

SMARTCATS Final Report

Theoretical Studies on the Combustion Mechanism of Cyclic Species Containing Oxygen

1. Details of the STSM

Applicant Details

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Home Institute

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Host Institute

Laboratoire Réactions et Génie de Procédés (LRGP), CNRS, Université de Lorraine,
ENSIC, 1 rue Grandville, BP 20451, 54001 Nancy Cedex, France

Person in Charge: Prof. Frédérique Battin-Leclerc

2. Objective

The purpose of this STSM is to start some scientific collaboration between the University of Lisbon (Lisbon – Portugal) and Laboratoire Réactions et Génie de Procédés (Nancy – France) within the Chemistry Smart Energy Carriers and Technologies (SMARTCATS) COST action (CM1404) in order to create synergies between both partners of the action inside the European Research Area (ERA). Moreover, such collaboration will allow the applicant to start having some independent collaboration. The objectives of the proposed project are to determine the reaction mechanisms for the combustion of cyclic species containing oxygen (1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran) by using computational tools (TSSCDS, DFT and CBS methods) and by applying the kinetic models developed Battin-Leclerc's group.

3. Timeline and activities

The stay at Prof. Frédérique Battin-Leclerc's group at Laboratoire Réactions et Génie de Procédés (LRGP), CNRS, Université de Lorraine, ENSIC, started on the 1st February and Finished the 31st March. During these two months, conformational searches at Molecular Mechanics (MM) level with Avogadro software, Transition State Search using Chemical Dynamics Simulations (TSSCDS) with the TSSCDS software, calculations by using the Density Functional Theory (DFT) and Complete Basis Set (CBS) with Gaussian09

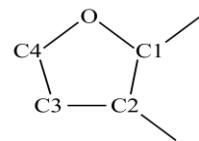
software, determination of enthalpies (H), entropies (S) and heat capacities at constant pressure (Cp) with thermo.pl and calculation of kinetic constants with ChemRate software were carried out in Prof. Frédérique Battin-Leclerc's group at Laboratoire Réactions et Génie de Procédés (LRGP), CNRS, Université de Lorraine, ENSIC. The main objective for all of these calculations is the determination of several pathways for the combustion of 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran and the determination of thermodynamic properties (H, S and Cp) at several temperatures and the determination of the kinetic constants. Many structures including reactants, products, intermediates and transition states were determined in order to build some map of the Potential Energy Surface (PES) for the combustion of 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran.

4. Methods and Computational Details

It is well-known that not many conformations can be found for cyclic structures as the case of tetrahydrofuran (THF). However, when substitution is produced the new group is able to give several conformations due to single-bond rotamers. This is the case of the hydroperoxyl group for which we have the rotamers associated to the C-O bond and those associated to O-O bond. Thus, in order to carry out some conformational search associated to such rotamers the following strategy was applied to obtain several rotamers. First, we performed a systematic conformational search by rotating 120° each single bonds associated to the hydroperoxyl group (C-O and O-O) taking into account the alternated conformations. That is 3 for the C-O single bond and 3 for the O-O single bond. Thus, we obtained a total of 9 rotamers which were subsequently optimized by means of DFT methods at B3LYP/6-31G(d,p) level. Radical structures were then obtained by subtraction of one H atom from several positions of the structure. Subsequently, the most stable structures were used to explore the PES for the combustion of 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran, trying to locate all the reactants, products, intermediates and transition states of the different pathways at CBS-QB3 level to obtain energies close to experimental data. Thermal corrections and thermodynamic properties were obtained from unscaled harmonic vibrational frequencies from the CBS-QB3 calculations. All calculations have been performed with Gaussian 09 package, whereas thermodynamic properties were obtained by using the thermo.pl script. The unrestricted formalism has been considered for the open shell systems. In all cases, spin contamination was found to be small since the S^2 expectation values were very close to 0.75.

5. Results

Table 1 and Table 2 show the results for the conformational search for 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran, (see Scheme 1 for the nomenclature of the carbons).



Scheme 1.

Table 1. Conformational Search (substitution position 1). Electronic energies and **Gibbs Free Energies** at B3LYP/6-31G(d,p) level in kcal mol⁻¹.

Hydroperoxyl						
Hydroperoxyl	0.0 0.0	1.2 1.1	2.7 2.0	3.4 2.9	3.5 3.0	4.2 3.6
-O [•]	0.0 0.0	0.4 0.1	0.5 0.6			
-C1 [•]	0.0 0.0	1.4 0.8	1.8 0.8			
-C2 [•]	0.0 0.0	1.8 1.6	2.2 1.8	2.7 2.5	4.7 4.1	4.9 4.3
-C3 [•]	0.0 0.0	1.8 1.4	2.5 2.0	3.4 3.1	3.9 3.5	4.5 4.0
-C4 [•]	0.0 0.0	0.2 0.0	1.0 1.1	1.1 1.1	2.5 2.0	2.8 2.2
	3.1 2.9	3.7 3.2	3.9 3.5	4.4 3.8	4.5 4.1	4.9 4.3

Table 2. Conformational Search (substitution position 2). Electronic energies and **Gibbs Free Energies** at B3LYP/6-31G(d,p) level in kcal mol⁻¹.

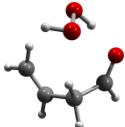
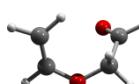
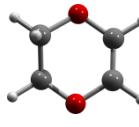
Hydroperoxyl						
	0.0 0.0	0.9 0.0	0.2 0.1	1.0 0.5	0.3 1.5	1.7 1.8
-O [•]						
	0.0 0.0	0.0 0.1	0.6 0.2	1.3 1.2	1.1 1.3	
-C1 [•]						
	0.0 0.0	1.8 0.1	0.5 0.3	2.1 0.7	1.5 0.9	2.8 2.2
-C2 [•]						
	0.0 0.0	0.0 0.0	-0.2 0.1			
-C3 [•]						
	0.0 0.0	0.6 0.5	0.9 0.7	1.1 1.0	1.3 1.1	1.0 1.2
-C4 [•]						
	0.0 0.0	0.3 0.1	0.3 0.2	0.6 0.3	0.5 0.4	0.6 0.5
	0.9 0.6	1.0 0.6	1.7 1.6	1.5 1.7	2.3 1.7	1.6 1.8

From the results of Table 1 and Table 2 it is observed that the different rotamers are located within an energy window of 5 kcal mol⁻¹ in the case of 1-hydroperoxyltetrahydrofuran, whereas for 2-hydroperoxyltetrahydrofuran such energy window is narrower (2 kcal mol⁻¹). We took into account the most stable structures to explore the PES for the combustion of both compounds: 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran.

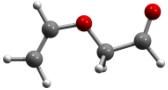
Table 3 shows the energies and the thermodynamic properties (H, S and Cp) at different temperatures for several structures located in the PES for the combustion of 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran.

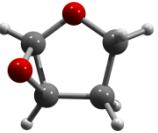
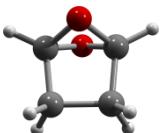
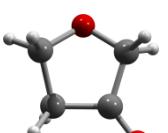
Table 3. Absolute Gibbs Free Energy (G) and thermodynamic properties (S, Cp and ΔH) at different temperatures (100 K, 200 K, 298.15, 300 K, 400 K, 500 K, 600 K, 700 K, 800 K, 900 K, and 1000 K) for the stationary points located in the PES.

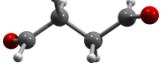
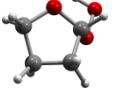
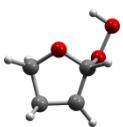
System	G (Hartrees)	S (J mol ⁻¹ K ⁻¹)	Cp (J mol ⁻¹ K ⁻¹)	ΔH (kJ mol ⁻¹)
	-305.908473	241.12 (100 K) 277.02 (200 K) 307.24 (298.15 K) 307.8 (300 K) 337.76 (400 K) 366.89 (500 K) 394.71 (600 K) 421.02 (700 K) 445.76 (800 K) 469.03 (900 K) 490.92 (1000 K)	43.78 (100 K) 63.64 (200 K) 90.19 (298.15 K) 90.72 (300 K) 118.52 (400 K) 142.69 (500 K) 162.49 (600 K) 178.62 (700 K) 191.93 (800 K) 203.05 (900 K) 212.45 (1000 K)	3.70 (100 K) 8.99 (200 K) 16.51 (298.15) 16.68 (300 K) 27.16 (400 K) 40.25 (500 K) 55.55 (600 K) 72.63 (700 K) 91.18 (800 K) 110.94 (900 K) 131.73 (1000 K)
	-305.973069	237.7 (100K) 270.19 (200 K) 297.38 (298.15 K) 297.89 (300 K) 325.76 (400 K) 353.57 (500 K) 380.56 (600 K) 406.30 (700 K) 430.65 (800 K) 453.64 (900 K) 475.30 (1000 K)	40.15 (100 K) 56.77 (200 K) 82.38 (298.15) 82.92 (300 K) 111.95 (400 K) 137.53 (500 K) 158.42 (600 K) 175.35 (700 K) 189.24 (800 K) 200.81 (900 K) 210.54 (1000 K)	3.52 (100 K) 8.30 (200 K) 15.07 (298.15) 15.22 (300 K) 24.97 (400 K) 37.49 (500 K) 52.32 (600 K) 69.04 (700 K) 87.29 (800 K) 106.81 (900 K) 127.39 (1000 K)
	-382.199291	261.51 (100 K) 312.56 (200 K) 353.90 (298.15 K) 354.64 (300 K) 393.64 (400 K) 430.63 (500 K) 465.58 (600 K) 498.47 (700 K) 529.37 (800 K) 558.42 (900 K) 585.77 (1000 K)	60.23 (100 K) 89.74 (200 K) 119.86 (298.15) 120.45 (300 K) 151.88 (400 K) 179.92 (500 K) 203.49 (600 K) 223.12 (700 K) 239.61 (800 K) 253.59 (900 K) 265.54 (1000 K)	4.37 (100 K) 11.90 (200 K) 22.16 (298.15 K) 22.39 (300 K) 36.02 (400 K) 52.64 (500 K) 71.85 (600 K) 93.21 (700 K) 116.37 (800 K) 141.05 (900 K) 167.02 (1000 K)

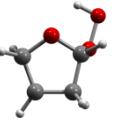
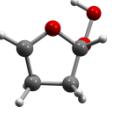
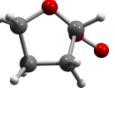
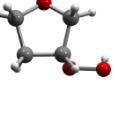
	-382.244971	296.49 (100 K) 366.21 (200 K) 416.81 (298.15 K) 417.69 (300 K) 462.12 (400 K) 502.41 (500 K) 539.42 (600 K) 573.61 (700 K) 605.34 (800 K) 634.92 (900 K) 662.59 (1000 K)	88.23 (100 K) 114.76 (200 K) 140.87 (298.15 K) 141.39 (300 K) 168.57 (400 K) 192.80 (500 K) 213.22 (600 K) 230.33 (700 K) 244.84 (800 K) 257.28 (900 K) 268.05 (1000 K)	6.14 (100 K) 16.35 (200 K) 28.87 (298.15) 29.13 (300 K) 44.64 (400 K) 62.74 (500 K) 83.07 (600 K) 105.28 (700 K) 129.05 (800 K) 154.17 (900 K) 180.45 (1000 K)
	-305.981878	252.92 (100 K) 297.90 (200 K) 332.73 (298.15 K) 333.35 (300 K) 365.67 (400 K) 395.95 (500 K) 424.32 (600 K) 450.87 (700 K) 475.71 (800 K) 498.99 (900 K) 520.87 (1000 K)	55.80 (100 K) 76.43 (200 K) 100.06 (298.15 K) 100.53 (300 K) 125.03 (400 K) 146.60 (500 K) 164.65 (600 K) 179.67 (700 K) 192.30 (800 K) 203.01 (900 K) 212.17 (1000 K)	4.26 (100 K) 10.86 (200 K) 19.50 (298.15 K) 19.69 (300 K) 30.98 (400 K) 44.59 (500 K) 60.18 (600 K) 77.42 (700 K) 96.04 (800 K) 115.82 (900 K) 136.59 (1000 K)
	-305.984610	238.63 (100 K) 272.09 (200 K) 300.57 (298.15 K) 301.10 (300 K) 329.70 (400 K) 357.80 (500 K) 384.85 (600 K) 410.54 (700 K) 434.80 (800 K) 457.68 (900 K) 479.25 (1000 K)	40.52 (100 K) 59.61 (200 K) 85.54 (298.15 K) 86.06 (300 K) 113.82 (400 K) 138.24 (500 K) 158.37 (600 K) 174.84 (700 K) 188.46 (800 K) 199.89 (900 K) 209.56 (1000 K)	3.53 (100 K) 8.46 (200 K) 15.55 (298.15 K) 15.71 (300 K) 25.72 (400 K) 38.35 (500 K) 53.22 (600 K) 69.91 (700 K) 88.09 (800 K) 107.52 (900 K) 128.01 (1000 K)
	-76.355126	152.43 (100 K) 175.48 (200 K) 188.79 (298.15 K) 189.00 (300 K) 198.70 (400 K) 206.39 (500 K) 212.86 (600 K) 218.49 (700 K) 223.52 (800 K) 228.10 (900 K) 232.31 (1000 K)	33.26 (100 K) 33.27 (200 K) 33.45 (298.15 K) 33.46 (300 K) 34.06 (400 K) 34.98 (500 K) 36.02 (600 K) 37.12 (700 K) 38.26 (800 K) 39.42 (900 K) 40.60 (1000 K)	3.33 (100 K) 6.65 (200 K) 9.92 (298.15) 9.98 (300 K) 13.36 (400 K) 16.81 (500 K) 20.36 (600 K) 24.01 (700 K) 27.78 (800 K) 31.67 (900 K) 35.67 (1000 K)

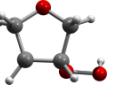
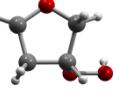
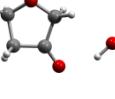
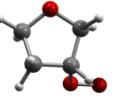
	-150.184523	173.23 (100 K) 193.40 (200 K) 205.05 (298.15 K) 205.23 (300 K) 213.73 (400 K) 220.49 (500 K) 226.19 (600 K) 231.14 (700 K) 235.54 (800 K) 239.50 (900 K) 243.10 (1000 K)	29.10 (100 K) 29.11 (200 K) 29.29 (298.15 K) 29.30 (300 K) 29.90 (400 K) 30.78 (500 K) 31.72 (600 K) 32.58 (700 K) 33.32 (800 K) 33.93 (900 K) 34.43 (1000 K)	2.91 (100 K) 5.82 (200 K) 8.68 (298.15 K) 8.74 (300 K) 11.69 (400 K) 14.73 (500 K) 17.85 (600 K) 21.07 (700 K) 24.36 (800 K) 27.73 (900 K) 31.15 (1000 K)
	-305.893149	257.8 (100 K) 304.49 (200 K) 340.72 (298.15 K) 341.37 (300 K) 374.62 (400 K) 405.58 (500 K) 434.50 (600 K) 461.50 (700 K) 486.71 (800 K) 510.32 (900 K) 532.47 (1000 K)	57.08 (100 K) 79.98 (200 K) 103.44 (298.15 K) 103.90 (300 K) 128.15 (400 K) 149.63 (500 K) 167.60 (600 K) 182.54 (700 K) 195.07 (800 K) 205.66 (900 K) 214.69 (1000 K)	4.44 (100 K) 11.31 (200 K) 20.29 (298.15 K) 20.48 (300 K) 32.10 (400 K) 46.02 (500 K) 61.90 (600 K) 79.43 (700 K) 98.33 (800 K) 118.38 (900 K) 139.41 (1000 K)
	-75.666646	146.48 (100 K) 166.66 (200 K) 178.27 (298.15 K) 178.45 (300 K) 186.83 (400 K) 193.32 (500 K) 198.64 (600 K) 203.15 (700 K) 207.08 (800 K) 210.58 (900 K) 213.75 (1000 K)	29.10 (100 K) 29.10 (200 K) 29.10 (298.15 K) 29.10 (300 K) 29.10 (400 K) 29.12 (500 K) 29.19 (600 K) 29.34 (700 K) 29.58 (800 K) 29.89 (900 K) 30.26 (1000 K)	2.91 (100 K) 5.82 (200 K) 8.68 (298.15 K) 8.73 (300 K) 11.64 (400 K) 14.55 (500 K) 17.47 (600 K) 20.39 (700 K) 23.34 (800 K) 26.31 (900 K) 29.32 (1000 K)
	-150.763270	192.28 (100 K) 215.36 (200 K) 228.88 (298.15 K) 229.10 (300 K) 239.36 (400 K) 247.84 (500 K) 255.17 (600 K) 261.67 (700 K) 267.52 (800 K) 272.85 (900 K) 277.75 (1000 K)	33.26 (100 K) 33.42 (200 K) 34.63 (298.15 K) 34.66 (300 K) 36.86 (400 K) 39.19 (500 K) 41.28 (600 K) 43.05 (700 K) 44.57 (800 K) 45.89 (900 K) 47.05 (1000 K)	3.33 (100 K) 6.66 (200 K) 9.98 (298.15 K) 10.05 (300 K) 13.62 (400 K) 17.42 (500 K) 21.45 (600 K) 25.67 (700 K) 30.05 (800 K) 34.58 (900 K) 39.22 (1000 K)

	-305.982024	254.53 (100 K) 300.04 (200 K) 334.92 (298.15 K) 335.54 (300 K) 367.78 (400 K) 397.97 (500 K) 426.27 (600 K) 452.76 (700 K) 477.56 (800 K) 500.83 (900 K) 522.69 (1000 K)	56.49 (100 K) 76.91 (200 K) 99.92 (298.15 K) 100.38 (300 K) 124.63 (400 K) 146.18 (500 K) 164.28 (600 K) 179.38 (700 K) 192.08 (800 K) 202.86 (900 K) 212.07 (1000 K)	4.32 (100 K) 11.00 (200 K) 19.65 (298.15 K) 19.84 (300 K) 31.10 (400 K) 44.67 (500 K) 60.22 (600 K) 77.42 (700 K) 96.02 (800 K) 115.78 (900 K) 136.54 (1000 K)
	-305.981881	252.94 (100 K) 297.94 (200 K) 332.76 (298.15 K) 333.38 (300 K) 365.71 (400 K) 395.99 (500 K) 424.36 (600 K) 450.91 (700 K) 475.75 (800 K) 499.03 (900 K) 520.91 (1000 K)	55.82 (100 K) 76.44 (200 K) 100.07 (298.15 K) 100.53 (300 K) 125.03 (400 K) 146.60 (500 K) 164.65 (600 K) 179.67 (700 K) 192.30 (800 K) 203.01 (900 K) 212.16 (1000 K)	4.26 (100 K) 10.87 (200 K) 19.51 (298.15 K) 19.69 (300 K) 30.98 (400 K) 44.60 (500 K) 60.19 (600 K) 77.42 (700 K) 96.04 (800 K) 115.82 (900 K) 136.59 (1000 K)
	-305.981455	260.20 (100 K) 306.90 (200 K) 342.43 /298.15 K) 343.06 (300 K) 375.72 (400 K) 406.19 (500 K) 434.68 (600 K) 461.30 (700 K) 486.19 (800 K) 509.51 (900 K) 531.42 (1000 K)	58.69 (100 K) 78.50 (200 K) 101.50 (298.15 K) 101.96 (300 K) 126.01 (400 K) 147.30 (500 K) 165.18 (600 K) 180.10 (700 K) 192.66 (800 K) 203.33 (900 K) 212.45 (1000 K)	4.56 (100 K) 11.41 (200 K) 20.22 (298.15 K) 20.41 (300 K) 31.82 (400 K) 45.51 (500 K) 61.16 (600 K) 78.45 (700 K) 97.10 (800 K) 116.92 (900 K) 137.72 (1000 K)
	-306.043775	241.95 (100 K) 277.03 (200 K) 305.78 (298.15 K) 306.31 (300 K) 334.87 (400 K) 362.84 (500 K) 389.75 (600 K) 415.32 (700 K) 439.49 (800 K) 462.30 (900 K) 483.83 (1000 K)	43.77 (100 K) 60.86 (200 K) 85.70 (298.15 K) 86.21 (300 K) 113.39 (400 K) 137.53 (500 K) 157.50 (600 K) 174.11 (700 K) 187.84 (800 K) 199.38 (900 K) 209.17 (1000 K)	3.70 (100 K) 8.85 (200 K) 16.00 (298.15 K) 16.16 (300 K) 26.15 (400 K) 38.73 (500 K) 53.52 (600 K) 70.13 (700 K) 88.25 (800 K) 107.63 (900 K) 128.07 (1000 K)

	-305.982822	237.12 (100 K) 268.65 (200 K) 295.61 (298.15 K) 296.12 (300 K) 324.04 (400 K) 351.96 (500 K) 379.03 (600 K) 404.82 (700 K) 429.19 (800 K) 452.17 (900 K) 473.84 (1000 K)	38.97 (100 K) 55.68 (200 K) 82.32 (298.15 K) 82.87 (300 K) 112.35 (400 K) 138.01 (500 K) 158.82 (600 K) 175.60 (700 K) 189.34 (800 K) 200.78 (900 K) 210.42 (1000 K)	3.48 (100 K) 8.12 (200 K) 14.84 (298.15 K) 14.99 (300 K) 24.77 (400 K) 37.33 (500 K) 52.21 (600 K) 68.96 (700 K) 87.23 (800 K) 106.75 (900 K) 127.32 (1000 K)
	-306.005931	261.98 (100 K) 308.08 (200 K) 342.93 (298.15 K) 343.55 (300 K) 375.49 (400 K) 405.37 (500 K) 433.43 (600 K) 459.72 (700 K) 484.37 (800 K) 507.51 (900 K) 529.27 (1000 K)	57.89 (100 K) 77.39 (200 K) 99.24 (298.15 K) 99.68 (300 K) 123.36 (400 K) 144.78 (500 K) 162.94 (600 K) 178.15 (700 K) 190.97 (800 K) 201.85 (900 K) 211.16 (1000 K)	4.62 (100 K) 11.38 (200 K) 20.02 (298.15 K) 20.20 (300 K) 31.36 (400 K) 44.80 (500 K) 60.21 (600 K) 77.29 (700 K) 95.76 (800 K) 115.42 (900 K) 136.08 (1000 K)
	-305.971410	234.84 (100 K) 263.51 (200 K) 288.90 (298.15 K) 289.40 (300 K) 316.68 (400 K) 344.40 (500 K) 371.43 (600 K) 397.24 (700 K) 421.65 (800 K) 444.67 (900 K) 466.37 (1000 K)	35.83 (100 K) 51.18 (200 K) 79.26 (298.15 K) 79.85 (300 K) 110.93 (400 K) 137.55 (500 K) 158.84 (600 K) 175.83 (700 K) 189.65 (800 K) 201.10 (900 K) 210.72 (1000 K)	3.38 (100 K) 7.60 (200 K) 13.93 (298.15 K) 14.08 (300 K) 23.64 (400 K) 36.11 (500 K) 50.97 (600 K) 67.74 (700 K) 86.03 (800 K) 105.59 (900 K) 126.19 (1000 K)
	-306.013198	243.50 (100 K) 279.62 (200 K) 309.35 (298.15 K) 309.90 (300 K) 339.16 (400 K) 367.62 (500 K) 394.87 (600 K) 420.71 (700 K) 445.08 (800 K) 468.05 (900 K) 489.71 (1000 K)	44.59 (100 K) 63.11 (200 K) 88.23 (298.15 K) 88.74 (300 K) 115.71 (400 K) 139.57 (500 K) 159.38 (600 K) 175.71 (700 K) 189.28 (800 K) 200.68 (900 K) 210.35 (1000 K)	3.76 (100 K) 9.08 (200 K) 16.47 (298.15 K) 16.63 (300 K) 26.87 (400 K) 39.67 (500 K) 54.65 (600 K) 71.43 (700 K) 89.70 (800 K) 109.21 (900 K) 129.77 (1000 K)

	-306.013429	269.19 (100 K) 317.30 (200 K) 352.60 (298.15 K) 353.22 (300 K) 385.15 (400 K) 414.89 (500 K) 442.81 (600 K) 469.01 (700 K) 493.61 (800 K) 516.74 (900 K) 538.51 (1000 K)	61.94 (100 K) 79.15 (200 K) 99.67 (298.15 K) 100.09 (300 K) 122.92 (400 K) 144.04 (500 K) 162.25 (600 K) 177.67 (700 K) 190.75 (800 K) 201.87 (900 K) 211.37 (1000 K)	4.97 (100 K) 12.01 (200 K) 20.75 (298.15 K) 20.93 (300 K) 32.09 (400 K) 45.46 (500 K) 60.80 (600 K) 77.81 (700 K) 96.25 (800 K) 115.90 (900 K) 136.57 (1000 K)
	-382.270039	258.28 (100 K) 304.67 (200 K) 342.74 (298.15 K) 343.43 (300 K) 380.71 (400 K) 416.89 (500 K) 451.46 (600 K) 484.14 (700 K) 514.91 (800 K) 543.86 (900 K) 571.13 (1000 K)	56.13 (100 K) 81.20 (200 K) 112.58 (298.15 K) 113.22 (300 K) 147.25 (400 K) 177.22 (500 K) 201.88 (600 K) 222.03 (700 K) 238.72 (800 K) 252.75 (900 K) 264.68 (1000 K)	4.26 (100 K) 11.10 (200 K) 20.56 (298.15 K) 20.77 (300 K) 33.81 (400 K) 50.07 (500 K) 69.07 (600 K) 90.30 (700 K) 113.36 (800 K) 137.96 (900 K) 163.84 (1000 K)
	-381.706912	278.41 (100 K) 330.03 (200 K) 370.99 (298.15 K) 371.73 (300 K) 410.22 (400 K) 446.41 (500 K) 480.28 (600 K) 511.91 (700 K) 541.43 (800 K) 569.04 (900 K) 594.94 (1000 K)	63.76 (100 K) 88.93 (200 K) 118.69 (298.15 K) 119.27 (300 K) 149.30 (400 K) 175.16 (500 K) 196.38 (600 K) 213.79 (700 K) 228.28 (800 K) 240.52 (900 K) 250.96 (1000 K)	4.82 (100 K) 12.41 (200 K) 22.58 (298.15 K) 22.80 (300 K) 36.25 (400 K) 52.52 (500 K) 71.13 (600 K) 91.67 (700 K) 113.79 (800 K) 137.25 (900 K) 161.83 (1000 K)
	-381.614579	263.40 (100 K) 311.34 (200 K) 350.80 (298.15 K) 351.52 (300 K) 389.40 (400 K) 425.45 (500 K) 459.40 (600 K) 491.17 (700 K) 520.84 (800 K) 548.58 (900 K) 574.59 (1000 K)	56.88 (100 K) 84.69 (200 K) 115.68 (298.15 K) 116.28 (300 K) 148.04 (400 K) 175.19 (500 K) 197.12 (600 K) 214.85 (700 K) 229.42 (800 K) 241.63 (900 K) 251.97 (1000 K)	4.25 (100 K) 11.32 (200 K) 21.13 (298.15 K) 21.34 (300 K) 34.58 (400 K) 50.79 (500 K) 69.45 (600 K) 90.07 (700 K) 112.31 (800 K) 135.88 (900 K) 160.57 (1000 K)

	-381.616019	264.42 (100 K) 313.67 (200 K) 353.48 (298.15 K) 354.20 (300 K) 392.17 (400 K) 428.26 (500 K) 462.25 (600 K) 494.04 (700 K) 523.75 (800 K) 551.53 (900 K) 577.57 (1000 K)	58.91 (100 K) 85.99 (200 K) 116.17 (298.15 K) 116.77 (300 K) 148.26 (400 K) 175.36 (500 K) 197.31 (600 K) 215.07 (700 K) 229.68 (800 K) 241.91 (900 K) 252.28 (1000 K)	4.33 (100 K) 11.59 (200 K) 21.47 (298.15 K) 21.69 (300 K) 34.96 (400 K) 51.19 (500 K) 69.86 (600 K) 90.51 (700 K) 112.77 (800 K) 136.37 (900 K) 161.09 (1000 K)
	-381.620578	261.64 (100 K) 308.56 (200 K) 347.48 (298.15 K) 348.19 (300 K) 385.70 (400 K) 421.50 (500 K) 455.27 (600 K) 486.90 (700 K) 516.48 (800 K) 544.15 (900 K) 570.09 (1000 K)	55.42 (100 K) 83.29 (200 K) 114.35 (298.15 K) 114.96 (300 K) 146.83 (400 K) 174.14 (500 K) 196.22 (600 K) 214.07 (700 K) 228.73 (800 K) 241.01 (900 K) 251.42 (1000 K)	4.16 (100 K) 11.08 (200 K) 20.75 (298.15 K) 20.96 (300 K) 34.08 (400 K) 50.17 (500 K) 68.73 (600 K) 89.28 (700 K) 111.44 (800 K) 134.94 (900 K) 159.58 (1000 K)
	-381.631403	265.53 (100 K) 310.23 (200 K) 346.15 (298.15 K) 346.81 (300 K) 381.87 (400 K) 415.90 (500 K) 448.44 (600 K) 479.22 (700 K) 508.20 (800 K) 535.46 (900 K) 561.13 (1000 K)	55.25 (100 K) 77.05 (200 K) 105.93 (298.15 K) 106.53 (300 K) 138.47 (400 K) 166.78 (500 K) 190.10 (600 K) 209.12 (700 K) 224.83 (800 K) 237.96 (900 K) 249.07 (1000 K)	4.33 (100 K) 10.90 (200 K) 19.82 (298.15 K) 20.02 (300 K) 32.28 (400 K) 47.59 (500 K) 65.47 (600 K) 85.46 (700 K) 107.18 (800 K) 130.34 (900 K) 154.71 (1000 K)
	-382.256262	265.80 (100 K) 314.34 (200 K) 353.26 (298.15 K) 353.97 (300 K) 391.60 (400 K) 427.95 (500 K) 462.62 (600 K) 495.38 (700 K) 526.22 (800 K) 555.22 (900 K) 582.53 (1000 K)	59.03 (100 K) 83.92 (200 K) 114.14 (298.15 K) 114.76 (300 K) 148.17 (400 K) 177.87 (500 K) 202.42 (600 K) 222.51 (700 K) 239.17 (800 K) 253.18 (900 K) 265.09 (1000 K)	4.52 (100 K) 11.67 (200 K) 21.33 (298.15 K) 21.55 (300 K) 34.71 (400 K) 51.05 (500 K) 70.11 (600 K) 91.39 (700 K) 114.49 (800 K) 139.13 (900 K) 165.06 (1000 K)

	-381.600448	266.23 (100 K) 316.63 (200 K) 357.03 (298.15 K) 357.76 (300 K) 396.03 (400 K) 432.29 (500 K) 466.37 (600 K) 498.23 (700 K) 527.97 (800 K) 555.78 (900 K) 581.84 (1000 K)	60.41 (100 K) 87.66 (200 K) 117.41 (298.15 K) 118.00 (300 K) 149.12 (400 K) 175.97 (500 K) 197.77 (600 K) 215.43 (700 K) 229.97 (800 K) 242.14 (900 K) 252.46 (1000 K)	4.41 (100 K) 11.83 (200 K) 21.86 (298.15 K) 22.08 (300 K) 35.46 (400 K) 51.76 (500 K) 70.48 (600 K) 91.17 (700 K) 113.46 (800 K) 137.09 (900 K) 161.83 (1000 K)
	-381.608394	265.05 (100 K) 314.34 (200 K) 354.02 (298.15 K) 354.74 (300 K) 392.53 (400 K) 428.46 (500 K) 462.30 (600 K) 493.98 (700 K) 523.59 (800 K) 551.28 (900 K) 577.25 (1000 K)	59.14 (100 K) 85.85 (200 K) 115.66 (298.15 K) 116.25 (300 K) 147.54 (400 K) 174.59 (500 K) 196.56 (600 K) 214.33 (700 K) 228.96 (800 K) 241.21 (900 K) 251.59 (1000 K)	4.34 (100 K) 11.61 (200 K) 21.46 (298.15 K) 21.67 (300 K) 34.88 (400 K) 51.03 (500 K) 69.63 (600 K) 90.21 (700 K) 112.39 (800 K) 135.92 (900 K) 160.57 (1000 K)
	-381.675893	287.24 (100 K) 341.34 (200 K) 384.14 (298.15 K) 384.90 (300 K) 424.59 (400 K) 461.56 (500 K) 495.96 (600 K) 527.96 (700 K) 557.76 (800 K) 585.59 (900 K) 611.65 (1000 K)	66.55 (100 K) 93.44 (200 K) 123.17 (298.15 K) 123.73 (300 K) 153.10 (400 K) 178.32 (500 K) 199.03 (600 K) 216.04 (700 K) 230.22 (800 K) 242.21 (900 K) 252.45 (1000 K)	5.16 (100 K) 13.12 (200 K) 23.73 (298.15 K) 23.96 (300 K) 37.83 (400 K) 54.44 (500 K) 73.34 (600 K) 94.12 (700 K) 116.46 (800 K) 140.09 (900 K) 164.84 (1000 K)
	-381.620908	268.60 (100 K) 313.66 (200 K) 349.56 (298.15 K) 350.22 (300 K) 385.20 (400 K) 419.18 (500 K) 451.70 (600 K) 482.47 (700 K) 511.45 (800 K) 538.72 (900 K) 564.39 (1000 K)	56.14 (100 K) 77.19 (200 K) 105.72 (298.15 K) 106.32 (300 K) 138.21 (400 K) 166.58 (500 K) 189.98 (600 K) 209.09 (700 K) 224.87 (800 K) 238.06 (900 K) 249.21 (1000 K)	4.45 (100 K) 11.07 (200 K) 19.98 (298.15 K) 20.18 (300 K) 32.42 (400 K) 47.70 (500 K) 65.57 (600 K) 85.55 (700 K) 107.27 (800 K) 130.44 (900 K) 154.82 (1000 K)

	-381.610564	261.22 (100 K) 309.54 (200 K) 349.33 (298.15 K) 350.05 (300 K) 388.03 (400 K) 424.07 (500 K) 457.98 (600 K) 489.69 (700 K) 519.31 (800 K) 547.00 (900 K) 572.95 (1000 K)	56.63 (100 K) 85.66 (200 K) 116.26 (298.15 K) 116.86 (300 K) 148.15 (400 K) 175.04 (500 K) 196.82 (600 K) 214.46 (700 K) 228.97 (800 K) 241.14 (900 K) 251.47 (1000 K)	4.16 (100 K) 11.29 (200 K) 21.18 (298.15 K) 21.39 (300 K) 34.67 (400 K) 50.87 (500 K) 69.50 (600 K) 90.10 (700 K) 112.29 (800 K) 135.81 (900 K) 160.46 (1000 K)
	-381.627927	270.62 (100 K) 315.31 (200 K) 352.75 (298.15 K) 353.44 (300 K) 390.62 (400 K) 426.53 (500 K) 460.52 (600 K) 492.37 (700 K) 522.11 (800 K) 549.93 (900 K) 575.98 (1000 K)	55.21 (100 K) 78.64 (200 K) 112.01 (298.15 K) 112.67 (300 K) 146.74 (400 K) 175.11 (500 K) 197.55 (600 K) 215.42 (700 K) 229.99 (800 K) 242.13 (900 K) 252.41 (1000 K)	4.47 (100 K) 11.05 (200 K) 20.36 (298.15 K) 20.57 (300 K) 33.58 (400 K) 49.72 (500 K) 68.40 (600 K) 89.08 (700 K) 111.37 (800 K) 135.00 (900 K) 159.74 (1000 K)
	-381.644824	278.28 (100 K) 327.02 (200 K) 366.57 (298.15 K) 367.29 (300 K) 405.41 (400 K) 441.69 (500 K) 475.83 (600 K) 507.72 (700 K) 537.48 (800 K) 565.29 (900 K) 591.34 (1000 K)	60.20 (100 K) 84.68 (200 K) 116.24 (298.15 K) 116.87 (300 K) 149.05 (400 K) 176.25 (500 K) 198.05 (600 K) 215.59 (700 K) 230.00 (800 K) 242.06 (900 K) 252.31 (1000 K)	4.77 (100 K) 11.94 (200 K) 21.77 (298.15 K) 21.98 (300 K) 35.31 (400 K) 51.62 (500 K) 70.38 (600 K) 91.09 (700 K) 113.39 (800 K) 137.01 (900 K) 161.74 (1000 K)
	-381.635983	280.52 (100 K) 329.92 (200 K) 369.56 (298.15 K) 370.28 (300 K) 408.25 (400 K) 444.38 (500 K) 478.40 (600 K) 510.22 (700 K) 539.93 (800 K) 567.71 (900 K) 593.75 (1000 K)	60.77 (100 K) 85.42 (200 K) 115.97 (298.15 K) 116.58 (300 K) 148.39 (400 K) 175.56 (500 K) 197.48 (600 K) 215.18 (700 K) 229.74 (800 K) 241.93 (900 K) 252.27 (1000 K)	4.82 (100 K) 12.09 (200 K) 21.94 (298.15 K) 22.15 (300 K) 35.42 (400 K) 51.67 (500 K) 70.36 (600 K) 91.02 (700 K) 113.29 (800 K) 136.89 (900 K) 161.62 (1000 K)

Several stationary points were determined for the PES and their thermodynamic properties (S , C_p and ΔH) at different temperatures (100 K, 200 K, 298.15 K, 300 K, 400 K, 500 K, 600 K, 700 K, 800 K, 900 K, and 1000 K). At this point we can start to build the PES for

the minimal structures but we have still to characterize the transition states that links all the minimal stationary points.

6. Perspective

During my stay at Laboratoire Réactions et Génie de Procédés (LRGP), CNRS, Université de Lorraine, ENSIC theoretical calculations were carried out to optimize, characterize and calculate the thermodynamic properties S, Cp, and ΔH at different temperatures: 100 K, 200 K, 298.15 K, 300 K, 400 K, 500 K, 600 K, 700 K, 800 K, 900 K, and 1000 K of several stationary points of the PES corresponding to the combustion of 1-hydroperoxyltetrahydrofuran and 2-hydroperoxyltetrahydrofuran. Gaussian 09 software and thermo.pl script were used for the study. We also started to calculate some transition states with TSSCDS program and some kinetic constant for some reaction by using ChemRate. Thanks to this STSM we have got a good starting point to go on with the collaboration between Universidade de Lisboa (Portugal) and Université de Lorraine (France) and in the next months we will go on with the collaboration and we will try to characterize the rest of the transition states that link the minimal stationary points. Moreover, I had the opportunity to improve my knowledge about the use of programs to calculate thermodynamic properties and how to obtain kinetic constants, whereas the people of the host institution has improve their knowledge about Gaussian 09 and TSSCDS software and thus, we also established some synergies thanks to this STSM.

7. Outputs resulting from the STSM

The work carried on in the framework of the STSM will be presented in some conference, probably in the 3rd MC meeting in Lisbon and we are planning to write some publication.