First Principle Study of the Anti– and Syn–Conformers of Thiophene–2–Carbonyl Fluoride and Selenophene–2–Carbonyl Fluoride in the Gas and Solution Phases

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Abstract. The anti- and syn-conformers of thiophene-2-carbonyl fluoride (**A**) and selenophene-2-carbonyl fluoride (**B**) have been studied in the gas phase. The transition states have also been obtained for the interconversion of the anti- and syn-conformers. The methods used are MP2 and DFT/B3LYP and the basis sets used for all atoms are 6-311++G(d,p). The optimized geometries, dipole moments, moment of inertia, energies, energy differences and rotational barriers are reported. This study has been extended to include solvent effect. Some of the vibrational frequencies of the conformers are reported with appropriate assignments. The results indicate that in the gas phase the syn conformer is more stable and the CCSD(T)//MP2 energy differences are 2.97 kJ/mol (**A**) and 3.02 kJ/mol (**B**) and barriers of rotation are 38.50 kJ/mol (**A**) and 36.89 kJ/mol (**B**). The structures and vibrational frequencies of (**A**) and (**B**) are not much affected by the solvents but the more polar conformer gets more stabilized. The major effect of the solvents is that energy difference decreases but rotational barrier increases. The peculiar characteristic of fluorine affecting conformational preference is not observed.

Keywords: Thiophene-2-carbonyl fluoride, Selenophene-2-carbonyl fluoride, MP2, DFT/B3LYP, energy difference, rotational barrier, solvent effect.

1 Introduction

2-Substituted carbonyl compounds and their analogues are known to show conformation isomerism [1] and thus exist as syn- and anti-conformers. In general, the anti conformer is more stable but the nature of substituents, in particular fluorine [2], and polarity of the medium [3], can affect the preference for a given conformer. In a previous communication [4], we reported a conformational study of the furfural, thiofurfural and selenofurfural in the gaseous and solution phases in order to understand the effect of substituting the oxygen of the carbonyl group with sulfur and selenium leaving the aromatic ring unchanged. In literature, there have been some attempts to look into the effect of changing the oxygen of the ring with sulfur and selenium. A brief survey of literature has been helpful to set the objectives of this work.

Braathen *et al.* [5] investigated the thiophene-2-aldehyde by microwave, infrared and Raman spectroscopy and by electron diffraction in the gaseous phase. They found that the syn-conformer is more stable than the anti-conformer. Han *et al.* [1] studied the rotational equilibria of 2-substituted furan and thiophene carbonyl derivatives using theoretical methods both in the gaseous and solution phases. They also found that the syn-conformer is always more stable and in the gaseous phase, MP2/6-31+G(d,p) level predicts that the syn form is more stable by 1.44 kcal/mol for thiophene-2-aldehyde and 0.14 kcal/mol for thiophene-2-carbonyl fluoride. Concistrè *et al.* [6] studied the structure and conformations of 2-thiophenecarboaldehyde from partially average dipolar couplings derived from proton NMR spectra. They found that the syn form of thiophene-2-aldehyde is more stable. Fleming *et al.* [7] studied the syn- and anti-conformers of thiophene-2-aldehyde using density functional method and normal coordinate analysis. They found that the results obtained theoretically are in agreement with experimental statements of the literature. Apart from these, there are increasing possibilities for the synthesis of selenophene-2-carbonyl [8] and derivatives of title compounds have wide applications in the industry [9,10].

Therefore although thiophene-2-carbonyl fluoride (**A**) has received attention, to the best of our knowledge, in literature, there is no conformational study for selenophene-2-carbonyl fluoride (**B**). We hereby report an extensive conformational study of (**A**) using higher level methods and extend our study to the selenium analogue. In this paper, the molecular structures, energy differences (ΔE) between the syn- and anti-conformers, rotational barriers, rotational thermodynamics, and vibrational spectra have been obtained for conformers of the title compounds, Fig 1, using theoretical methods. The findings of this work are hereby reported.
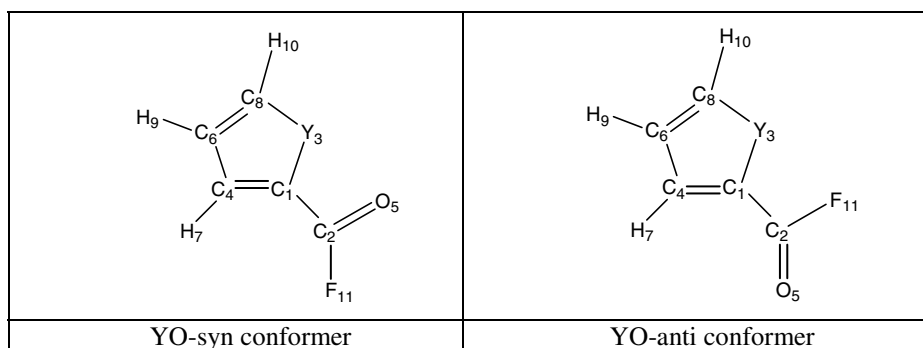

| YO-syn conformer | YO-anti conformer |

Fig. 1. Structures and atom labels of thiophene-2-carbonyl fluoride (Y=S) and selenophene-2-carbonyl fluoride (Y=Se) in C_s symmetry

2   Methods

All computations have been done using Gaussian 03W program suite [11] and Gauss View [12] has been used for visualizing the conformers.

DFT/B3LYP and MP2 methods have been used for molecular geometry optimization of the syn- and anti-conformers of (**A**) and (**B**). The basis sets used for all atoms are 6-311++G(d,p). The syn- and anti-conformers have been studied in C_s symmetry. The transition state arising from syn and anti isomerization has also been modeled. The transition state involves the planes containing $C_2O_5F_{11}$ and the ring containing hetero atom being at right angle and thus has been considered in the C_1 symmetry. Frequency computations have been carried out using the optimized structures to confirm the nature of the stationary points. Single point computations have also been carried out at the CCSD(T) level using the MP2/6-311++G(d,p) optimized structures.

Solvent effects have also been investigated by varying the dielectric constant from 1.92 (heptane) to 78.39 (water). All solution phase computations have been carried out using the integral equation formalism in the Polarizable Continuum model (IEF-PCM) [13-16] and all conformers have been fully optimized.

3 Results and Discussion

Some of the structural optimised parameters of the syn-, transition state and anti-conformers of the title compounds in the gas phase are reported in Table 1. Several conclusions can be drawn from Table 1. Firstly, there is little difference between the values of the different parameters obtained at B3LYP and MP2 level. Secondly, there is a good comparison between some of the computed parameters and those reported at HF/6-31+G(d,p) [1]. However, we believe that our structural parameters are more reliable due to the higher level of the methods used. Thirdly, the moment of inertias calculated for the conformers follow the order $I_A > I_B \approx I_C$. Fourthly, the syn conformer is more polar than the anti conformer due to opposing dipoles in the latter. Apart from these, comparing these conformers with parent molecules [4,17], it is found that hydrogen for fluorine substitution does not lead to much changes in the different optimized structural parameters except those where sulfur and selenium are involved. Further, it is interesting to note that the C1-C2 bond length is comparable in the syn- and trans-conformers but the same bond, about which rotation occurs for syn-anti isomerization, is longer in the transition state. However the other optimized structural parameters are almost comparable in the conformers for a given carbonyl fluoride.

Table 2 summarizes energies of the anti-, transition state and syn-conformers of the title compounds in the gas phase. Further, the energy differences between the anti- and syn-conformers (ΔE), the barriers of rotation between anti conformer and transition state (B1) and some thermodynamic functions (ΔH and ΔG) are also reported. The results from Table 2 indicate that (i) the syn conformers are more stable; (ii) the rotational barriers are larger than the energy differences; (iii) the energy differences and barriers of rotation are comparable for the three methods used; (iv) the effect of substituting hydrogen of the –CHO group by fluorine does not affect conformational preference but the rotational barriers and energy differences decrease; (v) the negative free energy changes indicates that the equilibrium favors the syn conformer and this is further reflected by the equilibrium being more populated with the syn conformer. The stability of the syn conformer of (**A**) is in agreement with the work of Han *et al.* [1] and they reported the energy difference as –0.59 kJ/mol computed at the MP2/6-31+G(d,p) level.

Table 1. Some optimized parameters of the syn-, transition state and anti-conformers of thiophene-2-carbonyl fluoride and selenophene-2-carbonyl fluoride computed in the gas phase

	OY-syn conformer		OY-transition state		OY-anti conformer	
	Y=S	Y=Se	Y=S	Y=Se	Y=S	Y=Se
B3LYP/6-311++G(d,p)						
Bond length (Å)						
$r(C_1-C_2)$	1.453 (1.462)	1.451	1.482 (1.464)	1.479	1.454	1.453
$r(C_1-Y_3)$	1.744 (1.730)	1.886	1.739 (1.731)	1.886	1.744	1.887
$r(C_1-C_4)$	1.378 (1.356)	1.374	1.368 (1.356)	1.364	1.378	1.374
$r(C_2-O_5)$	1.188 (1.172)	1.190	1.182 (1.171)	1.183	1.188	1.188
$r(C_2-F_{11})$	1.372 (1.326)	1.373	1.367 (1.327)	1.368	1.374	1.377
Angle (°)						
$\angle(C_2C_1Y_3)$	119.8 (111.7)	119.9	121.3 (127.3)	121.7	123.4	123.7
$\angle(C_2C_1C_4)$	128.7	128.5	127.0	126.7	125.3	124.9
$\angle(Y_3C_1C_4)$	111.5	111.6	111.7	111.6	111.4	111.4
$\angle(C_1C_2O_5)$	128.9 (127.6)	128.8	128.7 (127.3)	128.8	128.4	128.8
$\angle(C_1C_2F_{11})$	111.0 (111.7)	111.3	111.3 (112.0)	111.4	111.4	111.3
$\angle(O_5C_2F_{11})$	120.2	120.0	120.0	119.9	120.2	119.9
$\angle(C_1Y_3C_8)$	90.8 (90.7)	86.4	91.1 (90.7)	86.6	90.9	86.5
Rotational constant (GHz)						
A	3.664	2.646	3.687	2.595	3.688	2.627
B	1.394	1.177	1.240	1.086	1.412	1.225
C	1.010	0.815	1.102	0.880	1.021	0.836
Dipole moment (Debye)						
	4.594	4.535	3.600	3.648	4.487	4.491
MP2/6-311++G(d,p)						
Bond length (Å)						
$r(C_1-C_2)$	1.456	1.461	1.481	1.480	1.462	1.463
$r(C_1-Y_3)$	1.722	1.861	1.715	1.862	1.718	1.862
$r(C_1-C_4)$	1.385	1.388	1.385	1.382	1.391	1.388
$r(C_2-O_5)$	1.204	1.195	1.191	1.191	1.192	1.193
$r(C_2-F_{11})$	1.368	1.363	1.361	1.362	1.367	1.369
Angle (°)						
$\angle(C_2C_1Y_3)$	119.9	119.8	121.7	122.2	123.5	123.8
$\angle(C_2C_1C_4)$	128.1	128.2	126.3	126.0	124.7	124.4
$\angle(Y_3C_1C_4)$	112.1	112.0	112.1	111.8	111.9	111.8
$\angle(C_1C_2O_5)$	128.1	128.1	128.3	128.3	128.0	128.1
$\angle(C_1C_2F_{11})$	110.8	111.1	111.0	111.1	111.2	111.2
$\angle(O_5C_2F_{11})$	121.1	120.8	120.7	120.6	120.9	120.7
$\angle(C_1Y_3C_8)$	91.3	87.1	91.71	87.3	91.6	87.2
Rotational constant (GHz)						
A	3.654	2.651	3.686	2.603	3.695	2.638
B	1.405	1.187	1.248	1.092	1.418	1.230
C	1.015	0.820	1.110	0.886	1.025	0.839
Dipole moment (Debye)						
	3.955	3.963	4.052	3.353	3.937	3.939

(Parameters in bracket are those computed at the HF/6-31+G(d,p) level, [1])

Some of the calculated infrared raw vibrational frequencies, their intensities, Raman activities and assignments of the syn- and anti-conformers of the title compounds are reported in Table 3. The 27 modes of vibrations account for the irreducible

Table 2. Energies of the anti-, transition state and syn-conformers and thermodynamic parameters of thiophene-2-carbonyl fluoride and selenophene-2-carbonyl fluoride

Y	Anti / Hartrees	Syn / Hartrees	Transition state/ Hartrees	B1/ kJ/mol	ΔE/ kJ/mol	ΔH/ kJ/mol	ΔG/ kJ/mol
			DFT/6-311++G(d,p)				
S	-765.725585 (0.068659)	-765.725920 (0.068724)	-765.710483 (0.068117)	39.65	-0.88	-0.54	-0.40 (54.1)*
Se	-2769.053128 (0.067411)	-2769.053365 (0.067453)	-2769.038421 (0.066897)	38.61	-0.62	-0.54	-0.45 (54.6)
			MP2/6-311++G(d,p)				
S	-763.010428 (0.068082)	-764.233464 (0.067901)	-762.995765 (0.068138)	38.50	-0.77	-3.30	2.04 (21.5)
Se	-2766.477456 (0.066993)	-2766.477869 (0.066985)	-2766.465136 (0.066863)	32.34	-1.08	-1.04	-1.29 (72.7)
			CCSD(T) /6-311++G(d,p)// MP2/6-311++G(d,p)				
S	-763.010428	-763.011126	-762.995765	38.50	-1.83		
Se	-2765.263723	-2765.264482	-2765.249672	36.89	-1.99		

* Percentage of the syn conformer at 298.15 K

representations $\Gamma_v = 8A'' + 19A'$ of the C_s point group of the conformers. The infrared vibrational frequency and Raman activity are dominated by the high intensity of the carbonyl stretching frequency. The transition states have been confirmed by the one and only one negative frequency. The imaginary frequencies (cm^{-1}) for (**A**) and (**B**) computed at MP2 level are -88.83 and -81.02 and at B3LYP level are -90.49 and -84.58.

Table 3. Some infrared frequencies, their intensities, Raman activities and assignments for the syn and anti conformers of the title compounds computed at B3LYP/6-311++G(d,p) [*Values in bracket are those from MP2 computations]

Frequencies/ cm^{-1}	IR Intensity/ km mol^{-1}	Raman Activity/ Å^4 amu^{-1}	Symmetry	Assignment
		Syn thiophene-2-carbonyl fluoride		
84.5 (80.6)*	0.1 (0.1)	0.3	A"	Twisting $O_5C_2F_{11}$
1860.1 (1883.2)	526.3 (293.2)	155.0	A'	Stretching C_2O_5
755.8 (784.0)	4.1 (1.5)	4.9	A'	Scissoring $C_1C_4C_6$
725.1 (742.2)	2.5 (6.4)	24.5	A'	Scissoring $F_{11}C_2O_5$
645.1 (653.4)	9.5 (10.4)	3.9	A'	Scissoring $C_1S_3C_8$
463.5 (468.6)	0.1 (0.3)	3.3	A'	Scissoring $C_2C_1C_4$
365.1 (374.2)	2.9 (2.6)	3.7	A'	Bending $O_5C_2F_{11}$
178.0 (181.0)	1.6 (1.4)	0.2	A'	Bending C_1C_2
		Syn selenophene-2-carbonyl fluoride		
405.2 (371.9)	1.8 (2.6)	0.6	A"	Wagging $C_1Se_3C_8$
78.4 (59.0)	0.1 (0.1)	0.1	A"	Twisting $O_5C_2F_{11}$
1852.3 (1853.8)	508.5 (353.2)	152.7	A'	Stretching C_2O_5
942.5 (967.4)	210.5 (201.5)	4.0	A'	Stretching C_2F_{11}
699.9 (710.4)	8.3 (15.3)	20.5	A'	Scissoring $O_5C_2F_{11}$
565.2 (568.6)	3.7 (2.4)	12.2	A'	Bending $C_1C_2O_5$
389.7 (391.8)	0.2 (0.2)	3.4	A'	Bending $C_1Se_3C_8$
327.6 (334.0)	1.9 (1.8)	3.8	A'	Bending $C_2C_1C_4$
152.4 (156.1)	2.2 (1.7)	0.3	A'	Bending C_1C_2

Table 3. *(Continued)*

Trans thiophene-2-carbonyl fluoride				
454.5 (403.2)	0.8 (0.3)	0.5	A"	Wagging $C_1S_3C_8$
80.3 (58.2)	0.5 (0.2)	0.8	A"	Twisting $O_5C_2F_{11}$
1862.5 (1869.4)	533.0 (400.0)	165.7	A'	Stretching C_2O_5
991.4 (1014.0)	170.7 (165.3)	1.7	A'	Stretching C_2F_{11}
708.0 (724.0)	21.3 (20.8)	19.4	A'	Scissoring $O_5C_2F_{11}$
448.7 (458.1)	0.2 (0.1)	3.1	A'	Bending $C_2C_1S_3$
383.8 (385.9)	4.2 (3.7)	4.5	A'	Bending $O_5C_2F_{11}$
171.5 (175.8)	0.9 (0.8)	0.2	A'	Bending C_1C_2
Trans selenophene-2-carbonyl fluoride				
734.7 (713.4)	55.3 (92.6)	0.1	A"	Bending C_1C_2
407.4 (379.8)	2.1 (3.0)	1.0	A"	Wagging $C_1S_3C_8$
73.9 (60.2)	0.5 (0.3)	0.7	A"	Twisting $O_5C_2F_{11}$
1858.4 (1864.3)	538.1 (403.5)	175.9	A'	Stretching C_2O_5
971.4 (991.2)	161.5 (146.1)	2.6	A'	Stretching C_2F_{11}
691.2 (702.4)	30.8 (34.5)	15.5	A'	Scissoring $O_5C_2F_{11}$
380.9 (389.2)	1.0 (0.8)	4.7	A'	Bending $C_1C_2F_{11}$
352.8 (352.9)	3.1 (2.8)	4.0	A'	Bending C_2O_5
148.5 (151.4)	0.9 (0.7)	0.3	A'	Bending C_1C_2

Table 4. Solvent effect on rotational barriers, energy differences and thermodynamic parameters

Solvent	Dielectric constant	B1/ kJ/mol	ΔE/ kJ/mol	ΔH/ kJ/mol	ΔG/ kJ/mol	% of trans conformer at 298.15 K
Sulfur analogue						
Heptane	1.92	40.38	-0.68	-0.56	-0.83	58.31
Chloroform	4.90	41.00	-0.77	-0.54	-0.34	53.46
Tetrahydofuran	7.58	41.18	-0.80	-0.55	0.10	48.97
Dichloroethane	10.36	41.26	-0.82	-0.58	-0.31	53.17
Acetone	20.70	41.33	-0.87	-0.71	-0.49	54.88
Ethanol	24.55	41.30	-0.88	-0.63	-0.12	51.16
Methanol	32.63	41.21	-0.91	-0.66	0.52	44.78
Dimethylsulfoxide	46.70	41.42	-0.89	-0.64	-0.09	50.95
Water	78.39	41.24	-0.90	-0.80	0.29	47.10
Selenium analogue						
Heptane	1.92	38.91	-0.59	-0.51	-0.45	54.52
Chloroform	4.90	39.11	-0.59	-0.51	-2.19	70.77
Tetrahydofuran	7.58	39.17	-0.60	-0.43	-2.01	69.26
Dichloroethane	10.36	39.13	-0.60	-0.56	-2.64	74.33
Acetone	20.70	39.13	-0.62	-0.16	0.10	48.97
Ethanol	24.55	39.09	-0.62	-0.36	0.005	49.95
Methanol	32.63	39.13	-0.62	-0.42	-1.00	59.97
Dimethylsulfoxide	46.70	39.14	-0.63	-0.54	-1.99	69.06
Water	78.39	38.79	-0.62	-0.45	0.75	42.48

It is found that there are systematic changes in the structures of the conformers of the (**A**) and (**B**) when they are studied in different solvents but these are not significant. To be more precise, the largest change in bond length is 0.012 Å and the largest change in bond angle is 1.0°. Similarly there are only small changes in the infrared vibrational frequencies. The most apparent effect of the solvents is that due to solute-solvent interaction, stabilization of the conformers depends on the dipole moments. The net effect of the solvent is that energy difference between the conformers decreases but rotational barrier increases. However an increase in the polarity of the solvent leads to a leveling effect of the different parameters. The solvent effect on rotational barriers, energy differences, enthalpies and free energy changes are summarized in Table 4.

4   Conclusion

This work reports a systematic investigation of the syn-, transition state and anti-conformers of thiophene-2-carbonyl fluoride (**A**) and selenophene-2-carbonyl fluoride (**B**) in the gas and solution phases. Some of the results for (**A**) compare satisfactorily with literature and the results for (**B**) should be helpful for reference, as it has not been studied previously. An interesting outcome of this work is that fluorine is strongly electronegative and thus can affect conformational equilibrium [18]. However in this case, replacing hydrogen of the carbonyl group by fluorine does result in a change in conformational preference relative to the parent compounds and this can be explained on the basis of the opposite charges on sulfur or selenium and oxygen in (**A**) and (**B**). Hence the syn conformer to be more preferred for both (**A**) and (**B**).

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