Thermodynamic, pyrolytic, and kinetic investigation on the thermal decomposition of polyvinyl chloride in the presence of franklinite

Sanad Altarawneh[1],* Mohammad Al-Harahsheh[2], Chris Dodds[1], Adam Buttress[1], Sam Kingman[1]

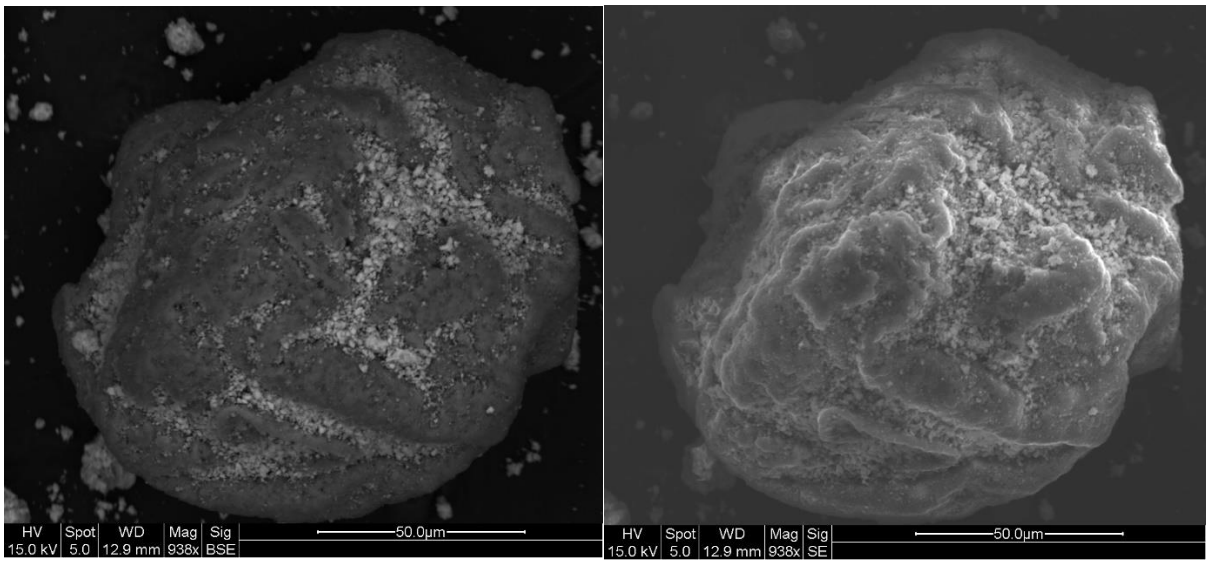
[1] Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, UK

[2] Chemical Engineering Department, Jordan University of Science and Technology, Irbid, 22110, Jordan

* corresponding author: sanad.altarawneh@nottingham.ac.uk

Supplementary material

1. SEM images of the $ZnFe_2O_4$-PVC powder before pyrolysis



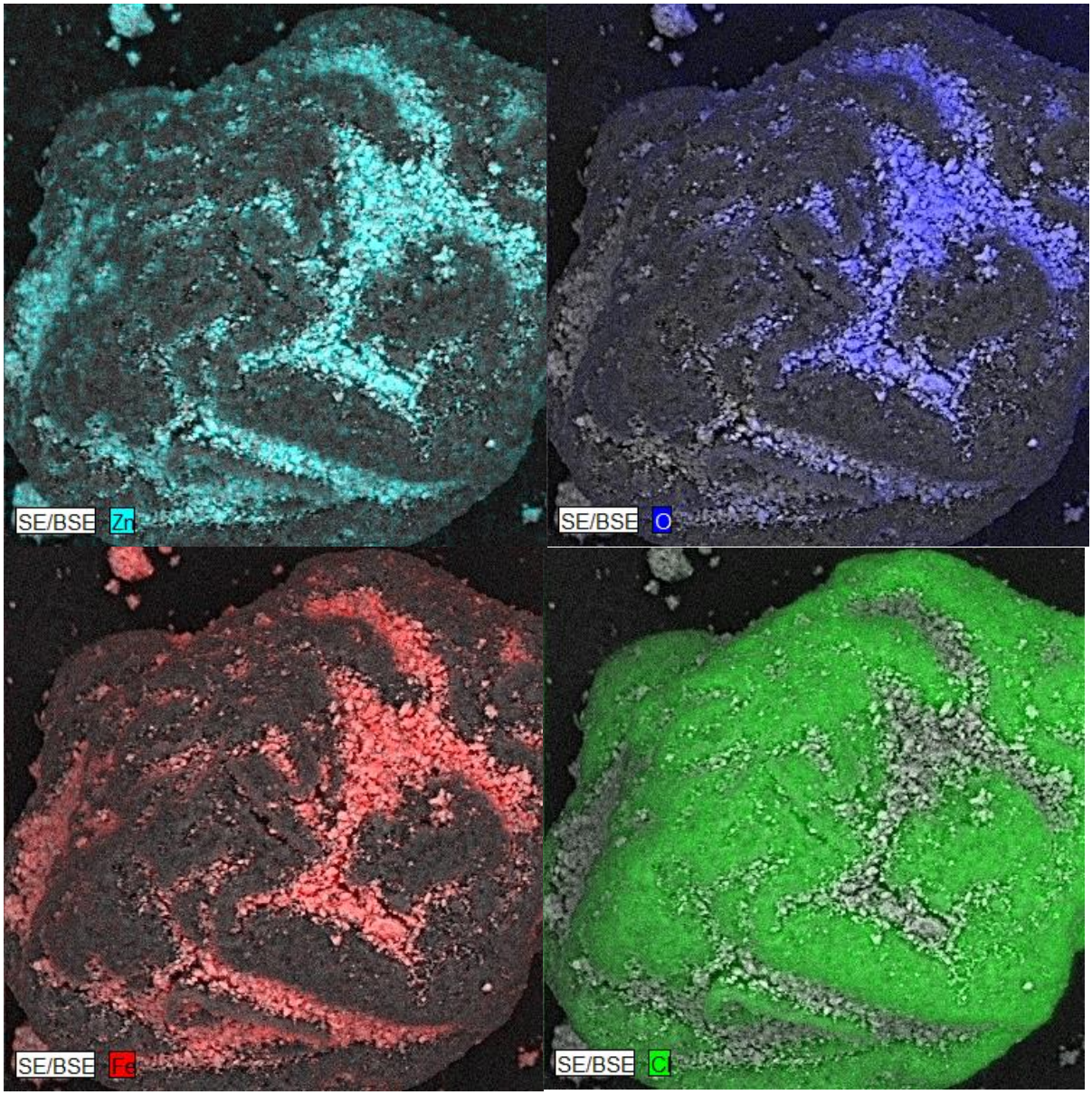


Figure S1: Secondary electron (SE), Back scattered electron (BSE), and EDS maps of a PVC particle covered with smaller particles of $ZnFe_2O_4$ confirming the formation of an interactive mixture.

2. TGA/DSC profile of pure PVC under air

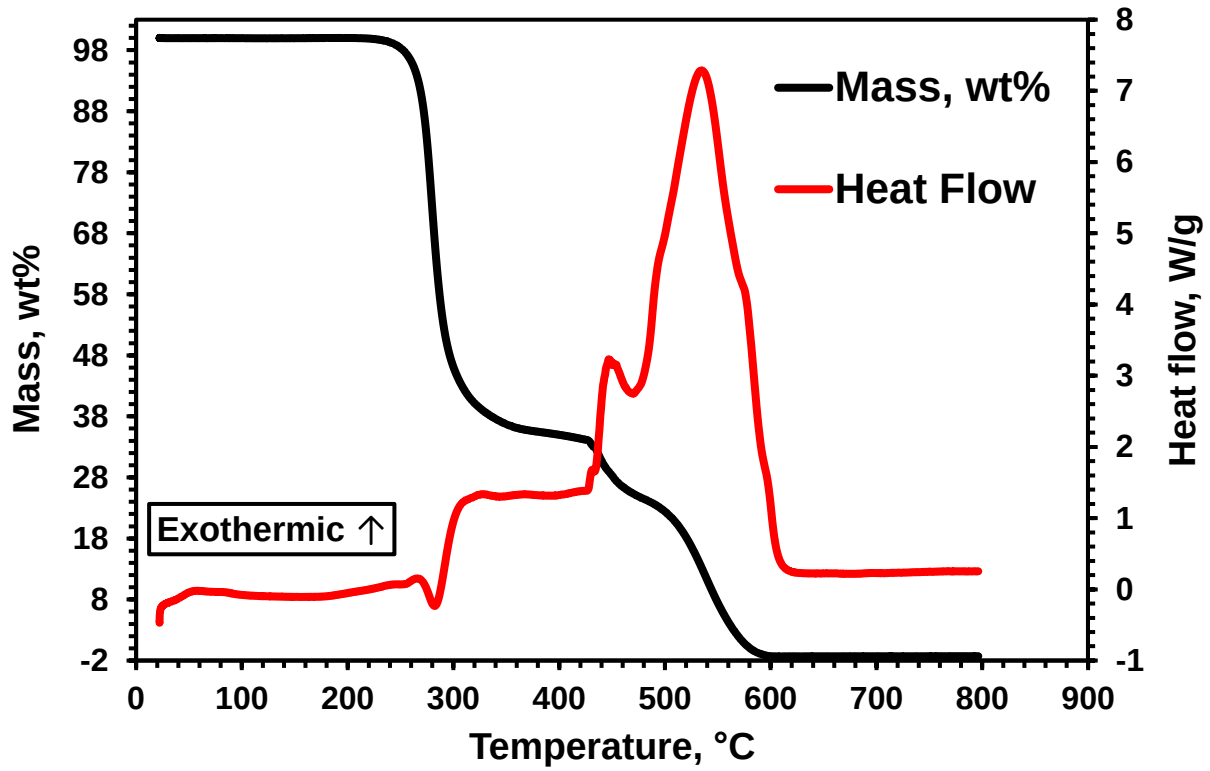
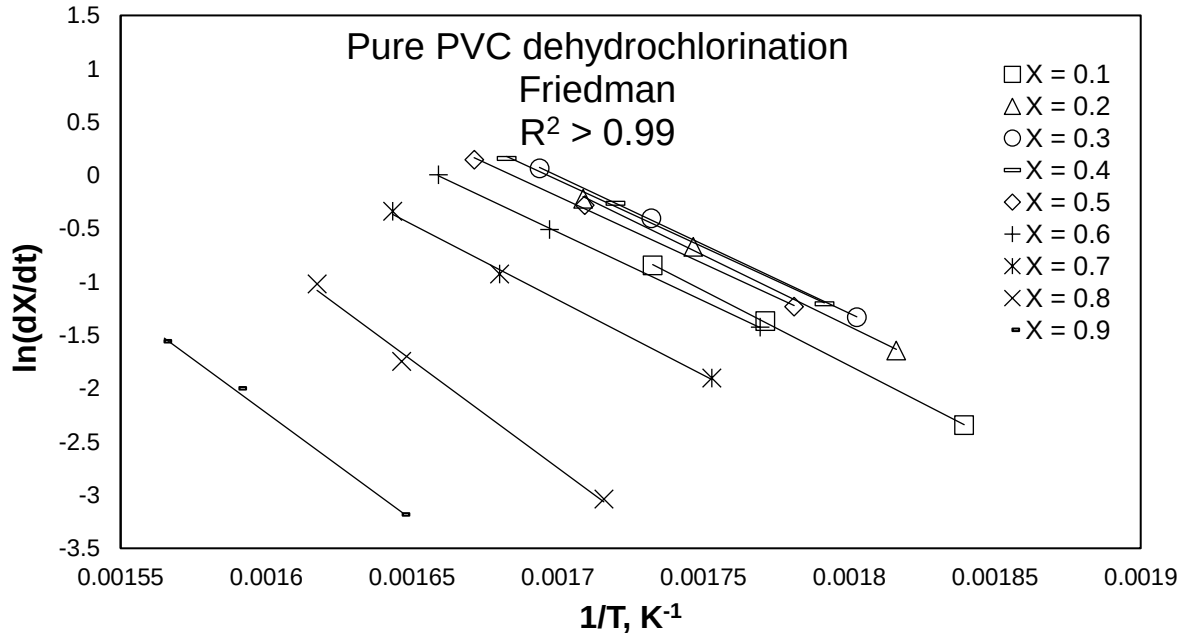


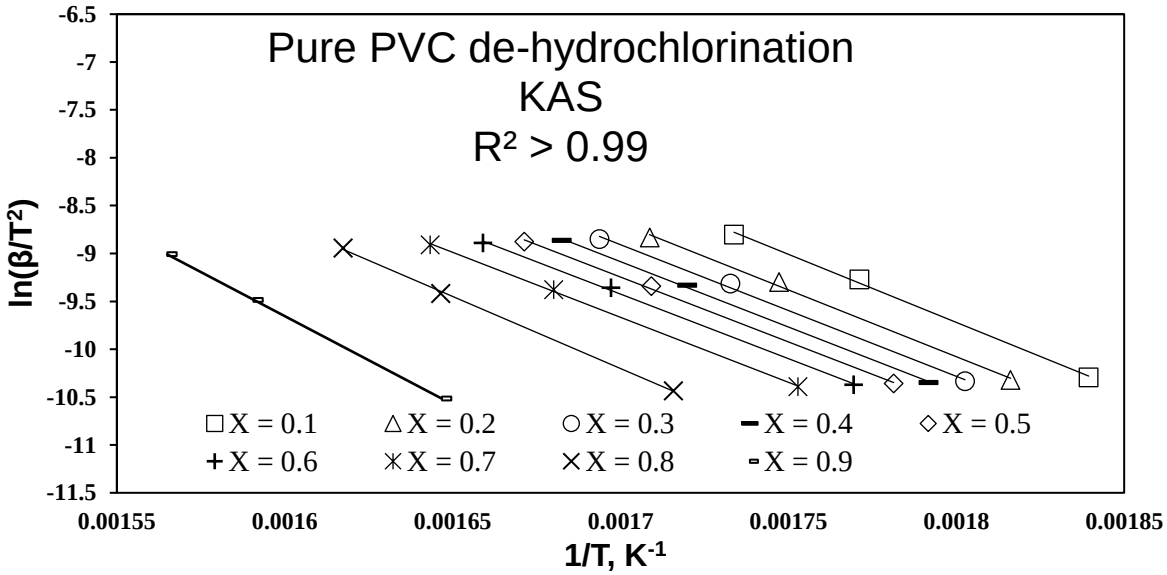
Figure S2: TGA/DSC profile of pure PVC under air at a heating rate of 10 °C/min.

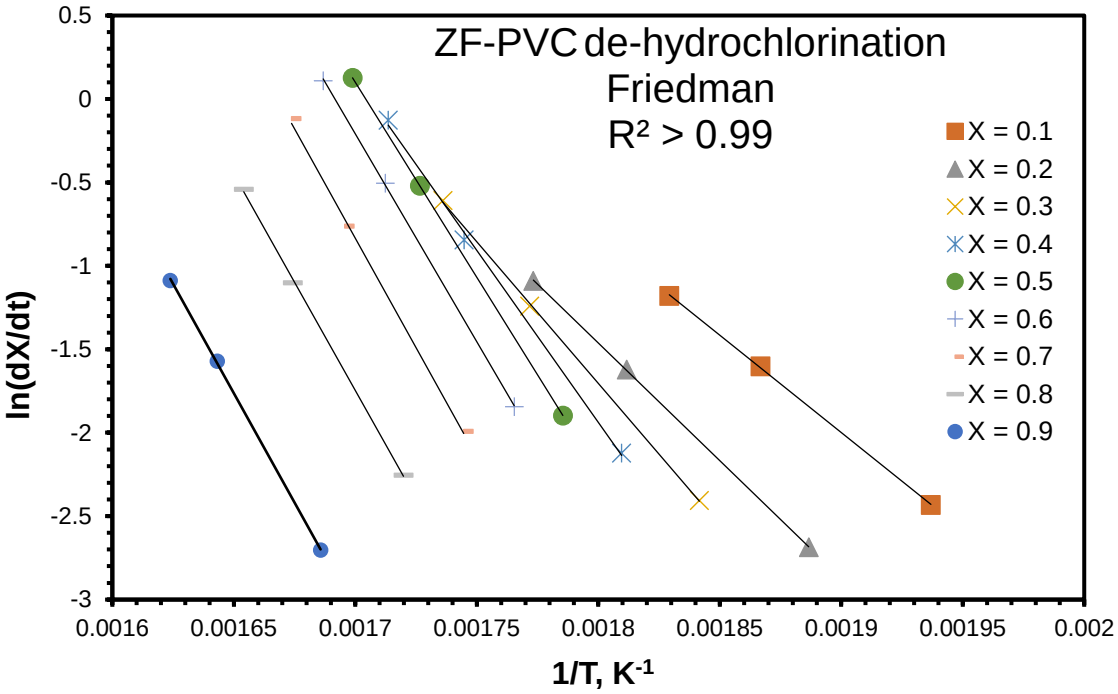
3. Kinetics data fitting

3.1. Data fitting for the extraction of the activation energy

3.1.1. De-hydrochlorination stage




Pure PVC de-hydrochlorination
KAS
R² > 0.99
ln(β/T²)
1/T, K-1
X = 0.1
X = 0.2
X = 0.3
X = 0.4
X = 0.5
X = 0.6
X = 0.7
X = 0.8
X = 0.9


ZF-PVC de-hydrochlorination
Friedman
R² > 0.99
ln(dX/dt)
1/T, K-1
X = 0.1
X = 0.2
X = 0.3
X = 0.4
X = 0.5
X = 0.6
X = 0.7
X = 0.8
X = 0.9

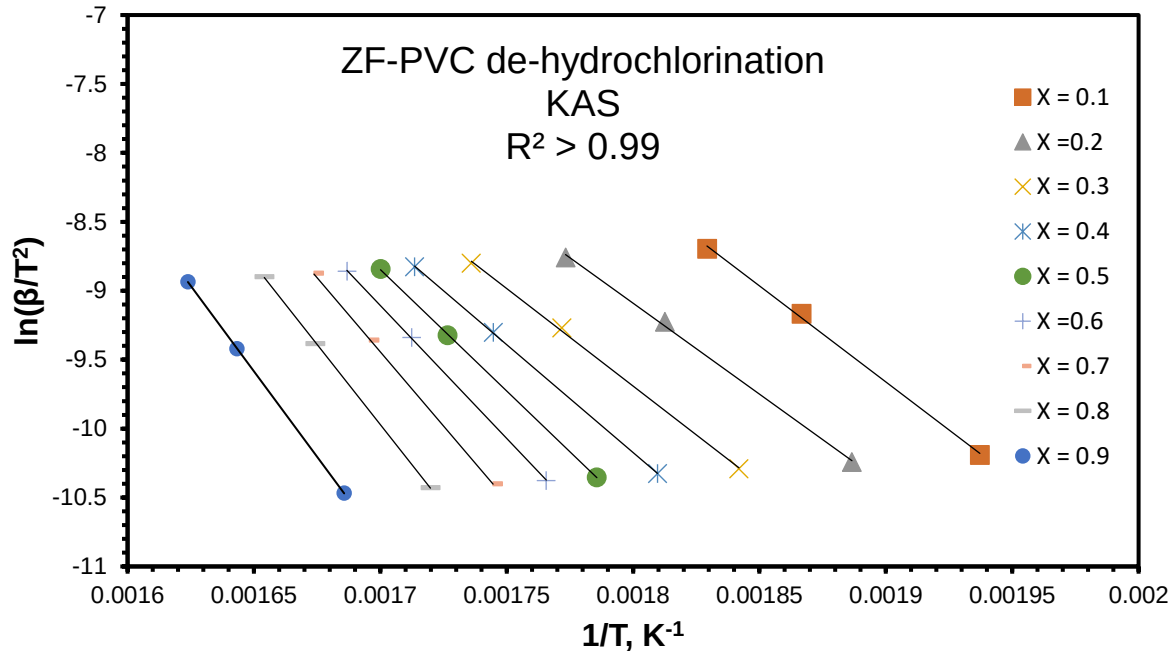
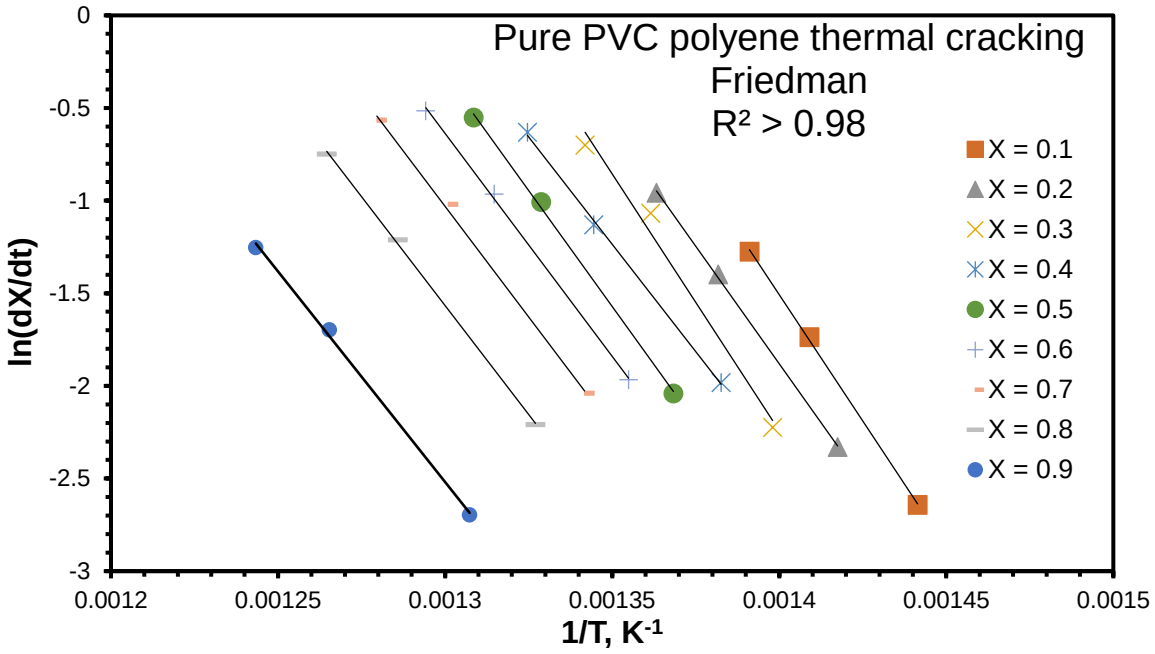
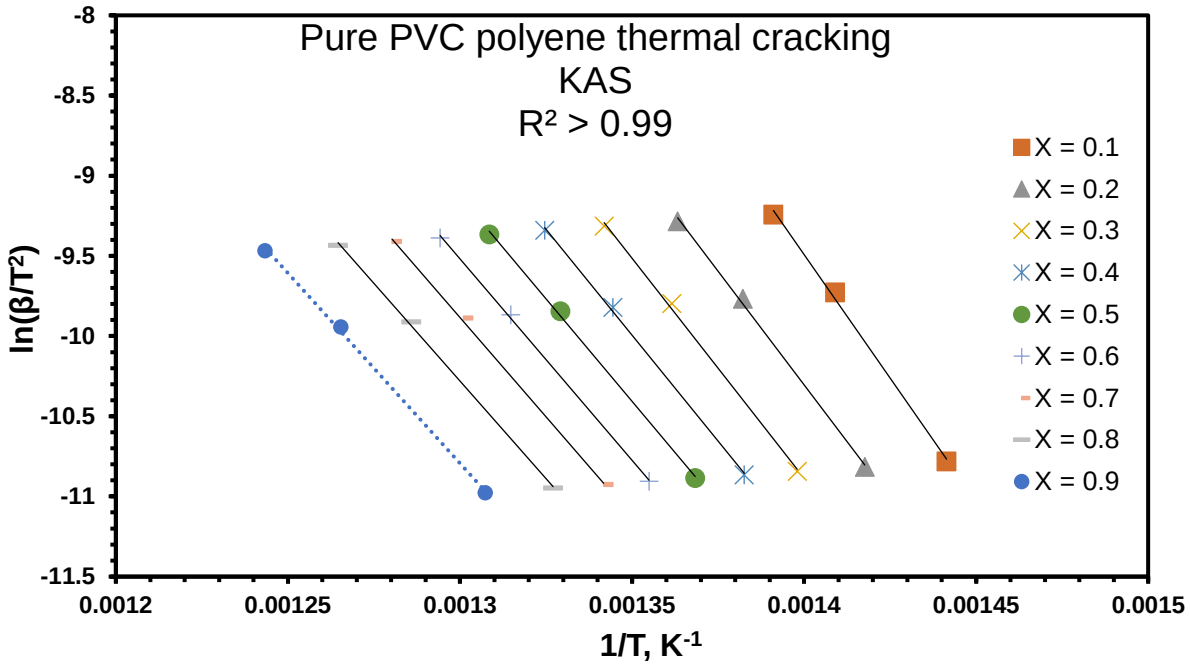
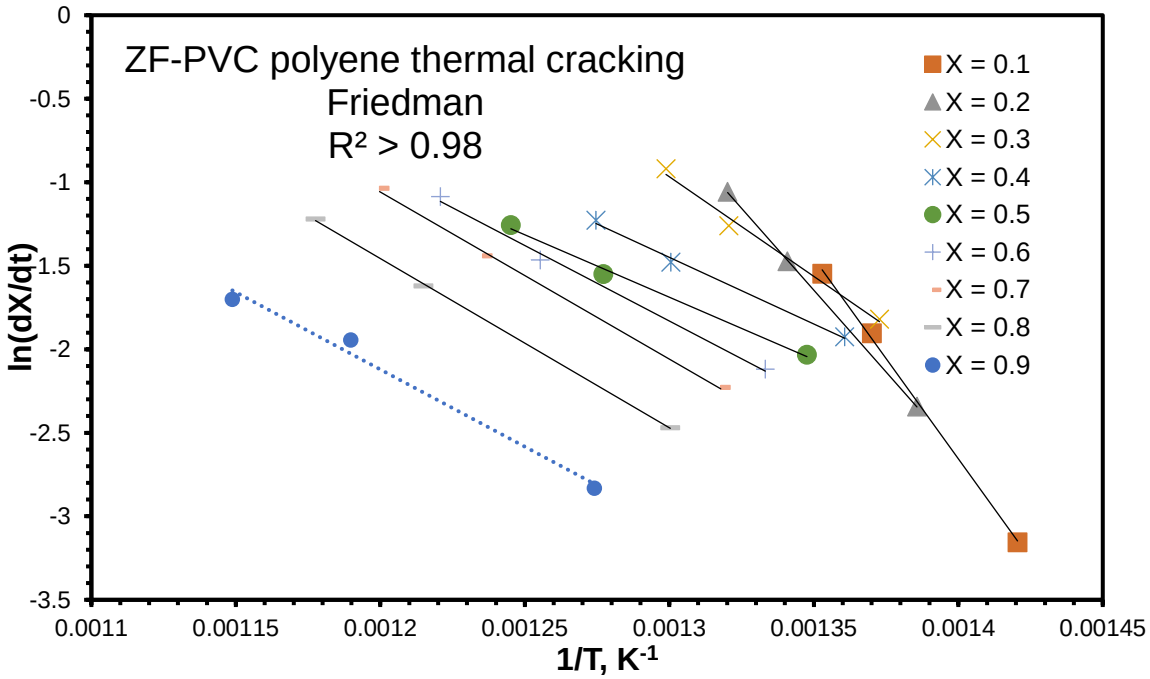


Figure S3: Data fitting using Friedman and KAS methods for the extraction of the activation energy for the de-hydrochlorination stage for PVC and ZF-PVC mixture.

3.1.2. Polyene thermal cracking stage




Pure PVC polyene thermal cracking
KAS
R² > 0.99
ln(β/T²)
1/T, K-1
-8
-8.5
-9
-9.5
-10
-10.5
-11
-11.5
0.0012
0.00125
0.0013
0.00135
0.0014
0.00145
0.0015
X = 0.1
X = 0.2
X = 0.3
X = 0.4
X = 0.5
X = 0.6
X = 0.7
X = 0.8
X = 0.9


ZF-PVC polyene thermal cracking
Friedman
R² > 0.98
ln(dX/dt)
1/T, K-1
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
0.0011
0.00115
0.0012
0.00125
0.0013
0.00135
0.0014
0.00145
X = 0.1
X = 0.2
X = 0.3
X = 0.4
X = 0.5
X = 0.6
X = 0.7
X = 0.8
X = 0.9

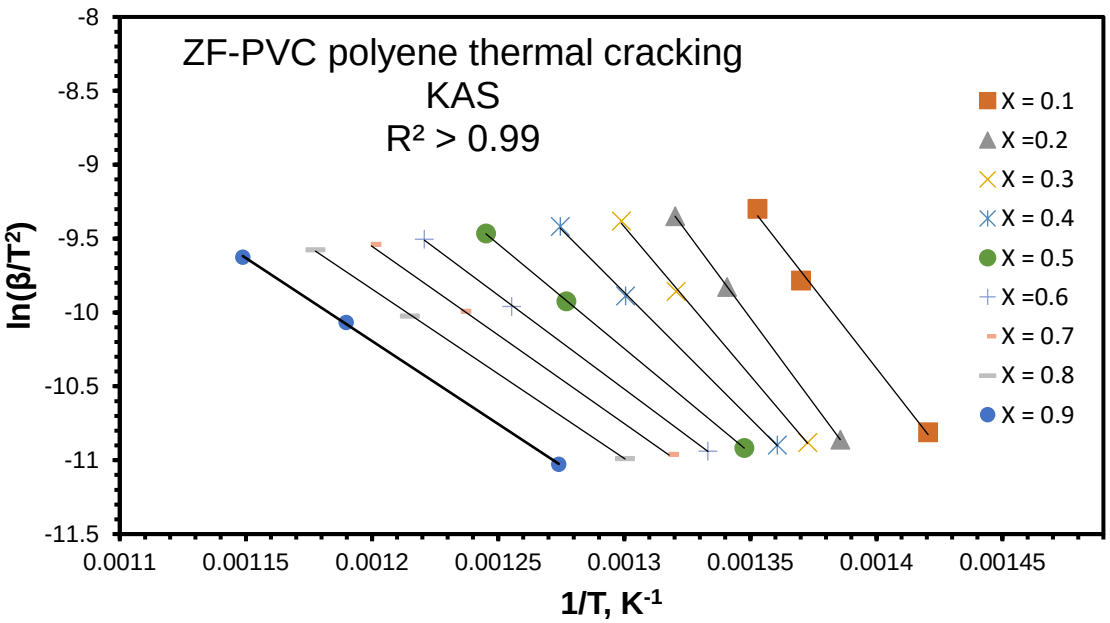
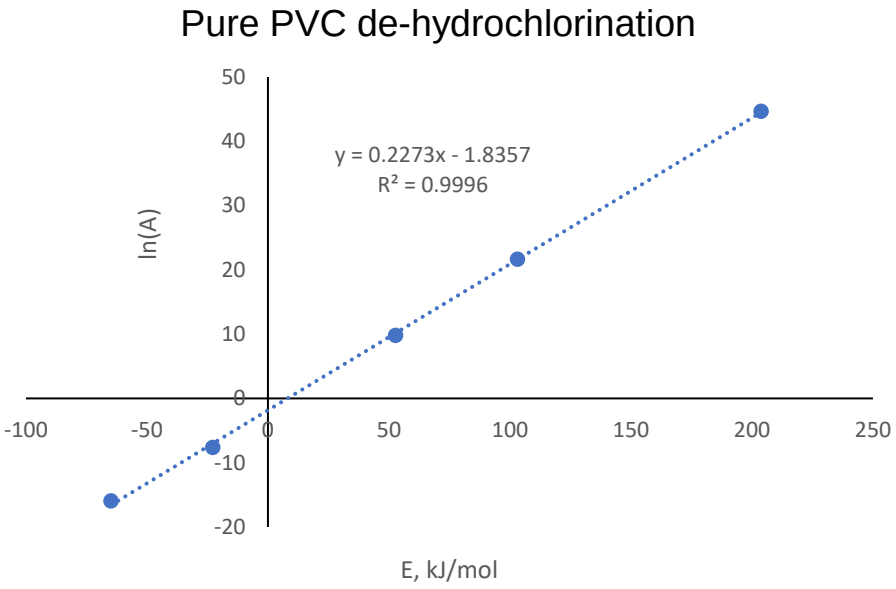
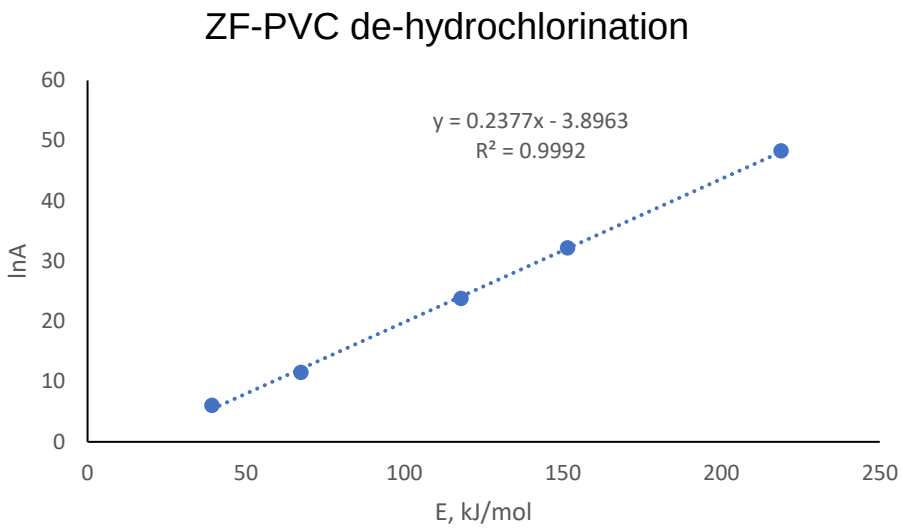
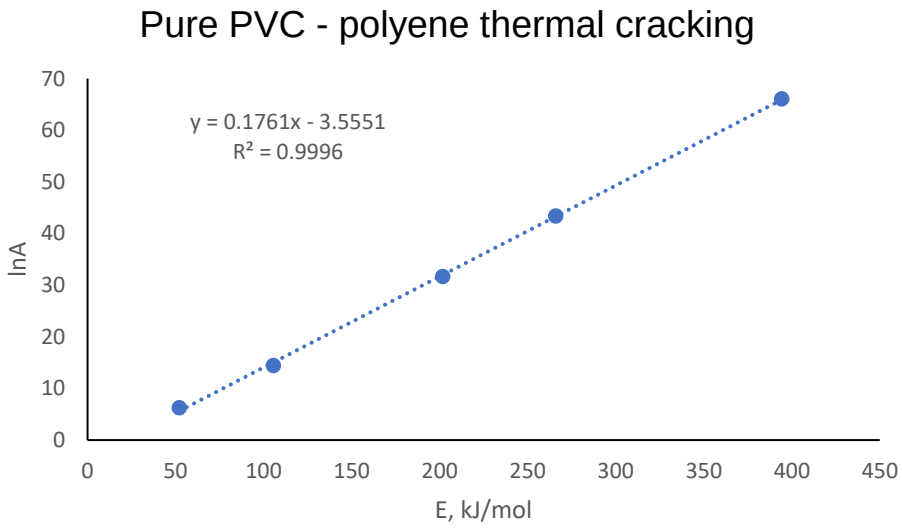


Figure S4: Data fitting using Friedman and KAS methods for the extraction of the activation energy for the polyene thermal cracking stage for PVC and ZF-PVC mixture.

3.2. Compensation charts for the extraction of the frequency factor







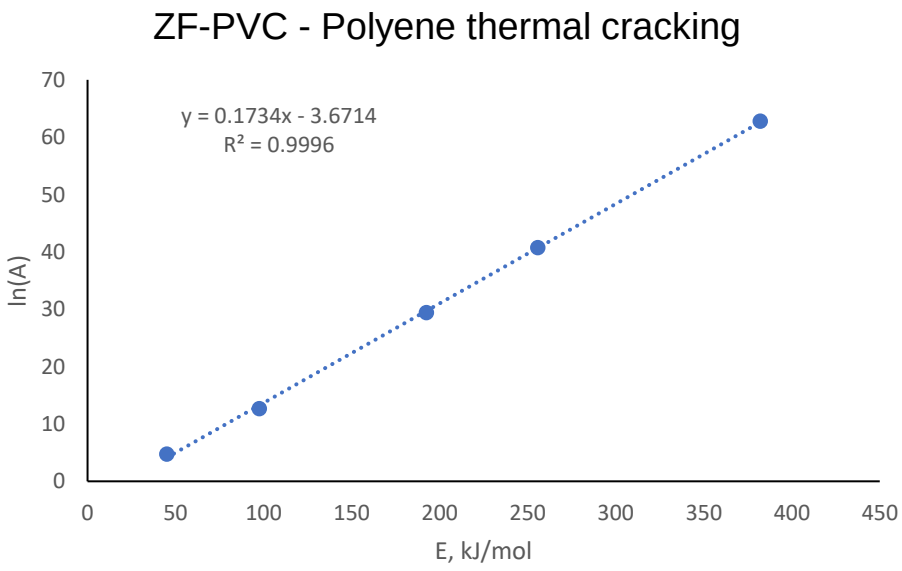
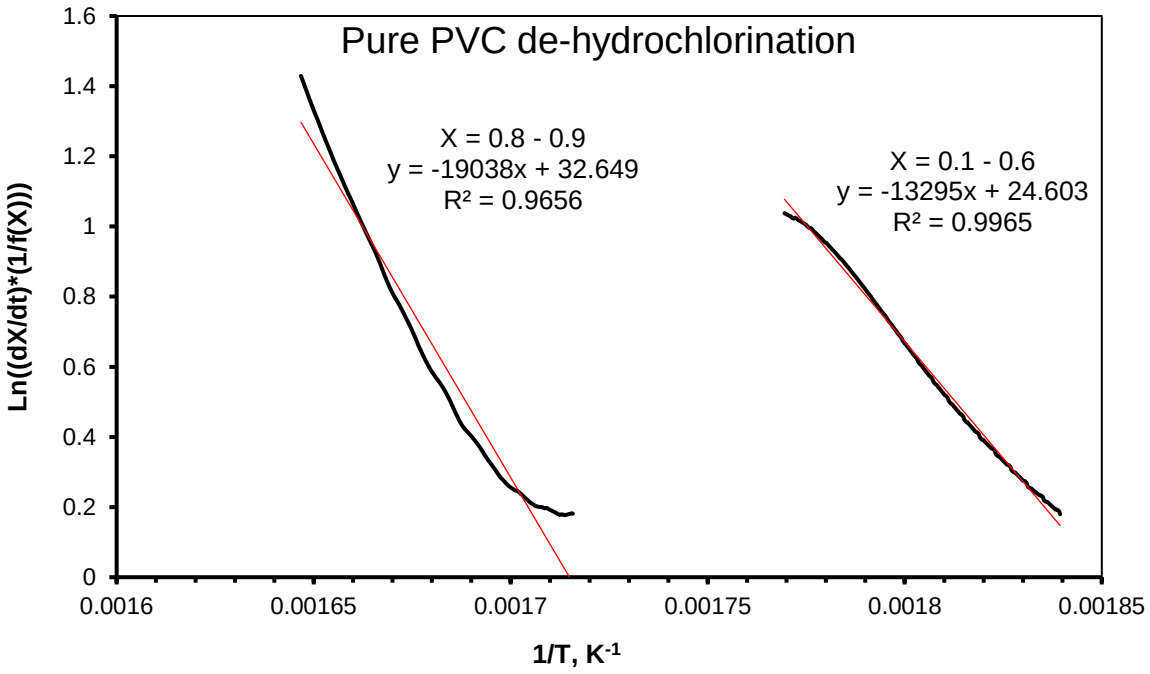
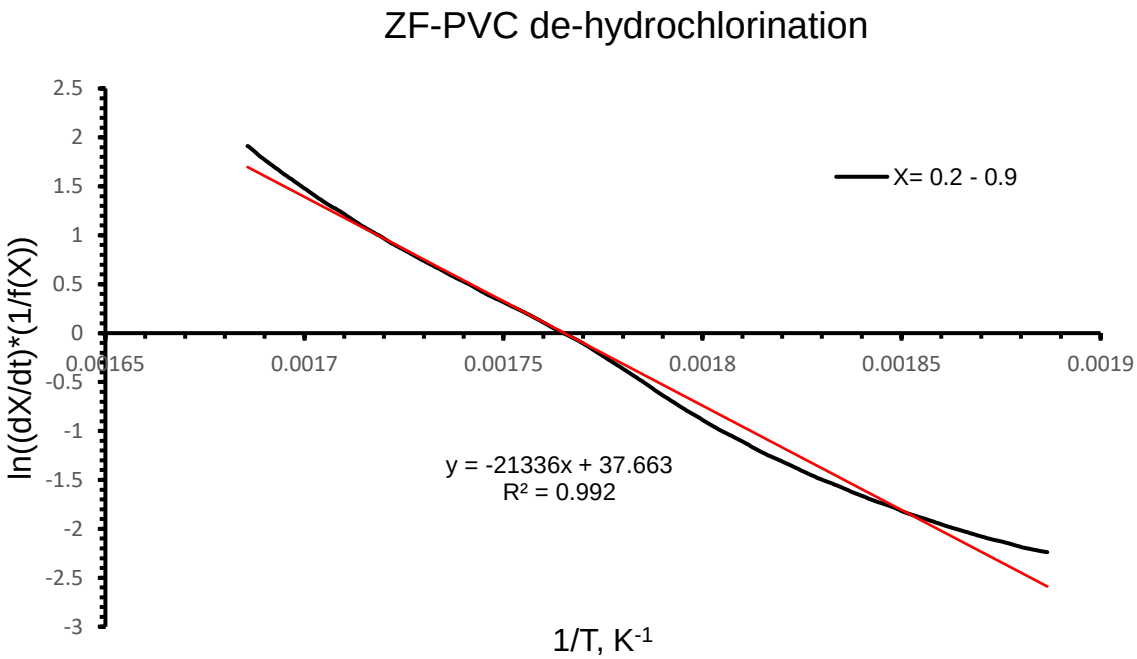


Figure S5: Compensation charts for the extraction of the frequency factor associated with the de-hydrochlorination and polyene thermal cracking stages for both PVC and ZF-PVC mixture.

3.3. Linear data fitting for the extraction of the reaction model





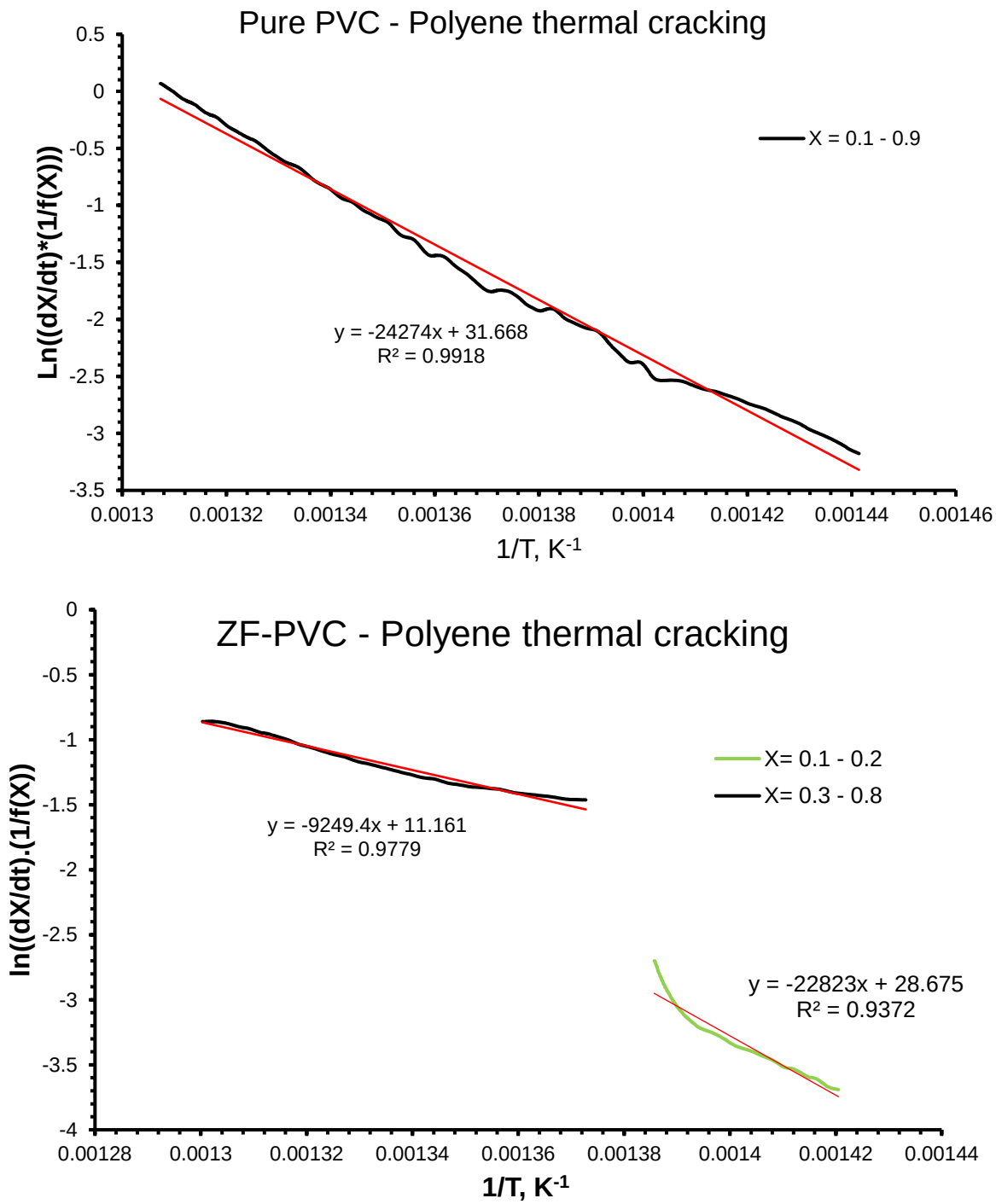


Figure S6: Data fitting for the extraction of the reaction model for the de-hydrochlorination and polyene thermal cracking stages for PVC and ZF-PVC mixture.

4. XRD of $ZnFe_2O_4$ up to 900 °C

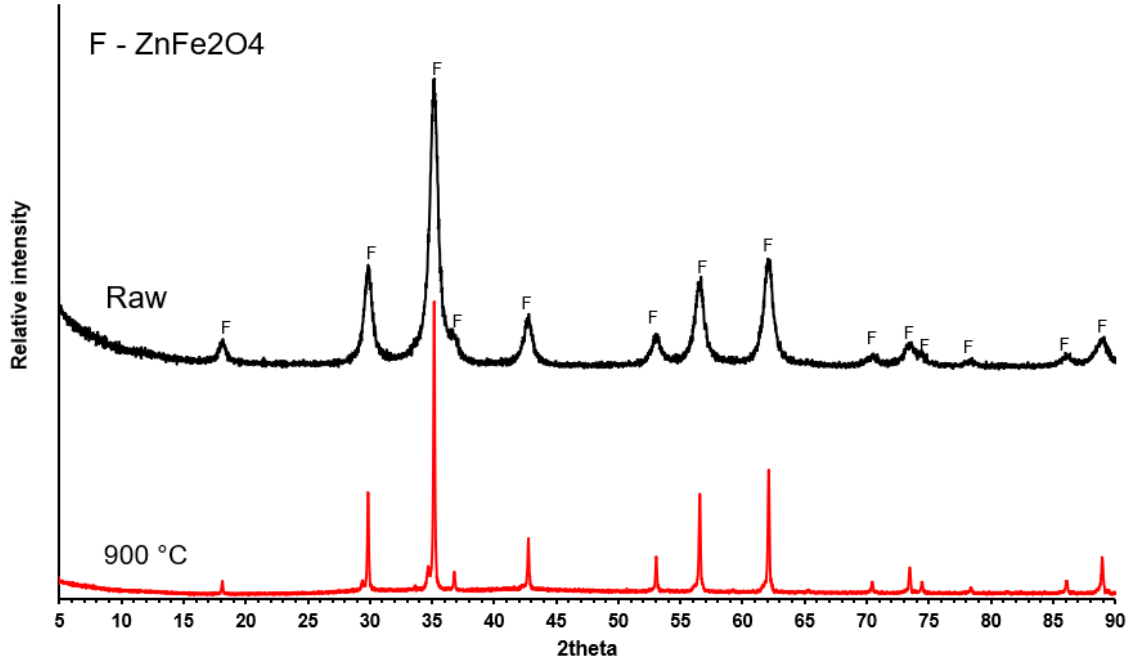


Figure S7: XRD pattern of $ZnFe_2O_4$ at room temperature and at a temperature of 900 °C

5. Mixture homogeneity and TGA repeatability

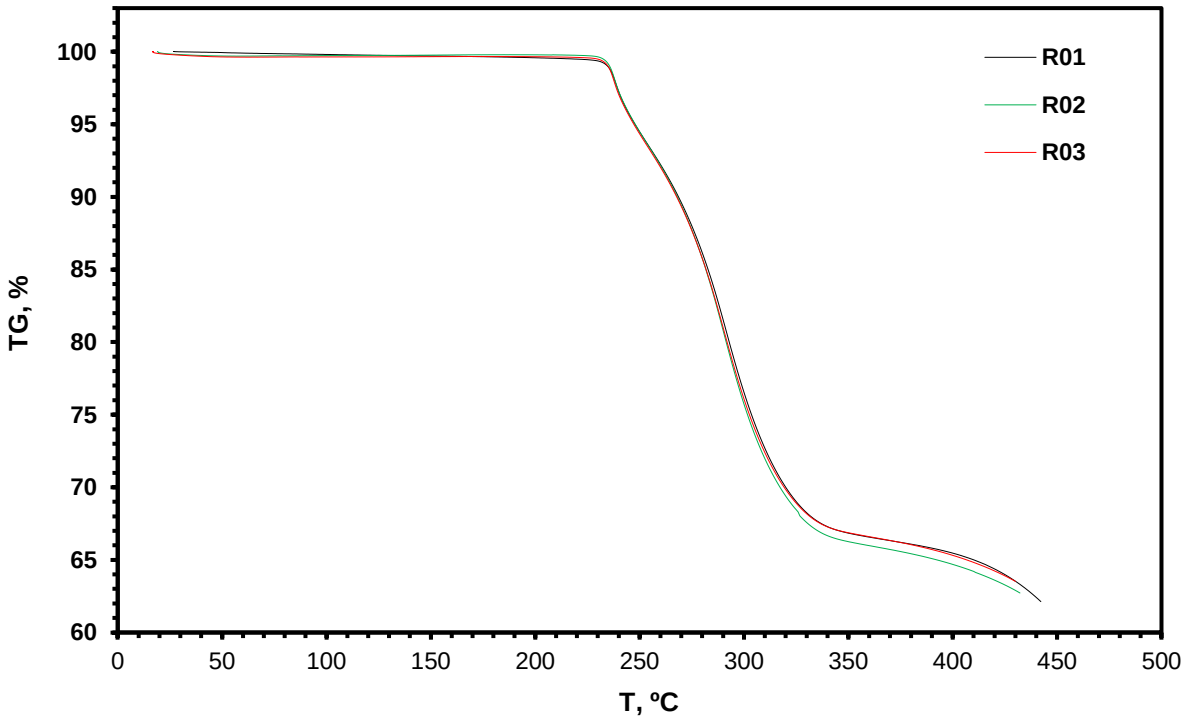


Figure S8: TGA repeats for the de-hydrochlorination stage of ZF-PVC mixture at a heating rate of 10 °C/min and under a nitrogen flow of 100 mL/min.