A Shock Tube and Chemical Kinetic Modeling Study of the Oxidation of 2,5-Dimethylfuran

Baptiste Sirjean,[1] René Fournet,[1,*]

Pierre-Alexandre Glaude,[1] Frédérique Battin-Leclerc,[1] Weijing Wang[2], Matthew A. Oehlschlaeger[2,*]

[1] *Laboratoire Réactions et Génie des Procédés (LRGP), Université de Lorraine, CNRS, BP 20451, 1 rue Grandville, 54001 Nancy, France*

[2] *Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY, USA*

*Authors to whom correspondence should be addressed:

René Fournet – rene.fournet@univ-lorraine.fr

Phone: +33 383175202

Matthew A. Oehlschlaeger – oehlsm@rpi.edu

Phone: 518.276.8115

Supplementary Data for "A Shock Tube and Chemical Kinetic Modeling Study of the Oxidation of 2,5-Dimethylfuran" by Sirjean et al.

Table S1. Experimental data: ignition delay time measurements for DMF/O_2/Ar mixtures. DMF: 2,5-dimethylfuran, φ: equivalence ratio, τ: ignition delay time.

φ	%-molar DMF	P [bar]	T [K]	τ [μs]
1	1	1.34	1403	1045
1	1	1.34	1474	463
1	1	1.26	1533	326
1	1	1.27	1663	122
1	1	1.19	1685	102
1	0.5	1.46	1387	1555
1	0.5	1.43	1424	1025
1	0.5	1.40	1485	574
1	0.5	1.33	1525	391
1	0.5	1.29	1636	173
1	0.5	1.23	1716	110
1	0.5	1.14	1792	75
1	0.5	1.06	1831	58
1	0.25	1.40	1433	1224
1	0.25	1.36	1469	826
1	0.25	1.36	1514	630
1	0.25	1.30	1530	577
1	0.25	1.34	1602	281
1	0.25	1.27	1701	148
1	0.25	1.21	1767	112
1	1	3.97	1310	1324
1	1	3.79	1357	682
1	1	3.57	1372	610
1	1	3.41	1388	525
1	1	3.30	1451	259
1	1	3.23	1571	118
1	1	2.96	1667	52
0.5	1	1.43	1318	1413
0.5	1	1.44	1397	618
0.5	1	1.36	1472	329
0.5	1	1.22	1521	197
0.5	0.5	1.44	1300	2306
0.5	0.5	1.40	1360	1325
0.5	0.5	1.50	1372	1124
0.5	0.5	1.39	1439	507
0.5	0.5	1.42	1547	198
0.5	0.5	1.31	1599	143
0.5	0.5	1.18	1664	100
1.5	1	1.32	1340	2455
1.5	1	1.24	1373	1668
1.5	1	1.32	1540	402
1.5	1	1.28	1632	195
1.5	1	1.20	1723	105
1.5	0.5	1.45	1392	2023
1.5	0.5	1.42	1427	1619
1.5	0.5	1.39	1477	977
1.5	0.5	1.34	1538	528
1.5	0.5	1.34	1690	206
1.5	0.5	1.20	1705	191

Table S2. Name and structure of the species involved in the detailed mechanism of the DMF oxidation.

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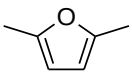
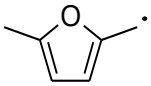
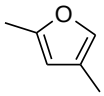
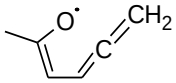
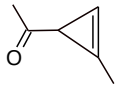
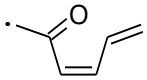
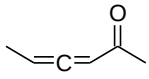
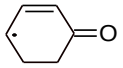
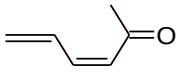
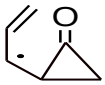
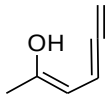
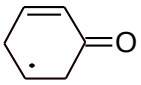
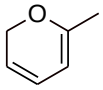
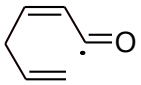
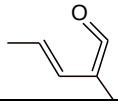
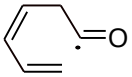
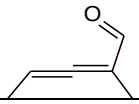
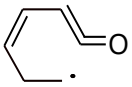
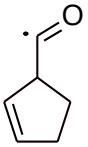
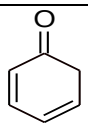
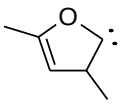
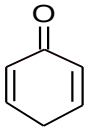
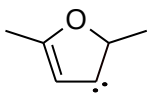
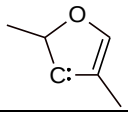
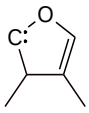
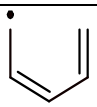
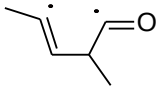
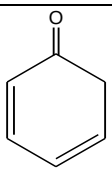
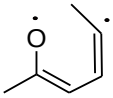
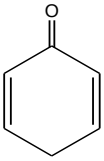
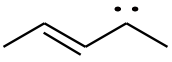
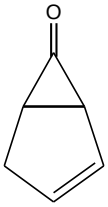
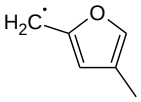
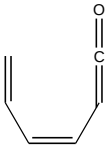
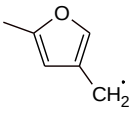
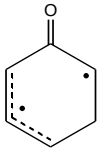
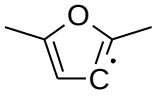
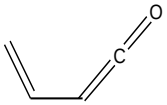
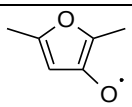
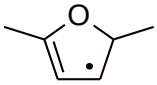
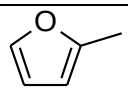
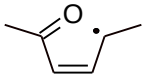
	DMF		R1C_6H_7O
	M2C_6H_8O		R2C_6H_7O
	M3C_6H_8O		R3C_6H_7O
	M4C_6H_8O		R4C_6H_7O
	M5C_6H_8O		R5C_6H_7O
	M6C_6H_8O		R6C_6H_7O
	M7C_6H_8O		R7C_6H_7O
	M8C_6H_8O		R8C_6H_7O
	M9C_6H_8O		R9C_6H_7O
	M10C_6H_8O		R10C_6H_7O
	M11C_6H_8O		M2C_6H_6O
	CA1		M3C_6H_6O

	CA2		$C_5H_7Y\#$
	CA3		C_5H_7
	CA4		C_5H_7Y
	B1		$M2C_6H_6O$
	B2		$M3C_6H_6O$
	B3		$M4C_6H_6O$
	M2-R1		$M5C_6H_6O$
	M2-R2		$B1C_6H_6O$
	DMF-3yl		C_4H_4O
	DMF-3ylO		$R1C_6H_9O$
	MF		$R3C_6H_9O$

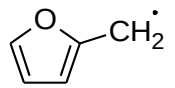
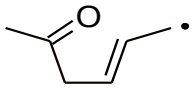
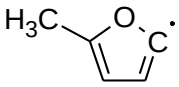
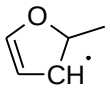
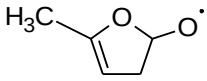
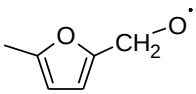
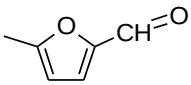
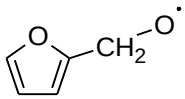
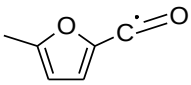
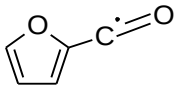
	furylCH2		R7C_6H_9O
	M5F-2yl		MFH
	M5F-2ylO		M5F-CH2O
	MF-CHO		furylCH2O
	MF-CO		furylCO

Table S3. Geometries, frequencies and RRKM parameters for the reactant and transition state involved in the reaction $CH_3CF_3 \rightarrow CH_2CF_2 + HF$
Geometries and frequencies obtained at the B3LYP/CBSB7 level of theory

CH_3CF_3 (Cartesian coordinates)

C 0.025794 1e-005 -2.6e-005
C -1.47728 8.8e-005 -3e-006
H -1.83923 0.853241 0.573577
H -1.83922 0.070152 -1.02565
H -1.83922 -0.92322 0.452083
F 0.526992 1.12745 -0.552796
F 0.526899 -0.084996 1.25276
F 0.52684 -1.04254 -0.699946

Transition state (Cartesian coordinates)

C -0.314717 0.189218 1.4e-005
C 0.494026 1.33579 4.5e-005
H 0.503768 1.89403 0.927649
H 1.41236 0.373914 -6.4e-005
H 0.50365 1.89417 -0.927481
F 1.32305 -0.888878 -4.4e-005
F -0.85571 -0.295171 1.07395
F -0.855738 -0.295077 -1.07396

CH_3CF_3 (Frequencies cm^{-1})

3116.37 3116.15 3035.19
1467.29 1467.11 1418.43
1268.81 1219.69 1219.49
957.793 957.432 816.949
588.369 529.868 529.121
358.358 358.161

230.877 (treated as hindered rotor) with a hindrance of V=3.1 kcal mol^{-1} and an internal symmetry σ_{int}=3.

Transition state (Frequencies cm^{-1})

3213.2 3115.8 1708.87
1546.04 1393.9 1379.94
1275.84 995.752 928.231
871.203 743.146 611.343
504.061 454.078 383.04
283.641 244.291
Imaginary frequency : -1781

RRKM parameters used in Chemrate

Lennard-Jones parameters for CH_3CF_3 : σ=5.29 Å and ε/k_B= 468.4 K
Ar as buffer gas (σ=3.54Å and ε/k_B= 39.95 K) and $\langle\Delta E\rangle_{down}$=750$cm^{-1}$
Neon as buffer gas (σ= 2.82 Å and ε/k_B=32.8 K) and $\langle\Delta E\rangle_{down}$=750$cm^{-1}$
Collision model: exponential down model
Time dependent solution (Divide and Conquer method)
Increment for energy: 25 cm^{-1}