kcal mol^{-1}) of cyclic structures and main geometric** and electronic parameters of the thiyrane fragments in compounds **5a**—**e**

Form	R_{ij}/Å				φ_{ijk}			$\theta_{ijk/jk}$		ρ_i (au)			ΔE
	3—4	3—5	2—3	5—6	deg			deg		S(4)	C(3)	C(5)	
					345	235	356	γ***	β				
5a	1.796	1.539	1.551	1.551	50.6	91.0	90.5	66.7	6.0	0.02	−0.11	−0.10	49.2
5b	1.934	1.495	1.469	1.471	47.3	105.4	104.9	0.0	128	0.49	−0.04	−0.05	9.6
5b'	1.857	1.521	1.493	1.493	49.6	108.3	108.3	128.7	~0	0.54	−0.04	−0.04	20.5
5c	1.795	1.553	1.542	1.533	51.1	91.5	91.4	61.0	3.4	0.04	−0.10	−0.09	113.1
5d	1.822	1.516	1.335	1.337	50.2	123.7	124.1	75.3	6.8	−0.06	−0.01	−0.02	25.4
5e	1.825	1.476	1.481	1.483	48.8	113.6	114.1	0.0	154.1	−0.04	−0.01	−0.01	197.6

* In the energy scale accepted for the initial rotamers of compound 5.

** See Footnote in Table 1.

*** In the determination of the angle of the shift of the thiirane cycle from the plane, because of the nonplanar structure of the C(2)C(3)C(5)C(6) fragment, averaging was performed: $\gamma = \{\gamma_1[\text{C(2)C(3)C(5)/C(3)C(5)S}] + \gamma_2[\text{C(3)C(5)C(6)/C(3)C(5)S}]\}/2$.

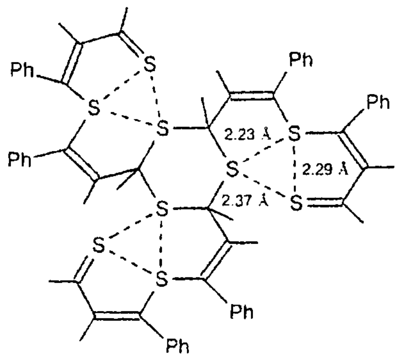


Fig. 1. Structure of the most probable trimer ($\alpha = 12^\circ$, $\beta = 15^\circ$, $\gamma = 172^\circ$).

the most stable of the trimers found. Taking into account a strong screening of the central skeleton by the phenyl substituents, this trimer can be characterized by its capability of activation under certain physicochemical conditions.

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