CONFORMATONAL AND VIBRATIONAL ANALYSIS OF 12-THIACROWN-4 AND 18-THIACROWN-6

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We used the combined conformational and vibrational analysis to predict the structure of free 12-thiacrown-4 (12t4) and 18-thiacrown-6 (18t6). Conformational analysis was performed using the efficient CONFLEX conformational search method of cyclic molecules. The ab initio computations were done at levels as high as the MP2/6-311G** level. Conformational analysis of free 12t4 predicted that 12t4 exists in the D_4 conformation, Fig. 1.[1] Conformational analysis of free 18t6 predicted a new C_2 conformation to be the ground state conformation, Fig. 1. At the MP2/6-311G** level this new C_2 conformation is more stable by 4.67 kcal/mol than the experimentally known C_2 conformation of 18t6. The factors affecting the structure of 12t4 and 18t6 are discussed.

The vibrational spectra, IR and Raman, of 12t4 and 18t6 were measured. The vibrational spectra were calculated at the HF, B3LYP, CAM-B3LYP and MP2 levels using the 6-311G** basis set. Comparison between the calculated and experimental results is made.

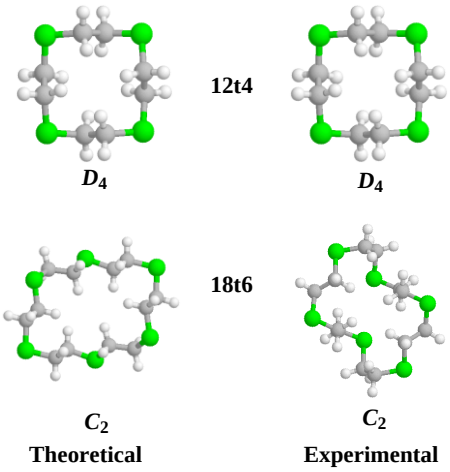

Figure 1. Structure of 12t4 and 18t6.

Keywords: Conformational analysis, vibrational analysis, thiacrown ethers.

References

[1] Al-Badri, N. I.; Al-Jallal, N. A.; El-Azhary, A. A. Theor. Chem. Acc., 130, **2011**, 919.