

Conformational Analysis of Electron Deficient Substituted Mesocyclic 1,4-Cyclodithioethers by *ab initio* Calculations

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Ab initio Hartree-Fock calculations at the HF/6-31G* level of theory for geometry optimization, MP2/6-31G*//HF/6-31G* and B3LYP/6-311G(2df,p)//HF/6-31G* levels for a single point total energy calculation are reported for the important energy minimum conformers of *trans* and *cis* isomers of 2,3-diacetyl-1,4-dithiane (**1**), 2,3-diacetyl-1,4-dithiepane (**2**) and 2,3-diacetyl-1,4-dithiocan (**3**). According to the HF/6-31G* calculations the *trans* di-equatorial of **2** and **3** are the most stable conformers but the *cis* form of **1** is more stable than the others.

Key Words: *Ab initio*, Conformational analysis, Cyclic disulfide, Stereochemistry.

INTRODUCTION

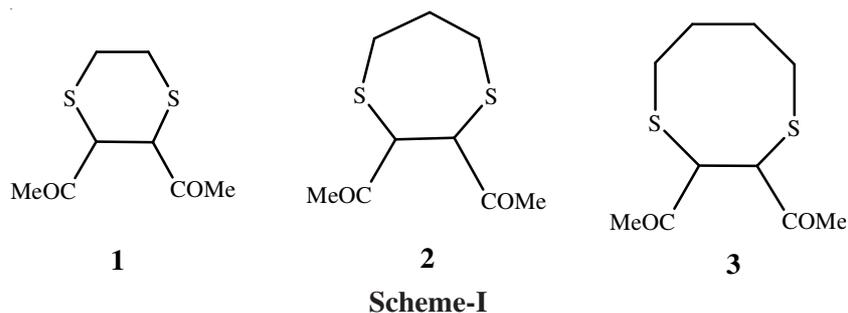
Ab initio calculations are iterative procedures based on self-consistent field (SCF) methods, that calculations are approached by the Hartree-Fock Closed-Shell approximation. One of the approximations inherent in essentially all *ab initio* methods is introduction of a basis set which an unknown linear combination of molecular orbital can be thought of as a function in the infinite coordinate system spanned by the complete basis set. The basis set of 6-31G(d) is a split valence basis where the core orbitals are a contraction of six Primitive Gaussian Type Orbitals (PGTOs) with a single *d*-type polarization that have been used in this investigation. Also these calculations have extensive configuration interaction terms at the Møller Plesset perturbation theory¹⁻³ second order (MP2) that are comparable in accuracy to B3LYP results which is based on density functional theory (DFT)⁴.

Heterocyclic compounds specially sulfur-containing heterocycles occupied a fundamental position in chemistry for many years. As we go down the periodic table (O, S, Se, Te) the inversion barriers become lower, probably because the difference in size, electronegativity and bond polarities associated with these elements are reflected in contrasting structural, conformational and reactivity behaviour for the corresponding heterocycles⁵.

In continuation of our interest in sulfur-containing heterocycles⁶⁻⁸, we wish to report the new results of computational calculation on π -deficient mesocyclic dithioethers. Thus, this study was undertaken in order to calculate geometry-optimized

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structures and configurational isomer energy differences of 2,3-diacetyl-1,4-dithiane (**1**), 2,3-diacetyl-1,4-dithiepane (**2**) and 2,3-diacetyl-1,4-dithiocan (**3**) by comparing their geometries and conformational energies using MP2/6-31G*//HF/6-31G* and B3LYP/6-311G(2df,p)//HF/6-31G* calculations (**Scheme-I**).



CALCULATIONS

Ab initio molecular orbital calculations were carried out using the GAUSSIAN 98 program⁹. Geometries for all structures were fully optimized by means of analytical energy gradients by Beryn optimizer with no geometrical constraint¹⁰. The restricted Hartree-Fock calculations with the split-valence 6-31G* basis set which include a set of d-type polarization functions on all non-hydrogen atoms were used in these calculations. Single point energy calculations at MP2/6-31+G*//HF/6-31+G* and B3LYP/6-311G//HF/6-31G* levels were used to evaluate the electron correlation effect in the energies and order of stability of conformers.

RESULTS AND DISCUSSION

2,3-Diacetyl-1,4-dithiane (1): Sulfur-containing six membered heterocycles (thiane) have important position in many biological and photographic processes¹¹⁻¹⁵, so the elucidation of intramolecular interactions and their relation to the physical and chemical properties of thiane derivatives are of interest. Thiane, dithianes and the sulfoxides derived from them adopt a chair conformation somewhat more puckered than of cyclohexane¹⁶.

When we studied the *cis* and *trans* of 2,3-diacetyl-1,4-dithiane (**1**) by *ab initio* calculations (**Scheme-II**), it is found that the *trans* (di-equatorial) isomer is more puckered conformer than the *cis* and *trans* (di-axial) forms that was confirmed by the relation between torsional angle (Φ) and valency angle (Θ) which is given in eqn. 1¹⁷.

$$\cos \Phi = -\cos \Theta / [1 + \cos \Theta] \quad (1)$$

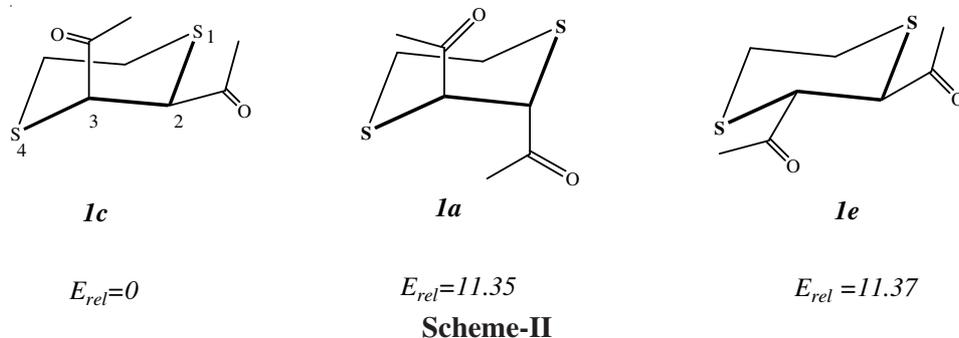
Applying eqn. 1, the average torsional angle for *trans* (di-equatorial) geometry (**1e**) that has been found in Table-1 ($\Phi_{1e} = 60.34$) is the highest value relative to the other structures ($\Phi_{1c} = 58.06$, $\Phi_{1a} = 55.20$), that exhibits the most puckered ring for **1e**. It may indicate additional attractive interactions of sulfur atoms with the electrons

TABLE-1
 CALCULATED HEATS OF FORMATION (kJ mol^{-1}), TOTAL AND ZERO-POINT VIBRATION (ZERO-POINT VIBRATION ENERGY IS SCALED BY A FACTOR OF 0.9135 TO ELIMINATE KNOWN SYSTEMATIC ERRORS IN CALCULATIONS) ENERGIES (HARTREE), RELATIVE ENERGY (INCLUDING ZERO-POINT ENERGY, kJ mol^{-1}) AND STRUCTURAL PARAMETERS FOR CHAIR CONFORMATION OF *trans*- AND *cis*-2,3-DIACETYL-1,4-DITHIANE

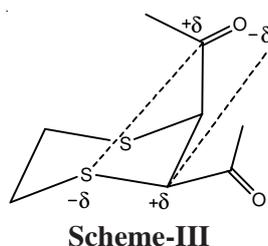
Structure	1e (<i>trans-ee</i>)	1a (<i>trans-aa</i>)	1c (<i>cis</i>)
HF/6-31G**//HF/6-31G	-1254.67532619	-1254.67532418	-1254.67980905
MP2/6-31G**//HF/6-31G*	-1254.67532619	-1254.67532418	-1254.67980905
B3LYP/6-311G//HF/6-31G*	-1258.85887576	-1258.85770275	-1258.86122857
ZPE	0.204839	0.204827	0.205005
$E_{\text{rel}}^{\text{a}}$	11.37	11.35	0.0
$E_{\text{rel}}^{\text{b}}$	11.37	11.35	0.0
$E_{\text{rel}}^{\text{c}}$	5.78	8.83	0.0
$S_1\text{-}C_2$	1.85	1.84	1.84
$C_2\text{-}C_3$	1.53	1.53	1.53
$C_3\text{-}S_4$	1.85	1.83	1.85
$S_4\text{-}C_5$	1.82 (1.81) ^d	1.81	1.82
$C_5\text{-}C_6$	1.51 (1.49)	1.51	1.51
$C_6\text{-}S_1$	1.82	1.82	1.82
$S_1\text{-}C_2\text{-}C_3$	112.38	115.38	111.81
$C_2\text{-}C_3\text{-}S_4$	112.42	116.10	116.39
$C_3\text{-}S_4\text{-}C_5$	102.10 (99.0)	104.09	102.57
$S_4\text{-}C_5\text{-}C_6$	113.39	112.52	114.45
$C_5\text{-}C_6\text{-}S_1$	113.51 (126.3)	113.84	113.15
$C_6\text{-}S_1\text{-}C_2$	102.18	105.90	103.08
$S_1\text{-}C_2\text{-}C_3\text{-}S_4$	64.71	51.60	60.06
$C_2\text{-}C_3\text{-}S_4\text{-}C_5$	-58.70	-52.90	-53.17
$C_3\text{-}S_4\text{-}C_5\text{-}C_6$	58.39	59.16	54.23
$S_4\text{-}C_5\text{-}C_6\text{-}S_1$	-64.74	-64.96	-64.53
$C_5\text{-}C_6\text{-}S_1\text{-}C_2$	58.20	54.04	60.09
$C_6\text{-}S_1\text{-}C_2\text{-}C_3$	-58.41	-46.71	-56.87
$C(\text{O})\text{-}C_2\text{-}C_3\text{-}C(\text{O})$	54.85	146.88	57.36
$\text{H}\text{-}C_2\text{-}C_3\text{-}\text{H}$	173.71	-82.78	53.84

^aThe relative energy with respect to the most stable conformation from HF/6-31G**//HF/6-31G* calculations; ^bThe relative energy with respect to the most stable conformation from MP2/6-31G**//HF/6-31G* calculations; ^cRelative energy with respect to the most stable conformation from B3LYP/6-311G//HF/6-31G* calculations; ^dX-ray data taken for 1,4-dithian

in the $\gamma\text{-C-C}$ bonds in there. As can be seen in Table-1, the calculated structural parameters for disubstituted 1,4-dithiane are in a good agreement with the X-ray data¹⁸.



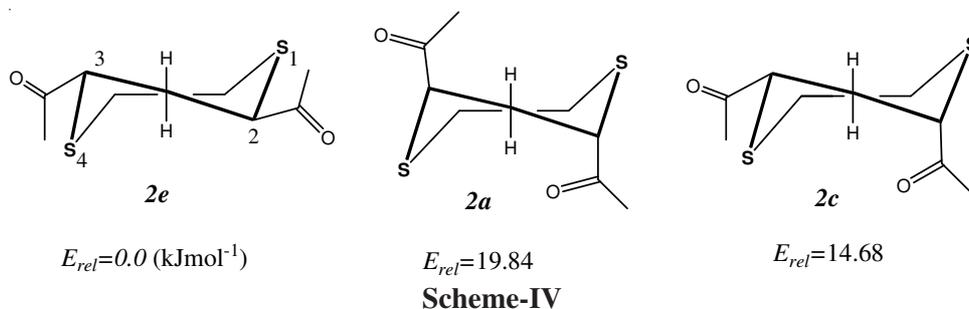
In the *cis*-isomer of this compound (**1c**) as preference conformer, since the acetyl substituents preferred the axial position. Therefore this effect was rationalized in terms of intramolecular electrostatic attraction (**Scheme-III**).



Since there is a repulsive interactions between lone pairs of the sulfur atoms and the oxygen of carbonyl group in *trans*-forms, so the structures **1a** and **1e** are about 11.36 kJ mol⁻¹ less stable than **1c** (Table-1).

2,3-Diacetyl-1,4-dithiepane (2): The conformational situation in cycloheptane was first unraveled by the classical study of Hendrickson¹⁹ which represents the first application of the computer to molecular mechanics calculation.

As we synthesized the 2,3-dibenzoyl-1,4-dithiepane²⁰, it is found that the *trans* isomer is more stable than the *cis* geometry based on the *ab initio* calculations that is corroborated by the NMR data. The energy minimum conformation of 1,4-dithiepane is twist-chair (TC) geometry and the preference of acetyl substituents are to occupy the equatorial positions on it (**Scheme-IV**).



As shown in Table-2, the *ab initio* calculations predict that the *trans* (di-equatorial) isomer **2e** is 14.68 kJ mol⁻¹ more stable than the *cis* geometry **2c**, while the same isomer is 19.84 kJ mol⁻¹ higher than the *trans* (di-axial) form (**2a**). The most significant structural difference observed among the compounds (Table-2) is the large variation in the ring torsion angle involving the S atoms ($\phi_{1234} = -41.96$) in **2a** relative to other forms.

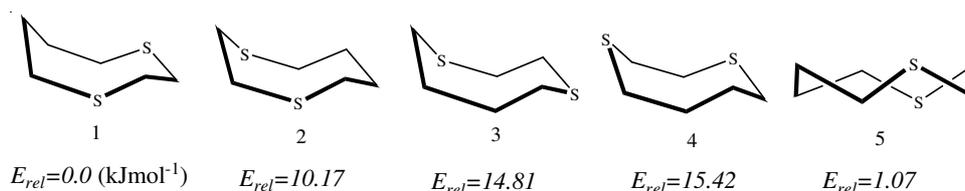
TABLE-2
CALCULATED HEATS OF FORMATION (kJ mol⁻¹), TOTAL AND ZERO-POINT VIBRATION (ZERO-POINT VIBRATION ENERGY IS SCALED BY A FACTOR OF 0.9135 TO ELIMINATE KNOWN SYSTEMATIC ERRORS IN CALCULATIONS) ENERGIES (HARTREE), RELATIVE ENERGY (INCLUDING ZERO-POINT ENERGY, kJ mol⁻¹) AND STRUCTURAL PARAMETERS FOR TC CONFORMATION OF *trans*- AND *cis*-2,3-DIACETYL-1,4-DITHIEPANE

Structure	2e (<i>trans-ee</i>)	2a (<i>trans-aa</i>)	2c (<i>cis</i>)
HF/6-31G**//HF/6-31G	-1293.71504042	-1293.70725761	-1293.70955017
MP2/6-31G**//HF/6-31G*	-1293.71504043	-1293.70725762	-1293.70955017
B3LYP/6-311G//HF/6-31G*	-1298.17610741	-1298.16968167	-1298.17174994
ZPE	0.235835	0.235589	0.235948
E _{rel} ^a	0.0	19.84	14.68
E _{rel} ^b	0.0	19.84	14.68
E _{rel} ^c	0.0	16.28	11.71
S ₁ -C ₂	1.85	1.84	1.84
C ₂ -C ₃	1.53	1.53	1.53
C ₃ -S ₄	1.85	1.84	1.85
S ₄ -C ₅	1.82	1.82	1.82
C ₅ -C ₆	1.52	1.52	1.52
C ₆ -C ₇	1.52	1.52	1.52
C ₇ -S ₁	1.82	1.82	1.82
S ₁ -C ₂ -C ₃	114.33	119.14	113.45
C ₂ -C ₃ -S ₄	114.20	120.95	117.49
C ₃ -S ₄ -C ₅	103.05	108.22	101.95
S ₄ -C ₅ -C ₆	115.63	116.39	116.57
C ₅ -C ₆ -C ₇	115.06	114.76	115.56
C ₆ -C ₇ -S ₁	115.56	115.06	116.33
C ₇ -S ₁ -C ₂	103.06	105.72	105.50
S ₁ -C ₂ -C ₃ -S ₄	-64.56	-41.96	-62.68
C ₂ -C ₃ -S ₄ -C ₅	74.71	57.24	75.46
C ₃ -S ₄ -C ₅ -C ₆	-93.37	-88.27	-91.53
S ₄ -C ₅ -C ₆ -C ₇	44.80	43.63	42.84
C ₅ -C ₆ -C ₇ -S ₁	46.03	48.58	47.31
C ₆ -C ₇ -S ₁ -C ₂	-93.57	-94.54	-91.85
C ₇ -S ₁ -C ₂ -C ₃	74.19	60.72	69.25
C(O)-C ₂ -C ₃ -C(O)	56.05	138.72	58.22
H-C ₂ -C ₃ -H	-177.14	94.14	54.95

^aThe relative energy with respect to the most stable conformation from HF/6-31G**//HF/6-31G* calculations; ^bThe relative energy with respect to the most stable conformation from MP2/6-31G**//HF/6-31G* calculations; ^cRelative energy with respect to the most stable conformation from B3LYP/6-311G//HF/6-31G* calculations.

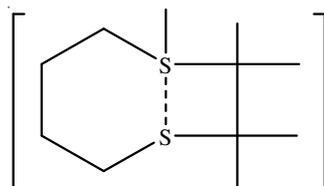
2,3-Diacetyl-1,4-dithiocan (3): Cyclooctane exhibits 10 symmetrical conformations which fall into four families that the first family (boat-chair and twist-boat-chair) of them represents the energy minimum²¹. But interconversion of this family into the one of the next-higher energy, the crown family, requires an activation energy calculated to be 47.7 kJ mol⁻¹. The conformational analysis of 5*H*, 8*H*-dibenzo[d,f][1,2]dithiocin²², the boat-chair (BC) conformer is more stable than twist-boat-chair (TBC) form of the same family. The main problem in the crown form, in addition to high symmetry and hence low entropy, is eclipsing strain, which is reduced in heterocyclooctanes.

So, we place the sulphur atoms in different position of the most stable conformers of 1,4-dithiocyclooctane and calculated the energy of them. We found there is four isomers of boat-chair conformation and one isomer of crown form are more stable than the others. The results of HF/6-31G* calculations have been shown in **Scheme-V**.



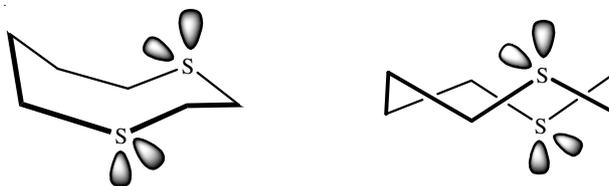
Scheme-V

On the other hand, according to the NMR data of 1-methyl-1-thion-4-thiacyclooctane²¹, there is an upfield shift of the S-methyl protons which would result from a transannular interaction (**Scheme-VI**).



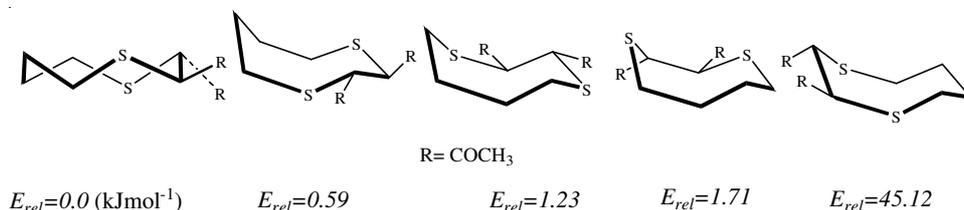
Scheme-VI

When we compare the structures **1** to **5** from energetic point of view, it seems that two structures of them (**1** and **5**) are more stable than the others. The sulfur lone pair of both of them are in *trans* position to each other as shown in **Scheme-VII**, so the repulsive interaction between them should in fact be at least. But S-C-C-S segment generally adopt anti conformation in crown isomer which is consistent with the decrease of repulsive gauche interaction²⁴. According to the *ab initio* calculations, the distance of two sulfur atoms in the crown form ($d = 3.81$ Å) is less than the boat-chair form ($d = 3.69$ Å) that confirm the same transannular effect in them.



Scheme-VII

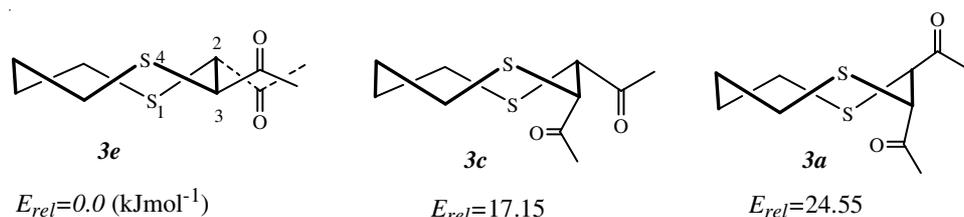
When we examined the same calculations on di-equatorial-2,3-diacetyl substituents of them, as the most stable form, surprisingly we found the crown form is more stable than the other structures as shown in **Scheme-VIII**.



Scheme-VIII

The existence of two electron deficient substituents on mesocyclic thioether changes the most stable conformation of them. But we choose the crown form and the first structure of boat-chair family as the starting points for our calculations because of the closeness of their energy.

As are shown in **Scheme-IX**, the *trans* (di-equatorial) isomer (**3e**) is the most stable form. The *cis*-isomer of 2,3-diacetyl-1,4-dithiocane **3c** is 7.4 kJ mol⁻¹ more stable than the *trans* (di-axial) conformer **3a**. The significant difference observed in Table-3 is the variation in the structural parameters of the *cis* isomer.



Scheme-IX

According to the results given in **Scheme-X**, the *trans* (di-equatorial) isomer (**4e**) is the most stable form. The *cis* isomer of 2,3-diacetyl-1,4-dithiocane **4c** is 9.06 kJ mol⁻¹ less stable than the *trans* (di-axial) conformer **4a**.

In looking more closely at the different conformations of disubstituted structures **3** and **4**, one finds that all of the isomer of the crown geometry is more stable than the boat-chair conformer. The results of this comparison are given in Table-4.

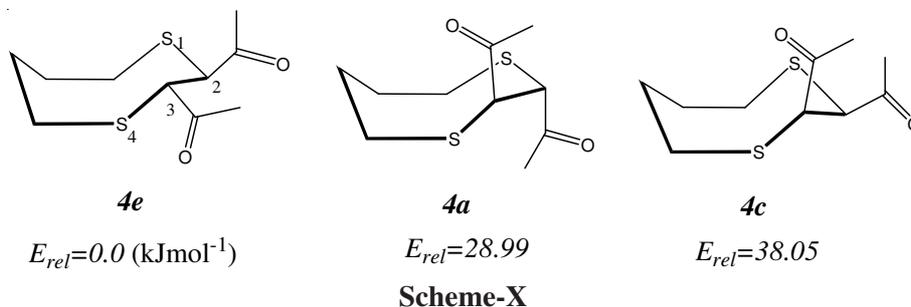
TABLE-3
CALCULATED HEATS OF FORMATION (kJ mol⁻¹), TOTAL AND ZERO-POINT VIBRATION (ZERO-POINT VIBRATION ENERGY IS SCALED BY A FACTOR OF 0.9135 TO ELIMINATE KNOWN SYSTEMATIC ERRORS IN CALCULATIONS) ENERGIES (HARTREE), RELATIVE ENERGY (INCLUDING ZERO-POINT ENERGY, kJ mol⁻¹) AND STRUCTURAL PARAMETERS CROWN CONFORMATION OF *trans*- AND *cis*-2,3-DIACETYL-1,4-DITHIOCAN

Structure	3e (<i>trans</i> -ee)	3a (<i>trans</i> -aa)	3c (<i>cis</i>)
HF/6-31G*//HF/6-31G	-1332.74219997	-1332.73264536	-1332.73573366
MP2/6-31G*//HF/6-31G*	-1334.6373510	-1334.63001731	-1334.63271770
B3LYP/6-311G//HF/6-31G*	-1337.6943208	-1337.68788750	-1337.69008511
ZPE	0.266410	0.266186	0.266483
E _{rel} ^a	0.0	24.55	17.15
E _{rel} ^b	0.0	19.26	12.17
E _{rel} ^c	0.0	16.89	11.12
S ₁ -C ₂	1.83	1.83	1.83
C ₂ -C ₃	1.53	1.54	1.53
C ₃ -S ₄	1.83	1.83	1.83
S ₄ -C ₅	1.83	1.83	1.83
C ₅ -C ₆	1.53	1.53	1.53
C ₆ -C ₇	1.53	1.53	1.53
C ₇ -C ₈	1.53	1.53	1.53
C ₈ -S ₁	1.83	1.83	1.83
S ₁ -C ₂ -C ₃	113.69	117.81	115.00
C ₂ -C ₃ -S ₄	113.69	117.80	117.86
C ₃ -S ₄ -C ₅	104.97	106.60	103.5
S ₄ -C ₅ -C ₆	113.53	111.94	112.73
C ₅ -C ₆ -C ₇	117.76	117.37	117.44
C ₆ -C ₇ -C ₈	117.75	117.37	117.72
C ₇ -C ₈ -S ₁	113.53	111.95	113.60
C ₈ -S ₁ -C ₂	104.97	106.60	107.38
S ₁ -C ₂ -C ₃ -S ₄	-71.82	51.88	-63.74
C ₂ -C ₃ -S ₄ -C ₅	87.11	-75.98	88.22
C ₃ -S ₄ -C ₅ -C ₆	-115.72	120.69	-117.33
S ₄ -C ₅ -C ₆ -C ₇	86.38	-84.48	82.99
C ₅ -C ₆ -C ₇ -C ₈	-57.46	50.54	-55.94
C ₆ -C ₇ -C ₈ -S ₁	86.38	-84.48	90.25
C ₇ -C ₈ -S ₁ -C ₂	-115.72	120.69	-115.54
C ₈ -S ₁ -C ₂ -C ₃	87.11	-75.96	75.30
C(O)-C ₂ -C ₃ -C(O)	53.03	149.27	-60.44
H-C ₂ -C ₃ -H	-174.80	-62.71	-66.89

^aThe relative energy with respect to the most stable conformation from HF/6-31G*//HF/6-31G* calculations; ^b The relative energy with respect to the most stable conformation from MP2/6-31G*//HF/6-31G* calculations; ^cRelative energy with respect to the most stable conformation from B3LYP/6-311G//HF/6-31G* calculations.

TABLE-4
AN ENERGITICAL COMPARISON OF DIFFERENT CONFORMATIONS OF STRUCTURE **3** AND **4**

Structure	Crown (3)	Boat-chair (4)
E _{rel} (kJ mol ⁻¹) for <i>trans</i> (di-equatorial)	0.0	0.59
E _{rel} (kJ mol ⁻¹) for <i>trans</i> (di-axial)	0.0	5.03
E _{rel} (kJ mol ⁻¹) for <i>cis</i>	0.0	21.48



Conclusion

We have examined diacetyl-substituted six-, seven- and eight-membered sulfur containing heterocycles using *ab initio* calculations from both structural and energetic aspects. For 2,3-diacetyl-1,4-dithiane (**1**) a *cis* preference of the acetyl groups has been predicted, while 2,3-diacetyl-1,4-dithiepane (**2**) or 2,3-diacetyl-1,4-dithiocane (**3**) show an *trans* (di-equatorial) preference of the $-\text{COCH}_3$ to be more stable than the other forms. On the other hand, if we plot the calculated energies of the most stable conformers of 1, 2 and 3 *versus* the number of atoms in mesocyclic thioethers, there will be a good linear correlation between them (Fig. 1). It may be concluded from present results, the energy of 1,4-dithiocloethers will be significantly decreased as the ring size increase. So we might expect analogous behaviour from the bigger-sized of them.

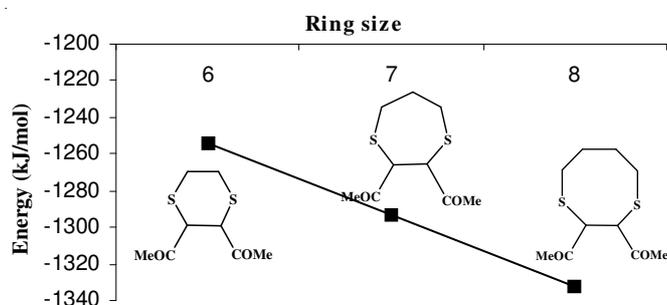


Fig. 1. Variation of energy with the change of the number of atoms

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