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LETTERS TO THE EDITOR

Conformational Transformations of 1,3-Diselenane

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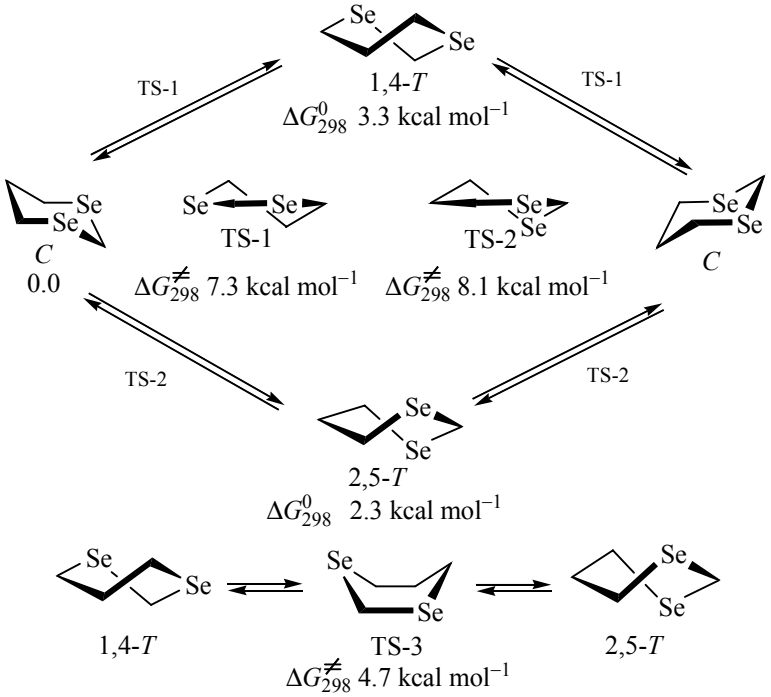
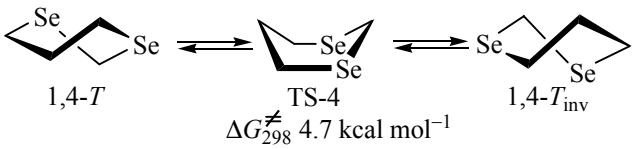
1,3-Diselenanes are of interest due to their structural features and the use as reactants in fine organic synthesis [1–4]. The X-ray analysis data shows the predominant *chair* conformation, which is characteristic of their molecules [5]. In [6, 7] the anomeric effect in 1,3-diselenanes containing phosphoryl and thioaryl substituents in the second position of the ring was mentioned. However, the conformational conversion of the compounds of this class so far remained unexplored. In this work we carried out a conformational analysis of the molecules of the unsubstituted 1,3-diselenane using the DFT-PBE/3z method (PRIRODA package [8]).

The potential energy surface of the test compound was found to contain several minima corresponding to the conformers *chair* (*C*) and also to the flexible 1,4- and 2,5-*twist* forms (1,4-*T*, 2,5-*T*). The main minimum corresponds to *chair* form, and the intermediate minima correspond to conformers 1,4-*T* and 2,5-*T*. Within the used approximation the form 2,5-*T* is the nearest minimum to the *chair* conformer on the potential energy surface, and the transition states of these reactions (TS-1 and TS-2) correspond to *semi-chair* forms. Besides, the conformers 1,4-*T* and 2,5-*T* are converted into each other via the unsymmetrical *boat* (TS-3).



There may also have two conformational transition associated with the interconversion of two enantiomeric forms of flexible 1,4-*T* and 2,5-*T* forms, respectively, via a symmetrical *boat* (TS-4) degenerate in energy with the form TS-3.



1,4-*T* TS-4 1,4-T_{inv}

$\Delta G^{\neq}_{298}$ 4.7 kcal mol^{-1}

2,5-*T* 2,5-T_{inv}

These results show that the *chair* conformation is dominant in the conformational equilibrium of unsubstituted 1,3-diselenane. At the same time its molecules are more conformationally flexible as compared with 1,3-dithiane [9].

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