Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Supplemental Material

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New insights in the oxidation of *n*-butane in a jet stirred reactor using cw-CRDS measurements

Phys. Chem. Chem. Phys., 2013.

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I/ Evolution with temperature of concentration of minor compounds of the oxidation of *n*-butane measured by gas chromatography

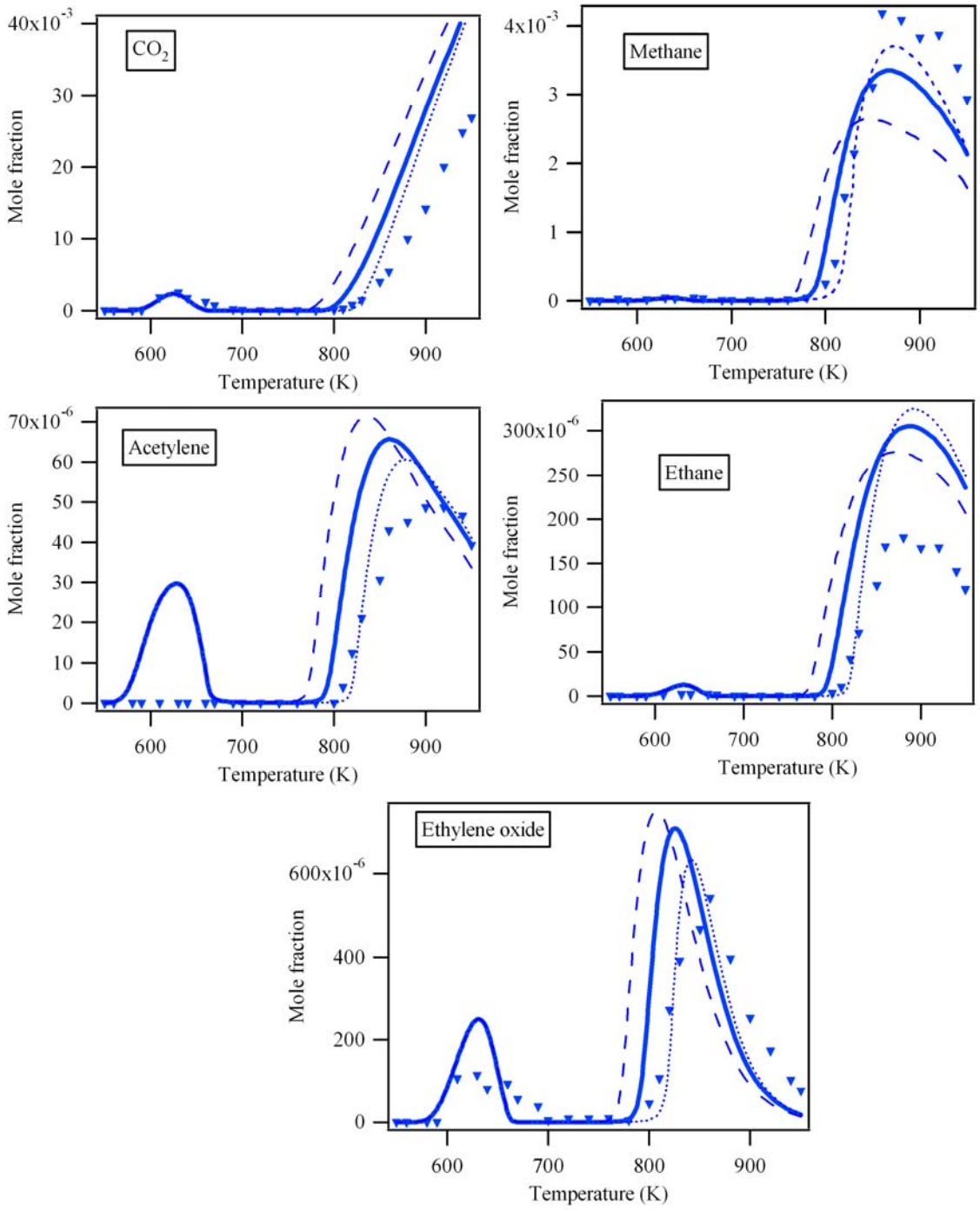


Figure S1: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of carbon dioxide, methane, acetylene and ethane.

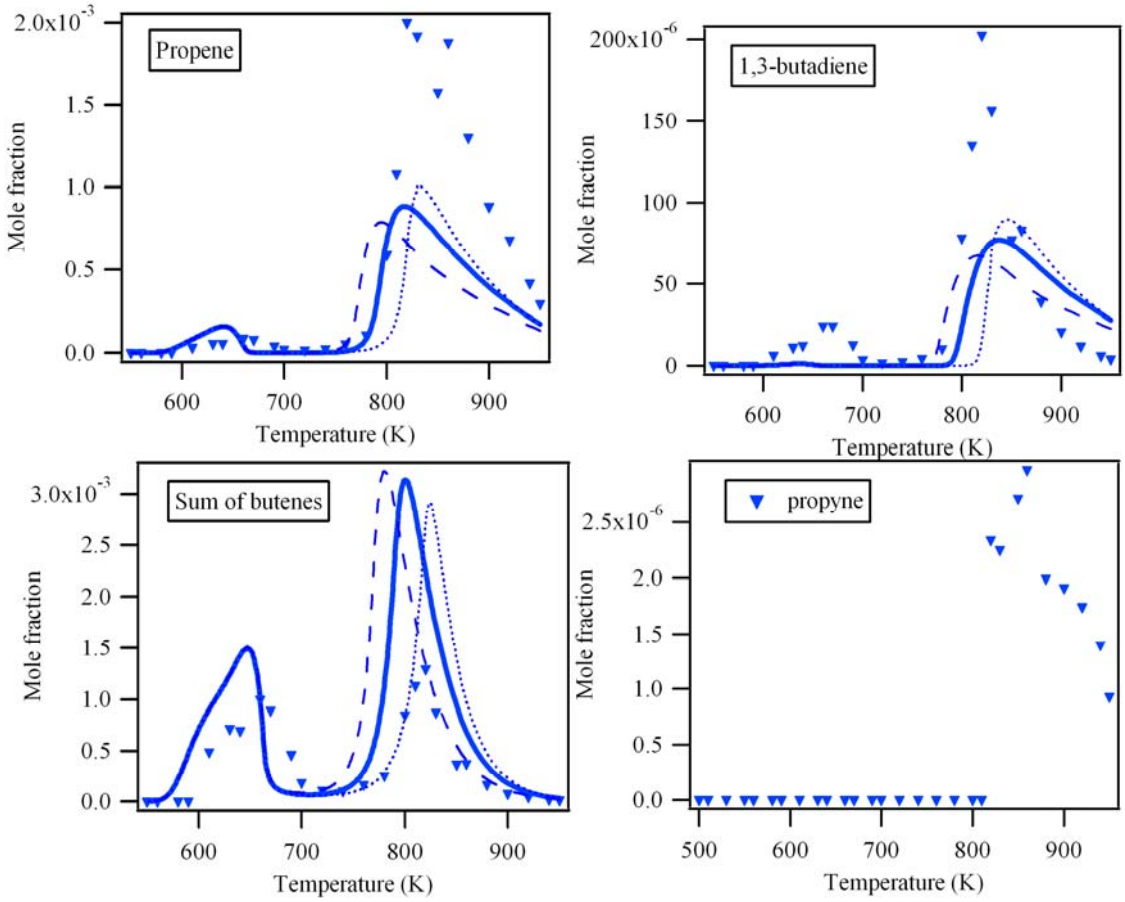


Figure S2: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of C_3-C_4 hydrocarbons. Propyne is not included in the used model.

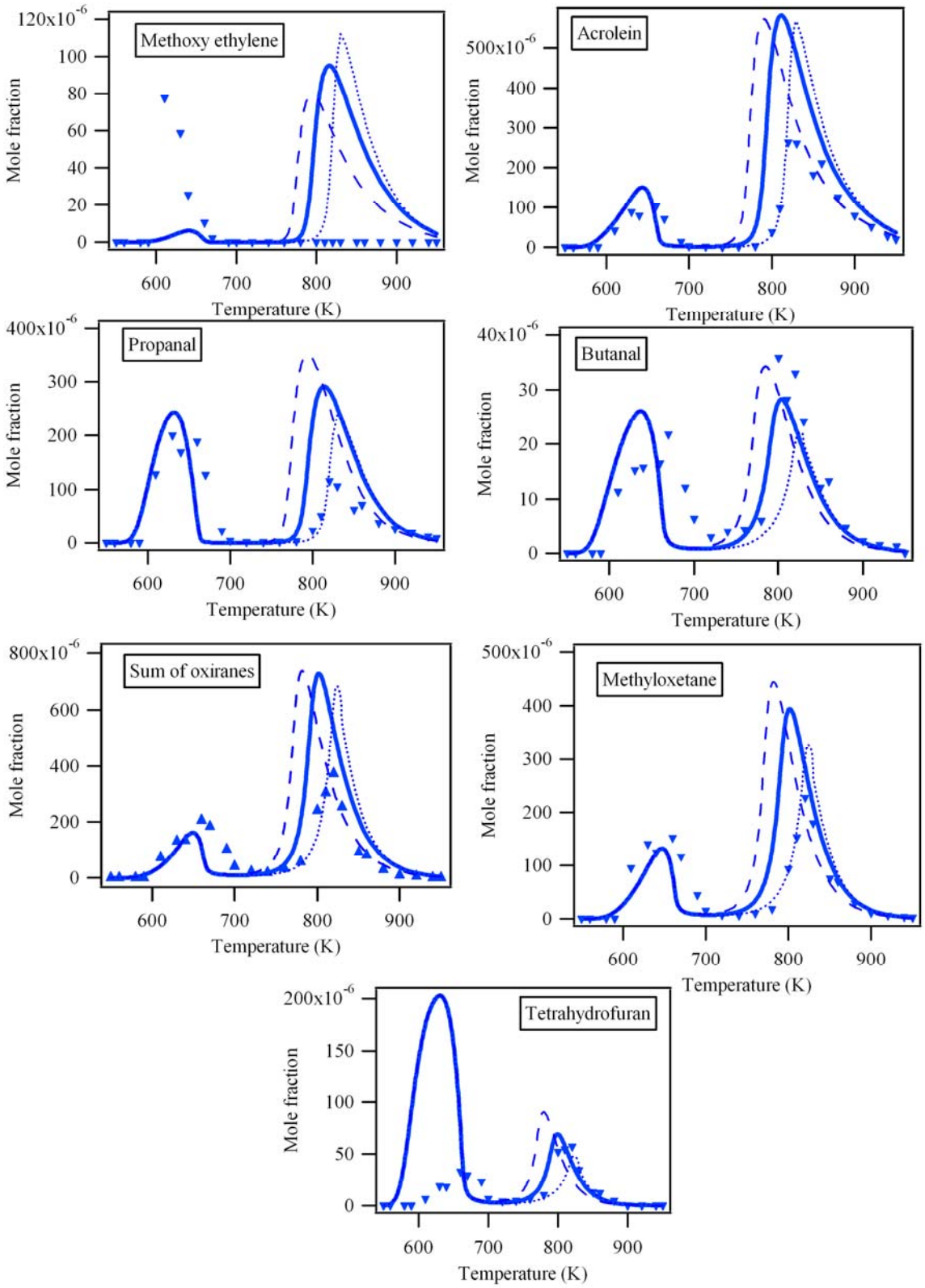


Figure S3: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of minor oxygenated species – part 1.

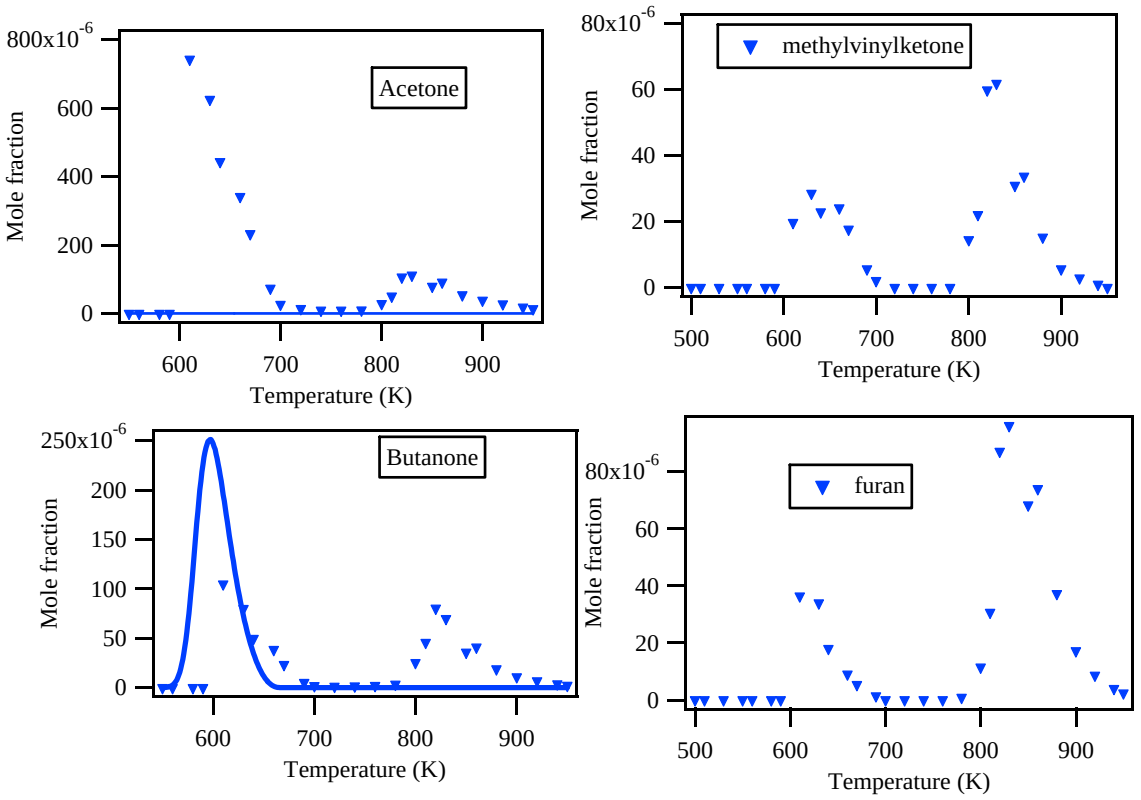
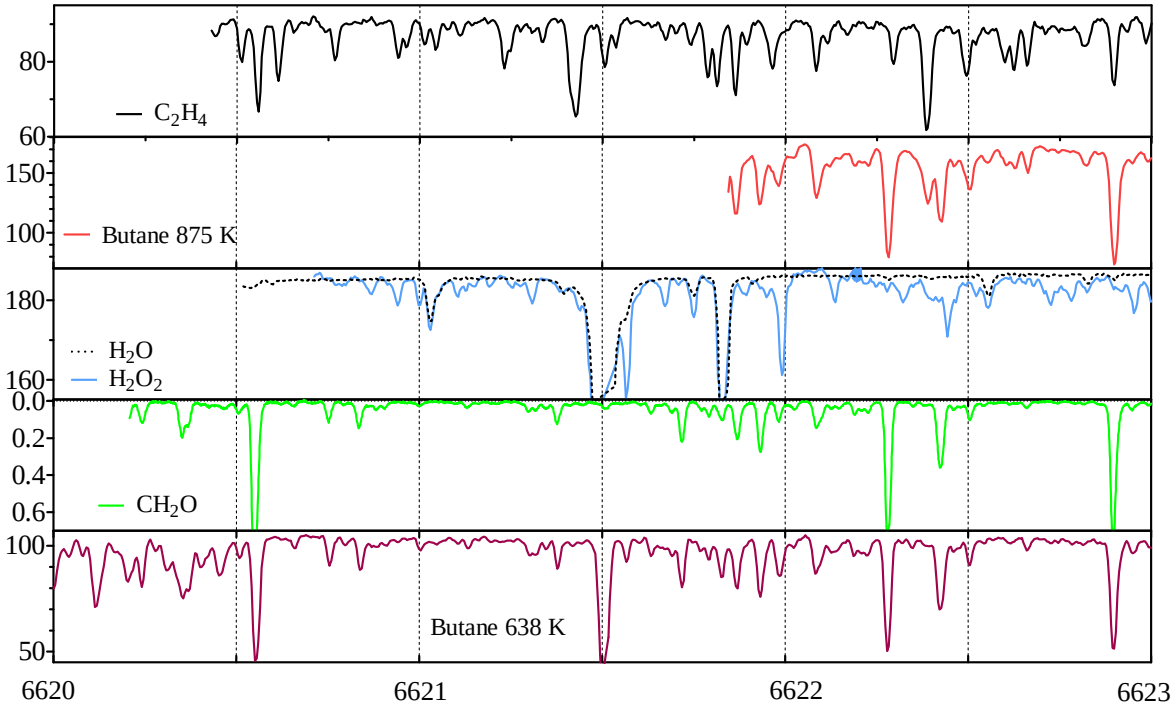
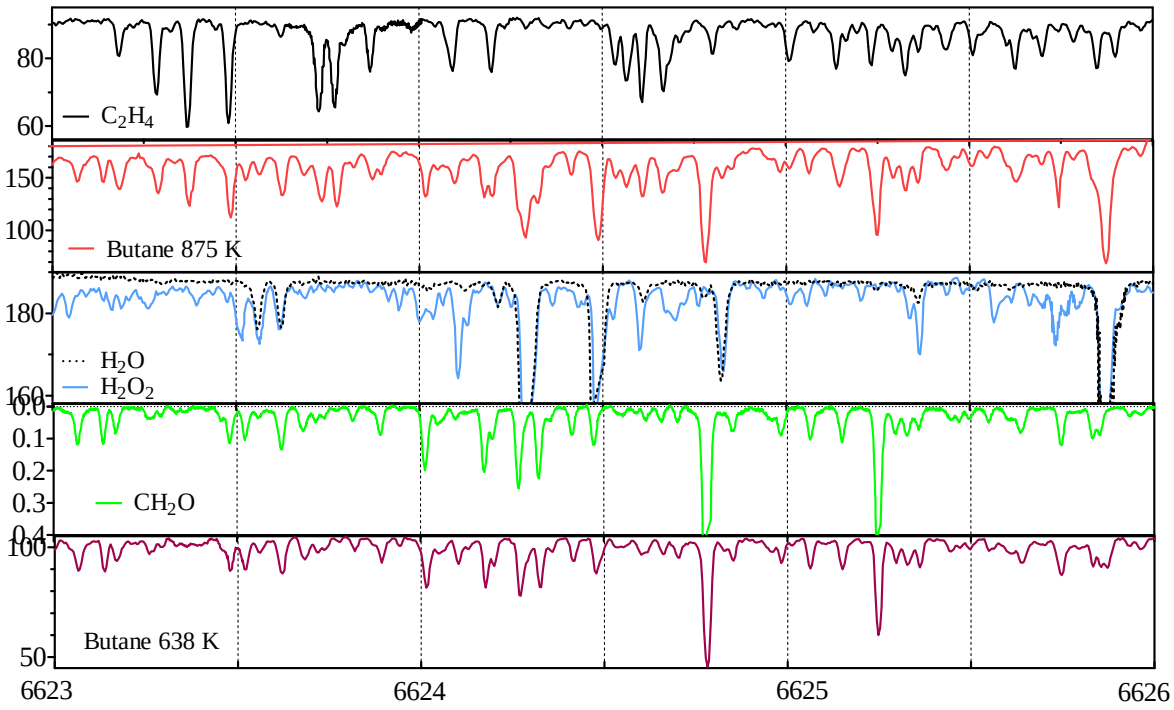


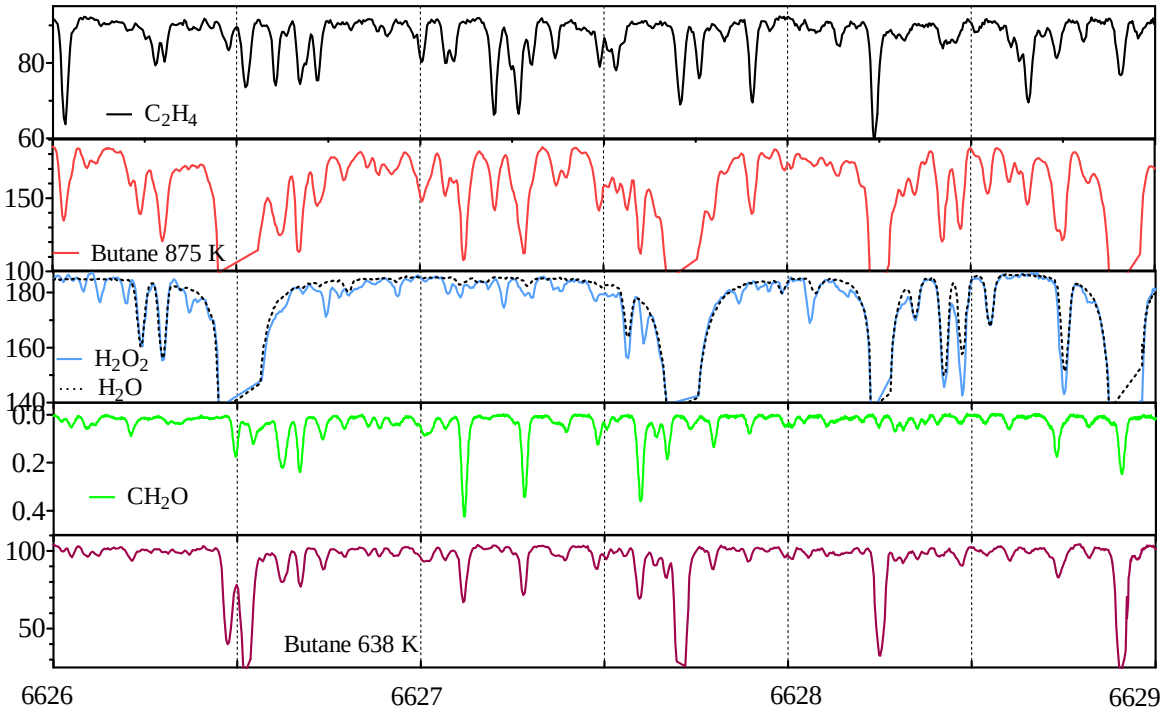
Figure S4: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of minor oxygenated species – part 2. Acetone, methylvinylketone and furan are not included in the used model.

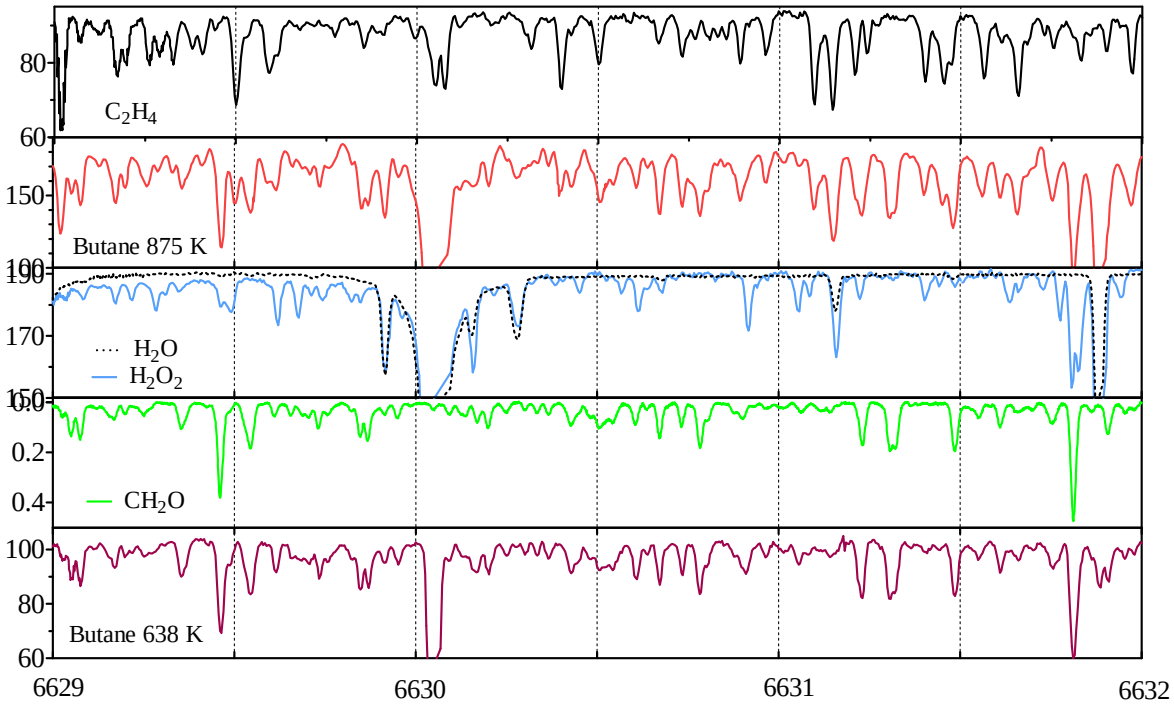
II/ Full absorption spectra

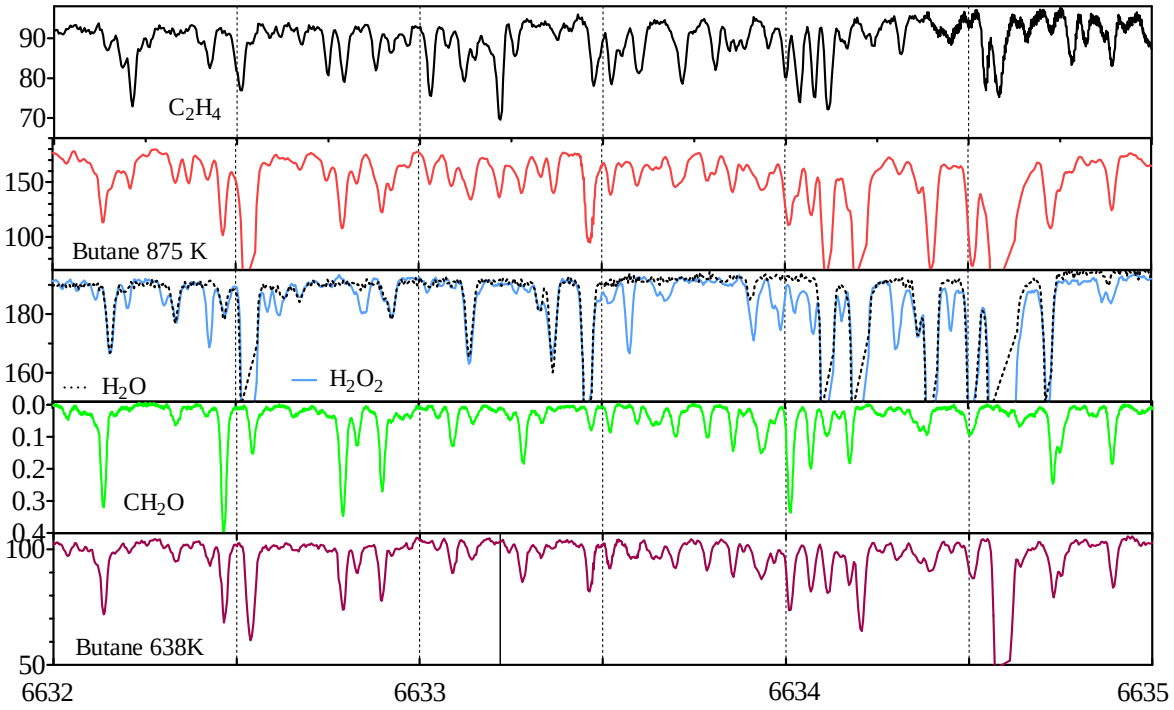
Figure S5 Absorption spectrum in the range 6620 - 6644 cm^{-1} for the major absorbing reaction products: units are ring down time τ as a function of wavenumber for H_2O_2, H_2O and C_2H_4, as well as the spectrum such as observed from the oxidation of n-butane at 638 K and 875 K, absorption cross sections σ in 20^{-21} cm^2 taken from Staak *et al*[1] for CH_2O

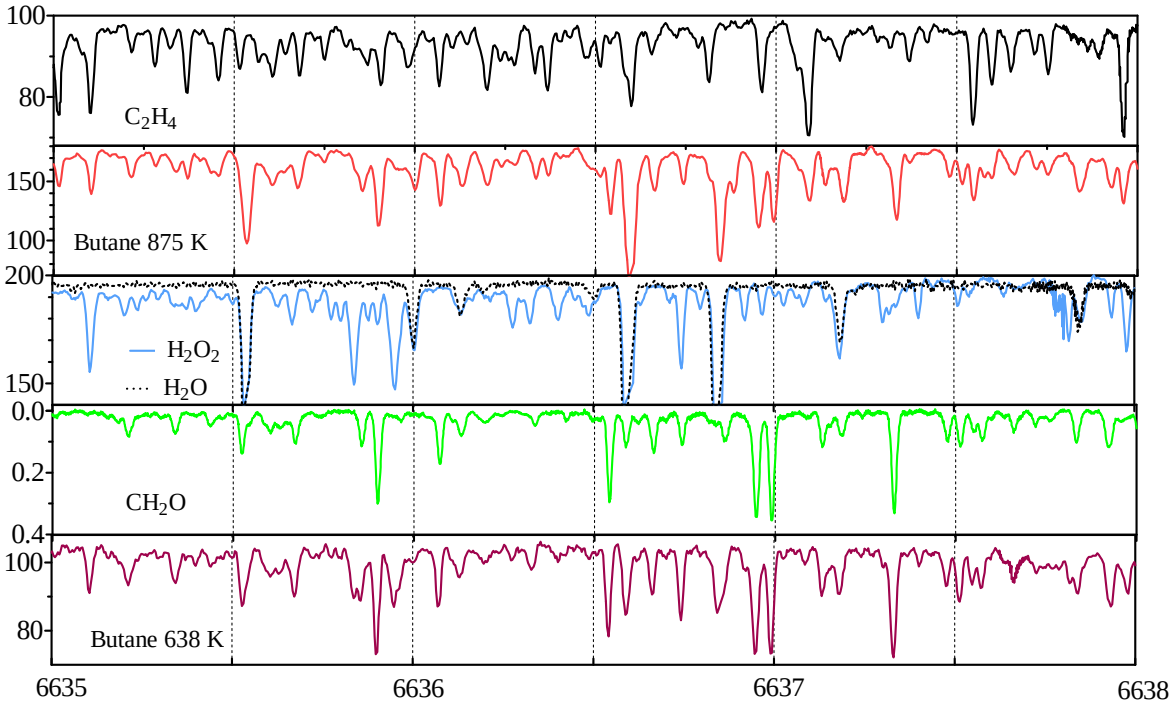


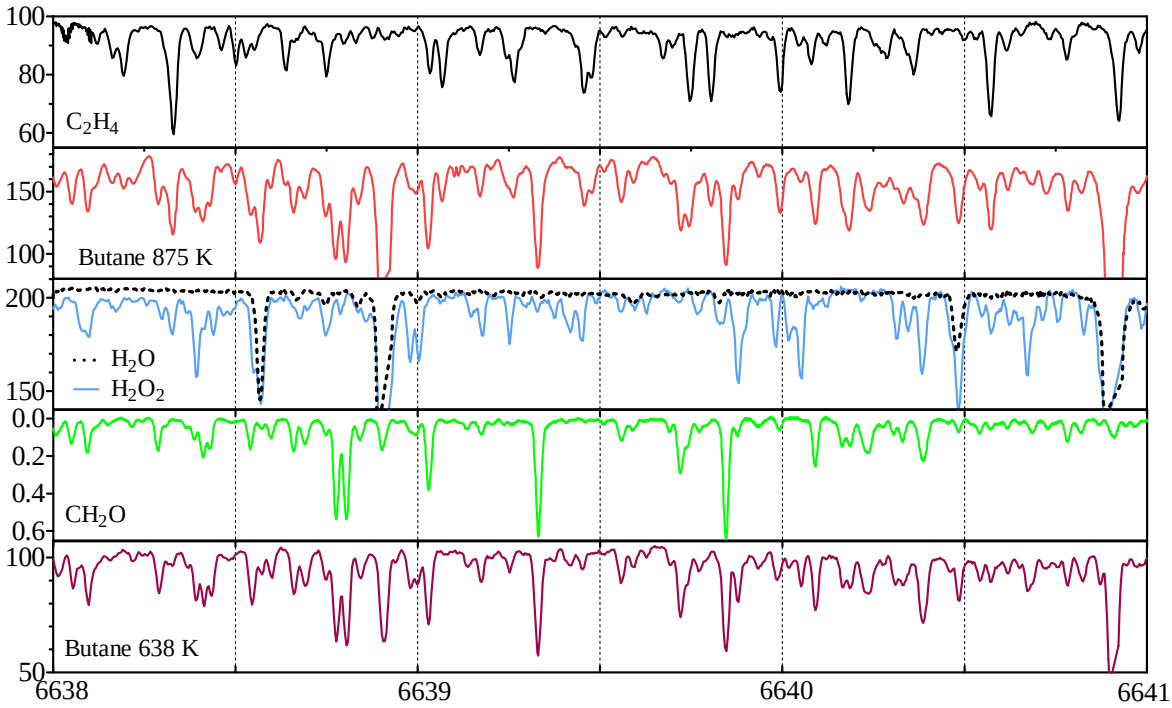

80
60
C2H4
150
100
Butane 875 K
180
160
H2O
H2O2
0.0
0.1
0.2
0.3
0.4
CH2O
100
50
Butane 638 K
6623
6624
6625
6626

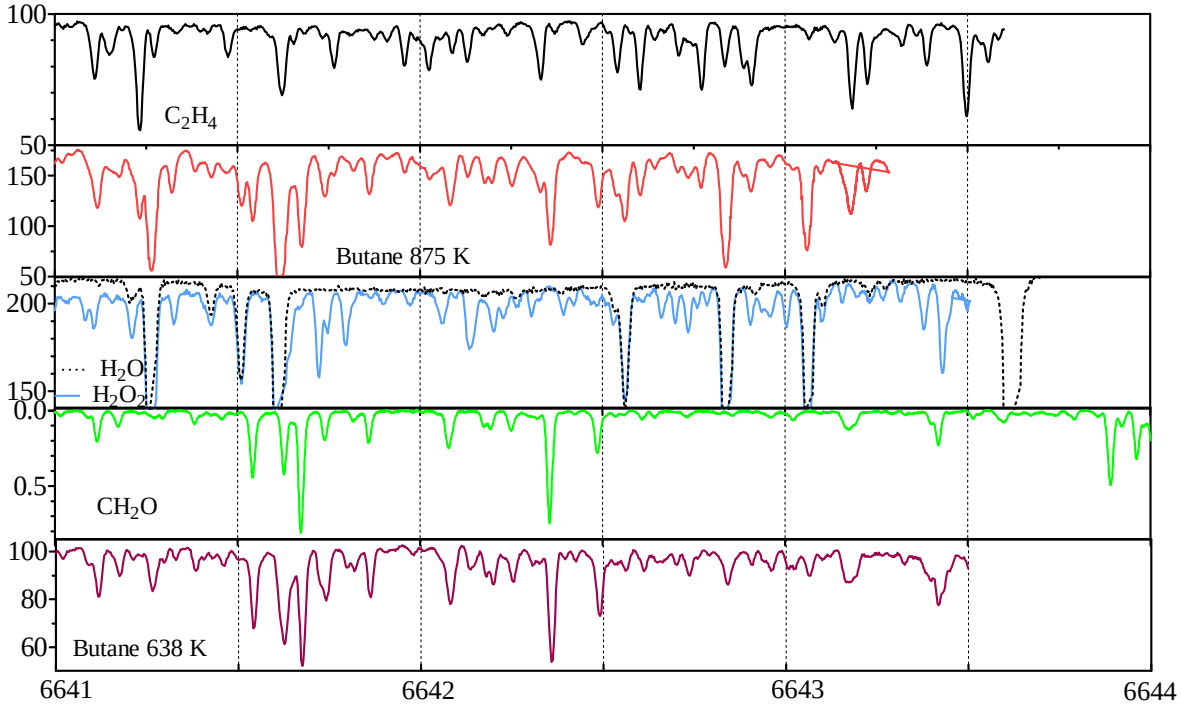

80
60
C2H4
150
100
Butane 875 K
180
160
140
H2O2
H2O
0.0
0.2
0.4
CH2O
100
50
Butane 638 K
6626
6627
6628
6629


80
60
C_2H_4
150
100
Butane 875 K
190
170
150
H_2O
H_2O_2
0.0
0.2
0.4
CH_2O
100
80
60
Butane 638 K
6629
6630
6631
6632


90
80
70
C_2H_4
150
100
Butane 875 K
180
160
H_2O
H_2O_2
0.0
0.1
0.2
0.3
0.4
CH_2O
100
50
Butane 638K
6632
6633
6634
6635


100
80
C2H4
150
100
Butane 875 K
200
150
H2O2
H2O
0.0
0.2
CH2O
0.4
100
80
Butane 638 K
6635
6636
6637
6638


100
80
60
C2H4
150
100
Butane 875 K
200
H2O
H2O2
150
0.0
0.2
0.4
CH2O
0.6
100
50
Butane 638 K
6638
6639
6640
6641


100
50
C_2H_4
150
100
50
Butane 875 K
200
150
H_2O
H_2O_2
0.0
0.5
CH_2O
100
80
60
Butane 638 K
6641
6642
6643
6644

VI/ Supplementary references

1. M. Staak, E. W. Gash, D. S. Venables and A. A. Ruth, *J. Mol. Spectrosc.*, 2005, **229**, 115-121.