TÉCNICO LISBOA

CQE Química Estrutural

Low Temperature Thermal Energy Storage

Insights into odd-even n-alkane systems

Maria C.M. Sequeira, **Bernardo A. Nogueira**, **Timur Nikitin**, **Fernando J.P. Caetano**, **Hermínio P. Diogo**, **João M.N.A. Fareleira**, **Rui Fausto**

IATP 2024 Boulder

UNIVERSIDADE AbERTA www.uab.pt

IATP Meeting 2024, Boulder, USA, June 23rd, 2024

Contents

Overview

PCM systems for TES at low T

Cold Storage and Transportation

Phase Equilibrium Studies

n – Alkanes
n – alkyl adipates

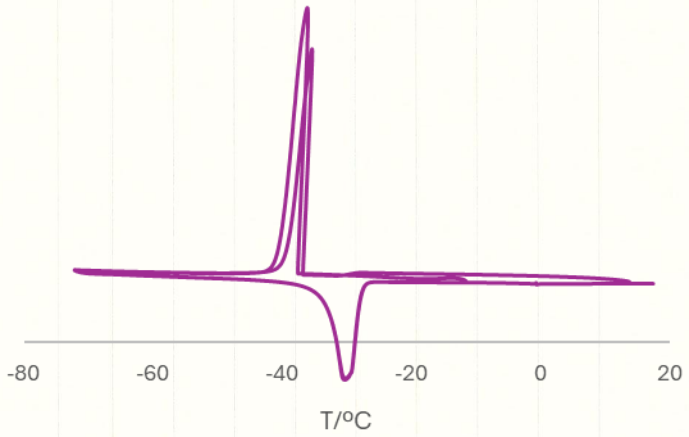
4 different alkane systems

Odd and Even alkyl chains

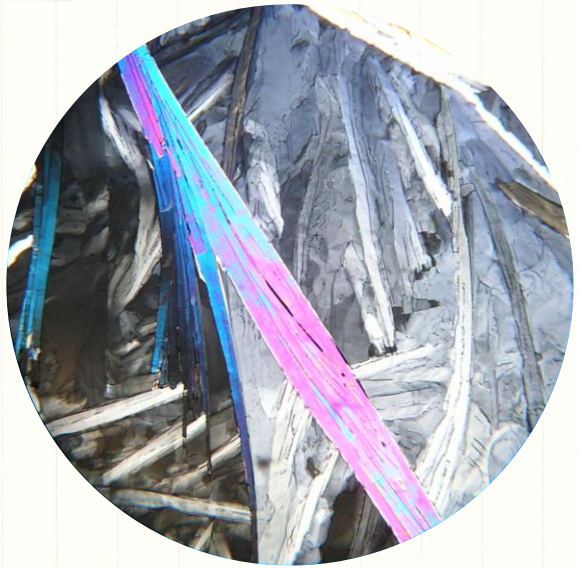
Good potential as PCMs for low T

Experimental Work

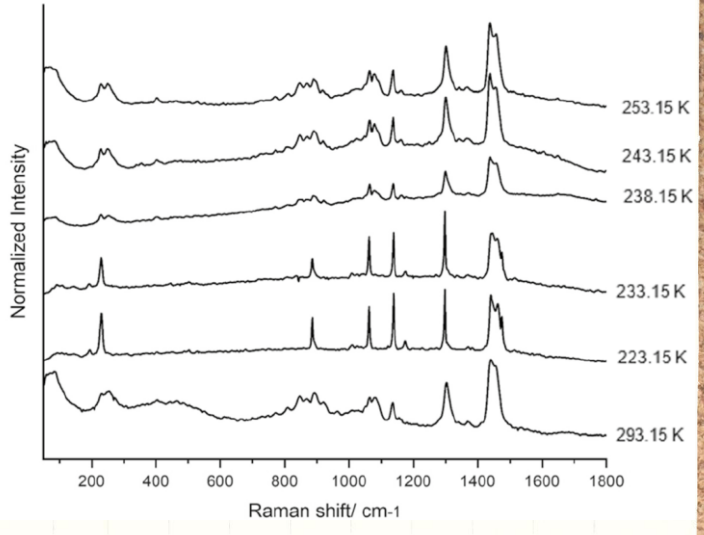
1 Differential Scanning Calorimetry (DSC)



2 Hot Stage Microscopy (HSM)



3 Raman Spectroscopy



1 Differential Scanning Calorimetry (DSC)

$C_{10} + C_{12}$

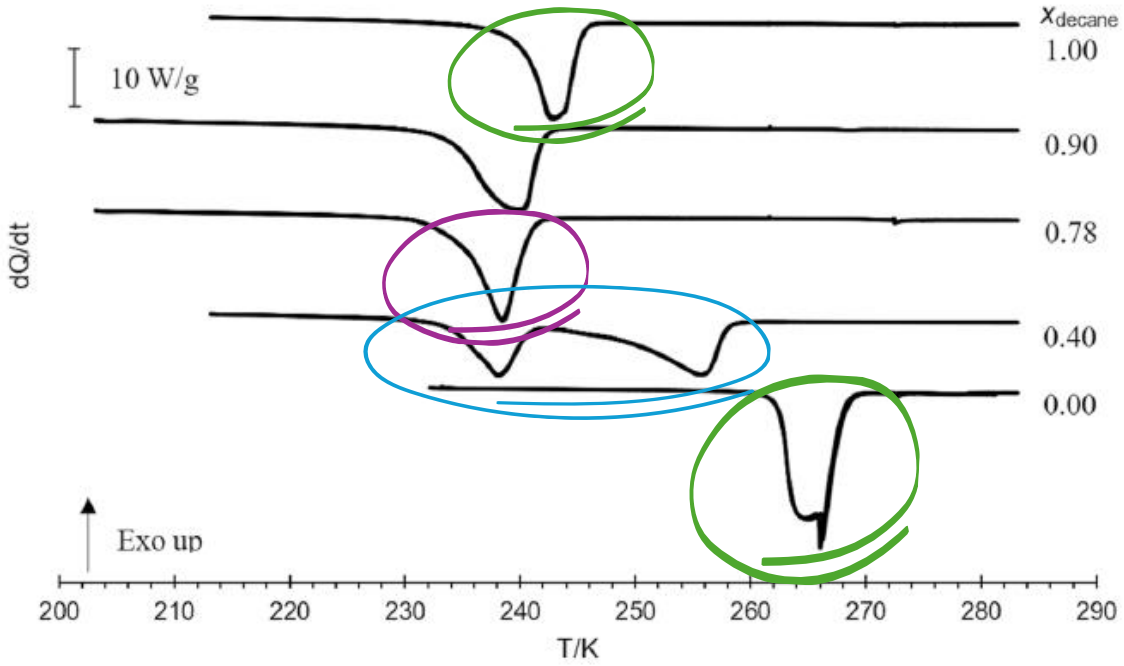


Fig. 1 – DSC heating curves of pure *n*-decane, *n*-dodecane, and of selected binary mixtures, with octane molar fraction x_{decane}.

$C_9 + C_{11}$

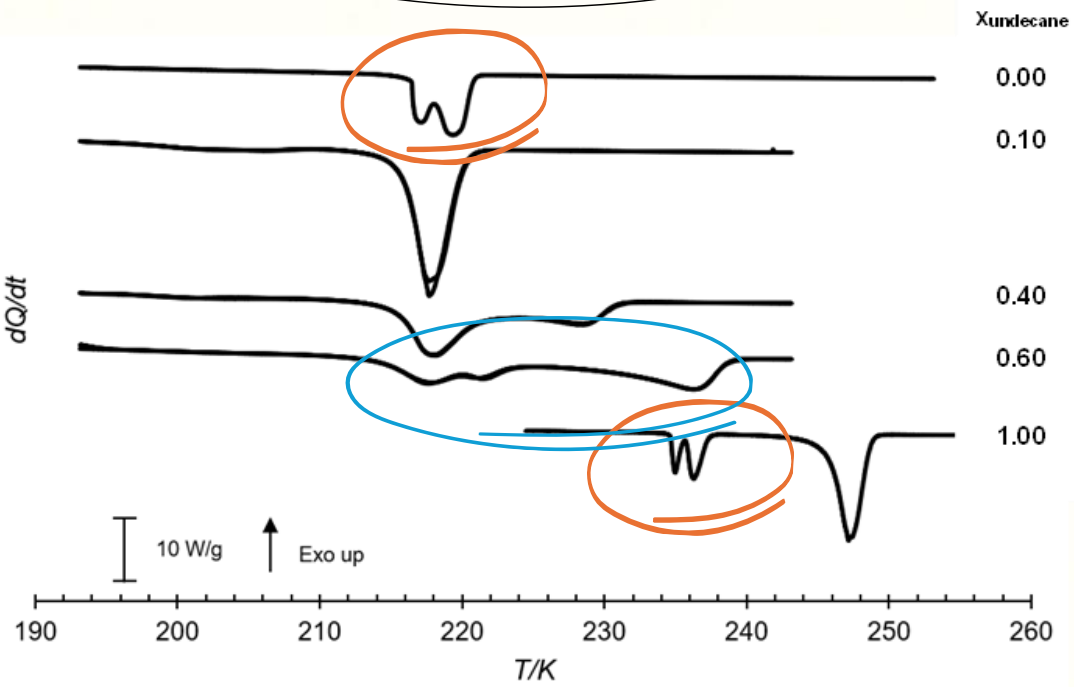
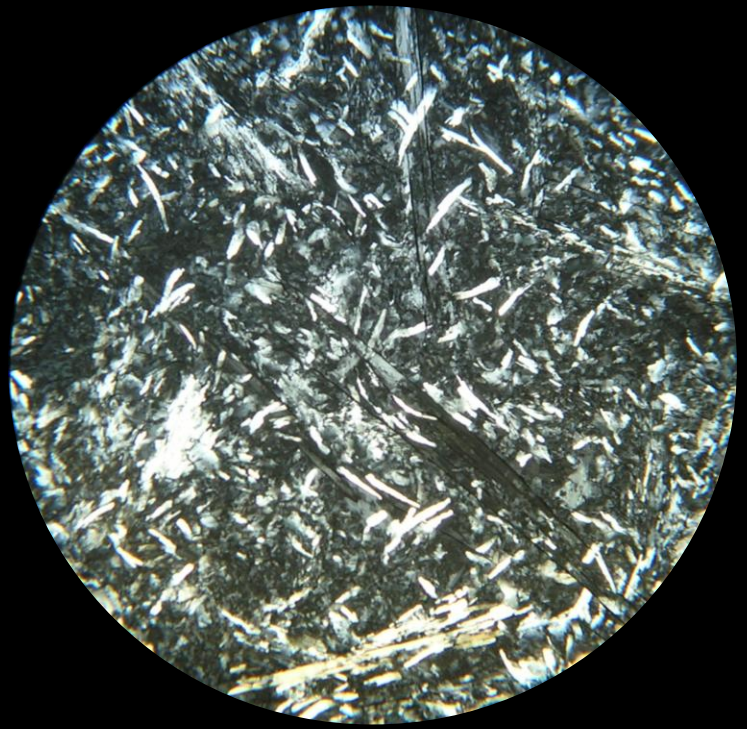


Fig. 2 – DSC heating curves of pure *n*-nonane, *n*-undecane, and of selected binary mixtures, with undecane molar fraction $x_{undecane}$.

2 Hot Stage Microscopy (HSM)

193.15 K



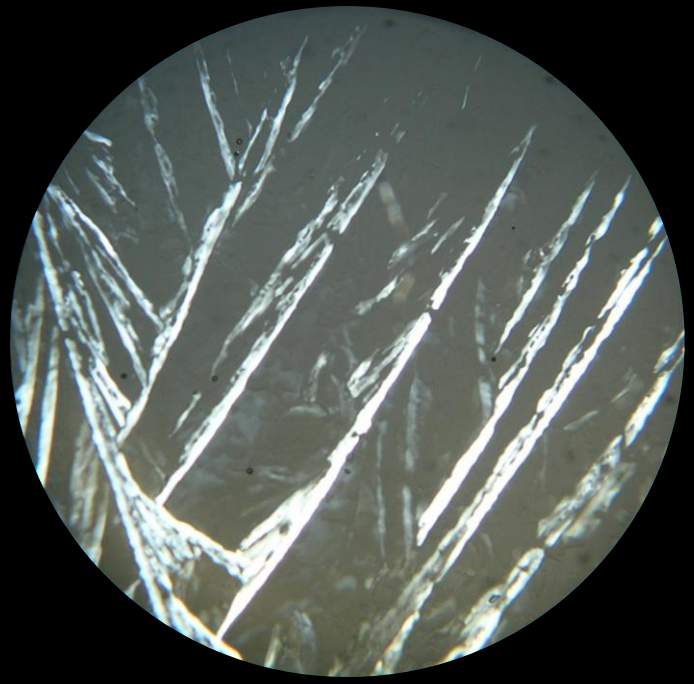
215.65 K

Fig. 3 – HSM images for the polymorphic transition of pure *n*-C_9 .

2 Hot Stage Microscopy (HSM)

193.15 K

240.15 K



245.15 K

Fig. 4 – HSM images for the phase transition of pure *n*-C_{11} .

3

Raman Spectroscopy

Pure compounds

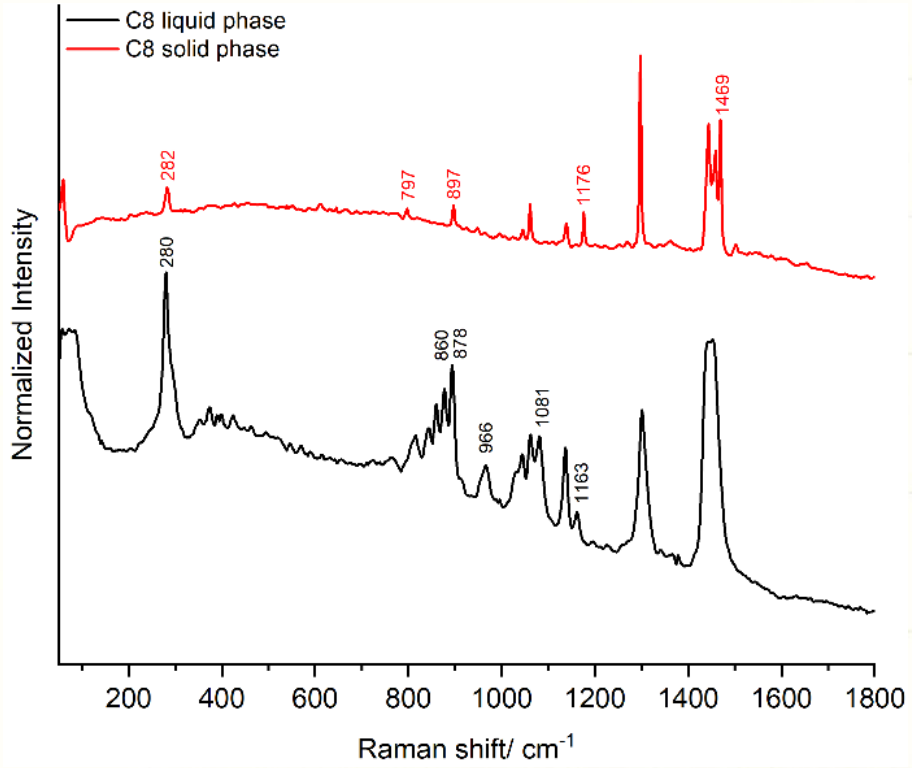


Fig. 5 – Raman spectra of solid and liquid phases samples of *n*-C_8

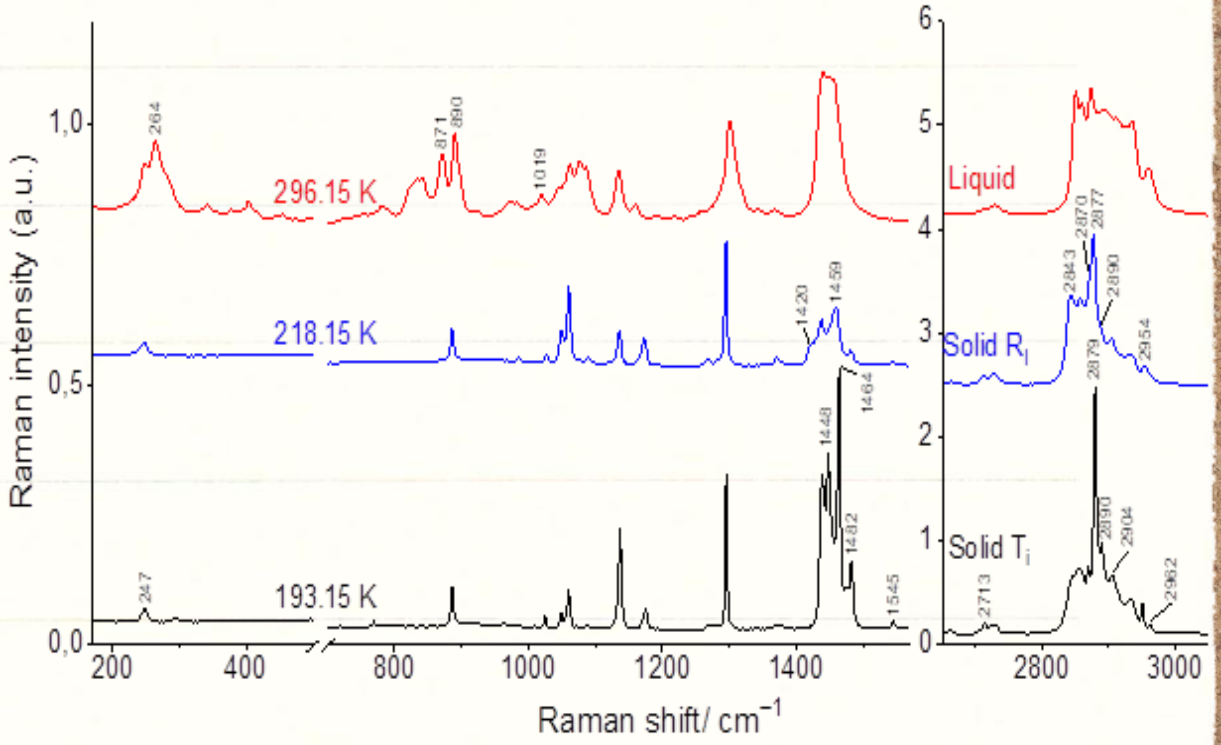


Fig. 6 – Raman spectra of solid and liquid phases samples of *n*-C_9

3 Raman Spectroscopy

Binary Mixtures

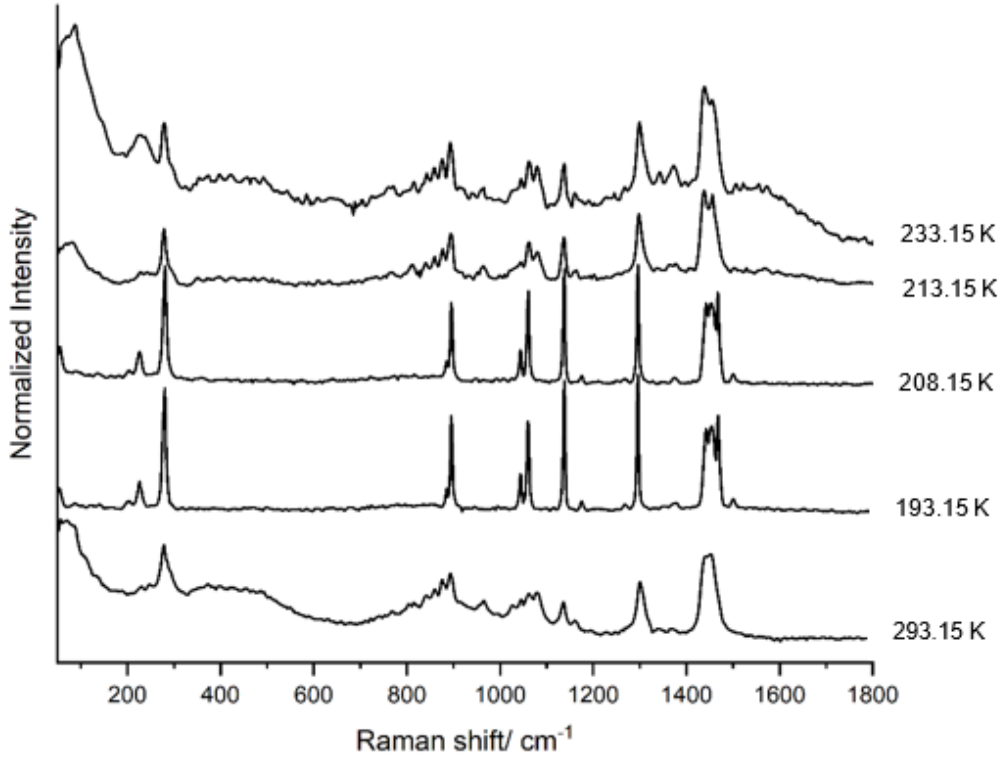


Fig. 7 - Temperature-variation Raman spectra for the eutectic mixture of the C_8/C_{10} binary system.

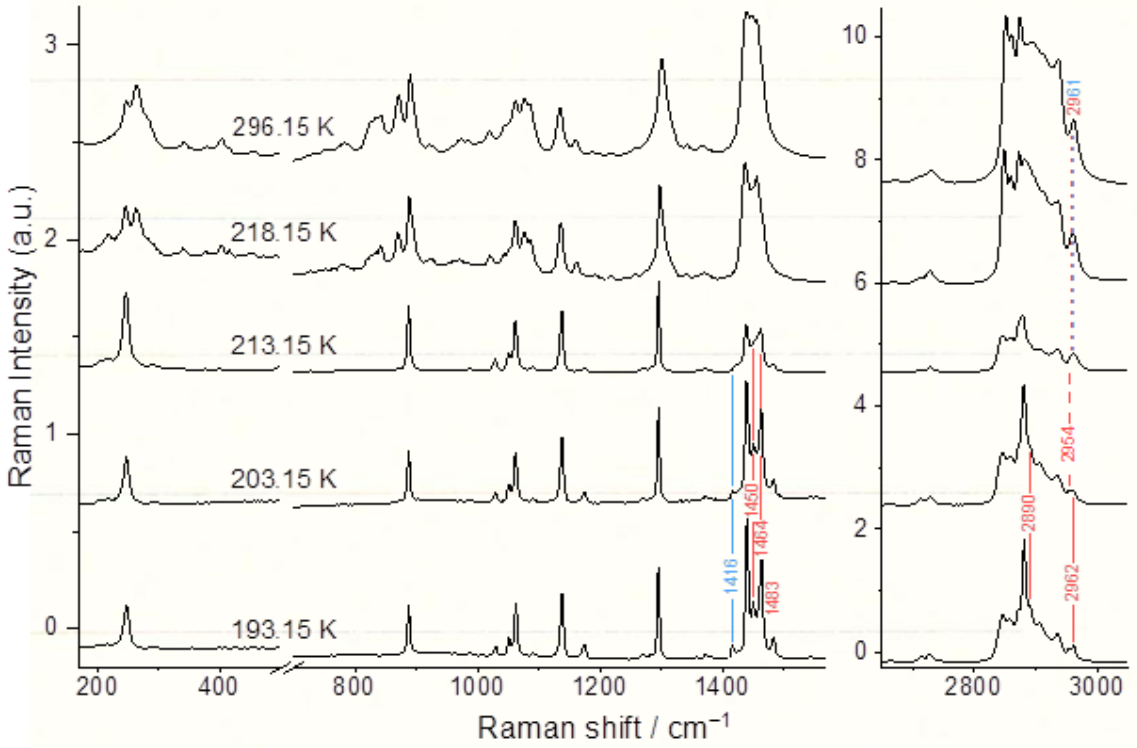


Fig. 8 - Temperature-variation Raman spectra for the congruent melting mixture of the C_9/C_{11} binary system.

Binary Phase Diagrams

$C_8 + C_{10}$

$C_{10} + C_{12}$

$C_9 + C_{11}$

$C_9 + C_{10}$

Binary Phase Diagrams

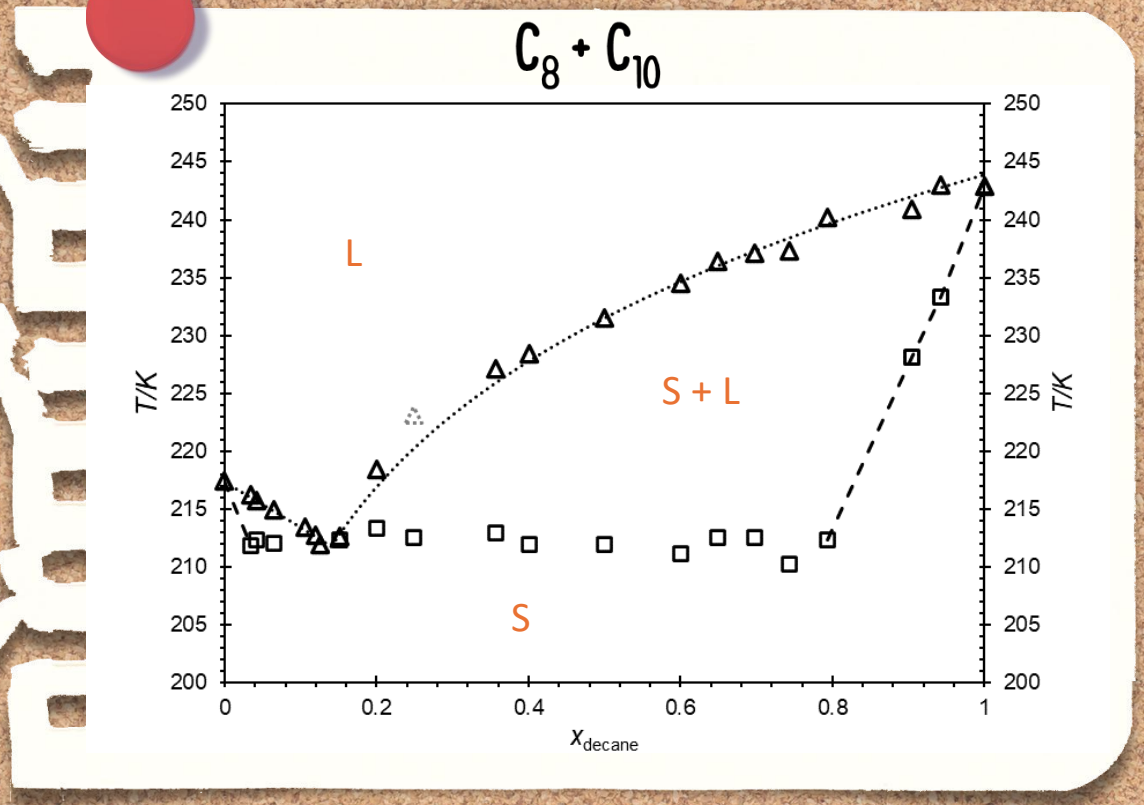


Fig. 9 - Binary solid-liquid phase diagram of *n*-C_8 and *n*-C_{10}.

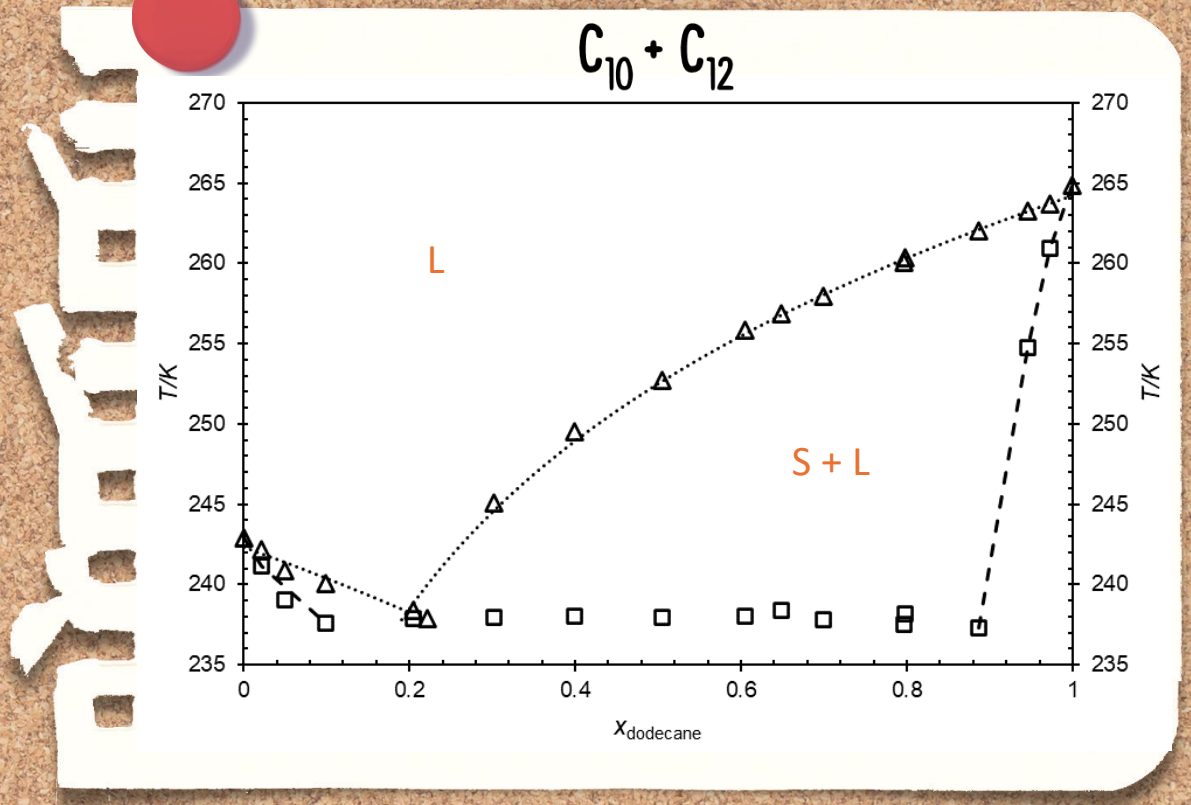


Fig. 10 - Binary solid-liquid phase diagram of *n*-C_{10} and *n*-C_{11}.

Results published in the International Journal of Thermophysics. DOI: 10.1007/s10765-023-03317-9

Binary Phase Diagrams

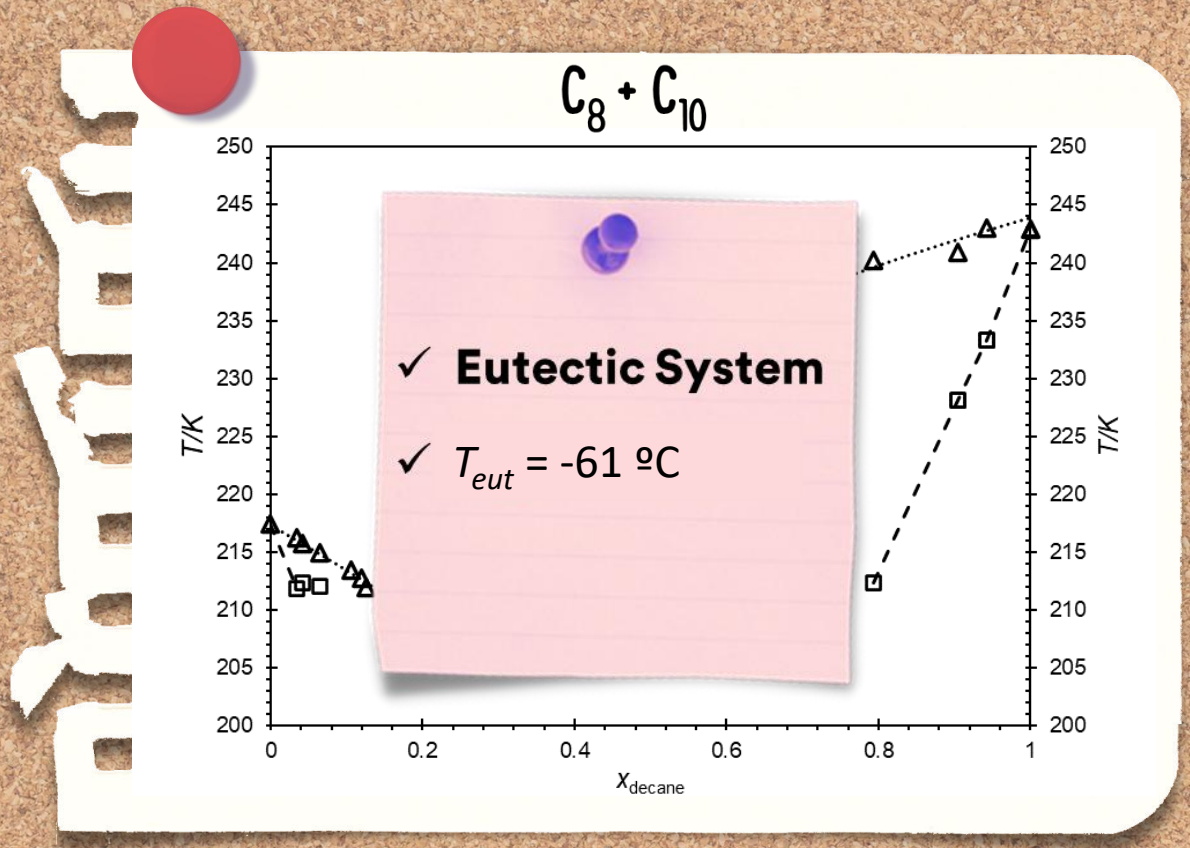


Fig. 9 - Binary solid-liquid phase diagram of *n*-C_8 and *n*-C_{10}.

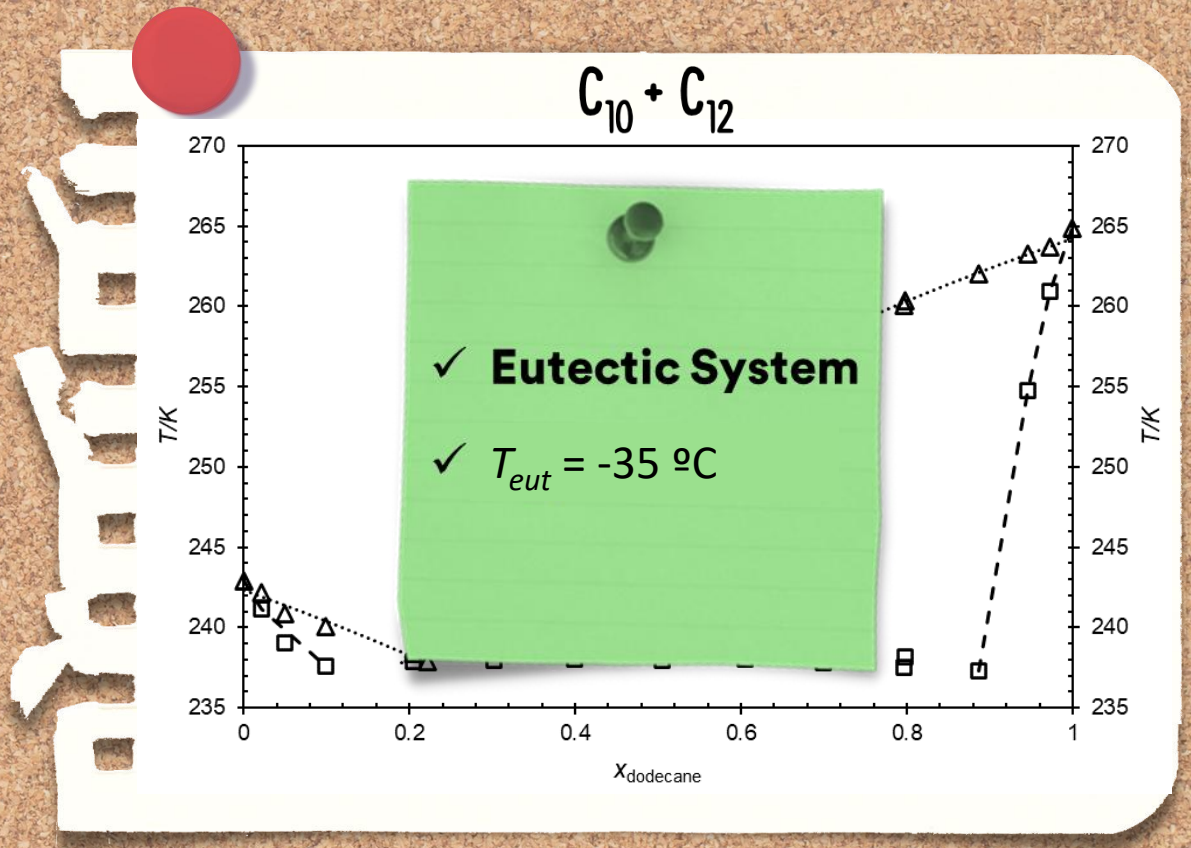


Fig. 10 - Binary solid-liquid phase diagram of *n*-C_{10} and *n*-C_{11}.

Results published in the International Journal of Thermophysics. DOI: 10.1007/s10765-023-03317-9

IATP Meeting 2024, Boulder, USA, June 23rd, 2024

Binary Phase Diagrams

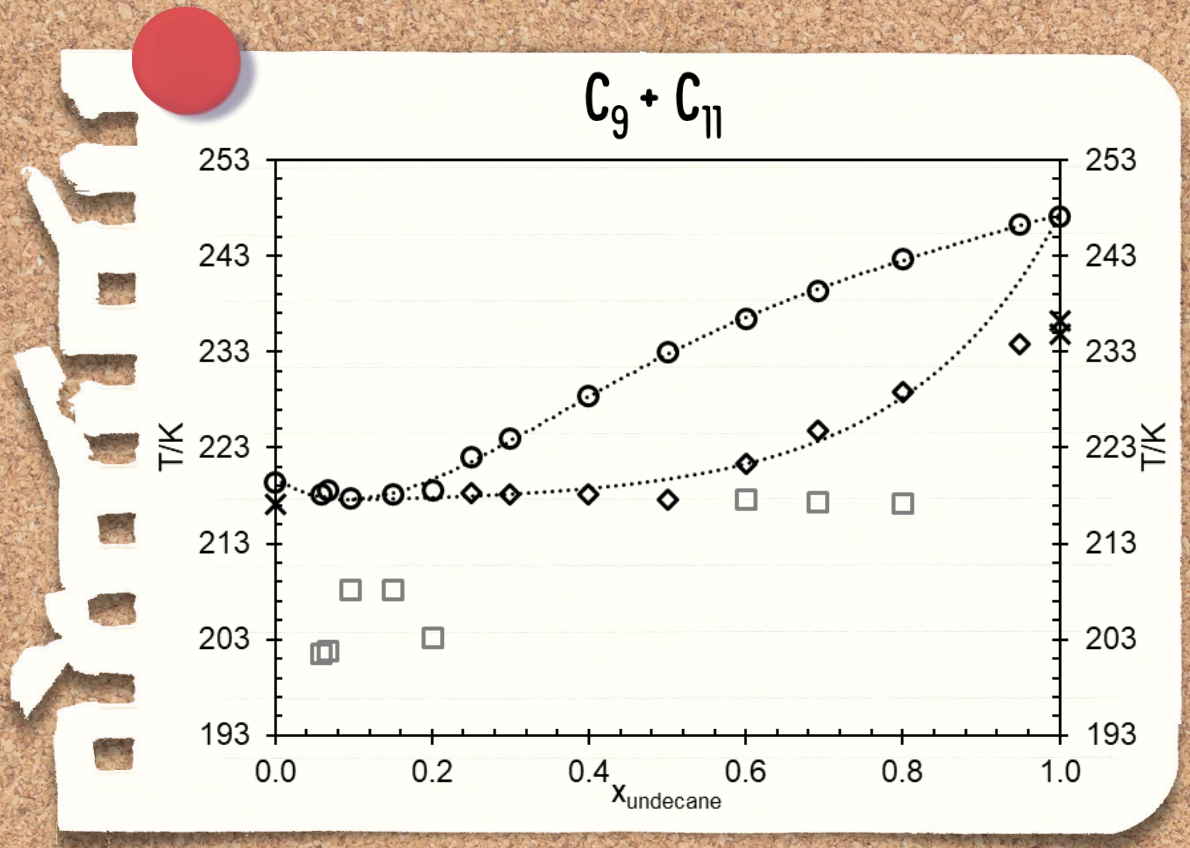


Fig. 11 – Binary solid-liquid phase diagram of *n*-C_9 and *n*-C_{11} (submitted to the International Journal of Thermophysics)

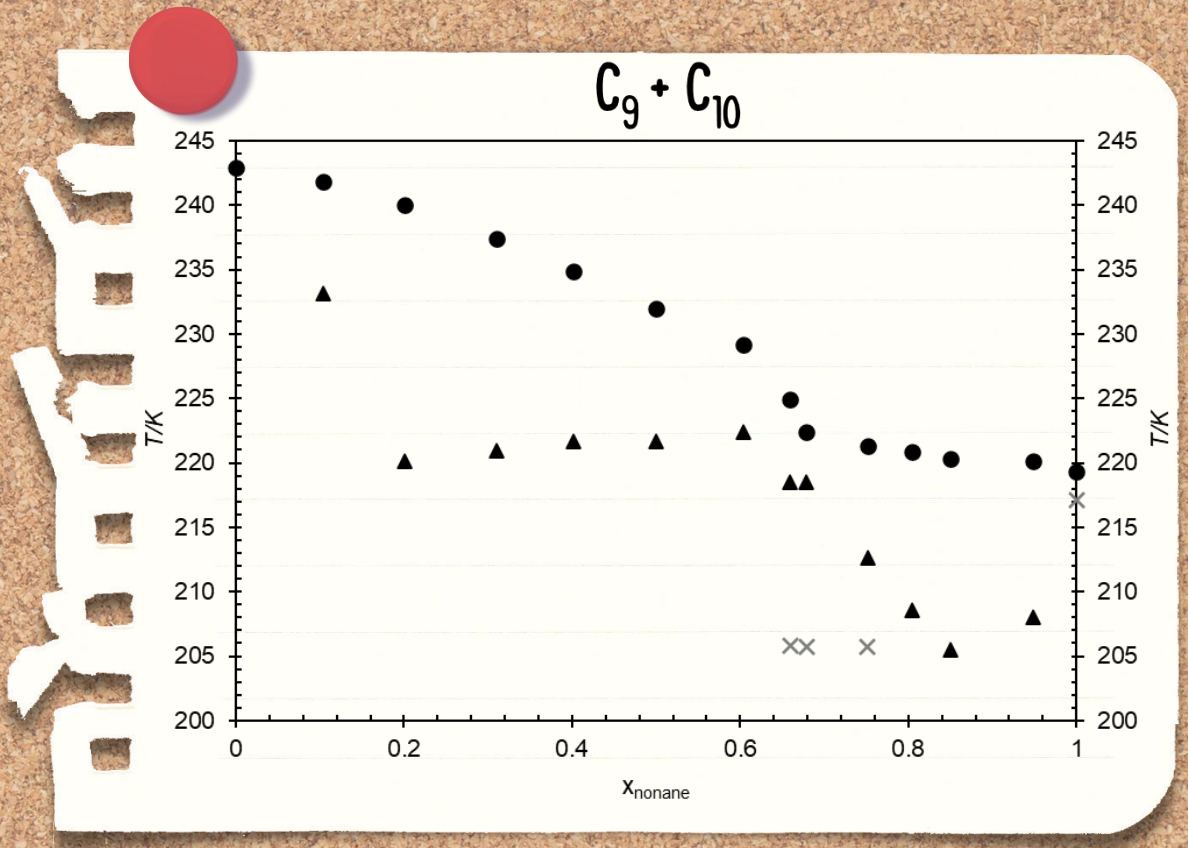


Fig. 12 – Preliminary binary solid-liquid phase diagram of *n*-C_9 and *n*-C_{10}.

Binary Phase Diagrams

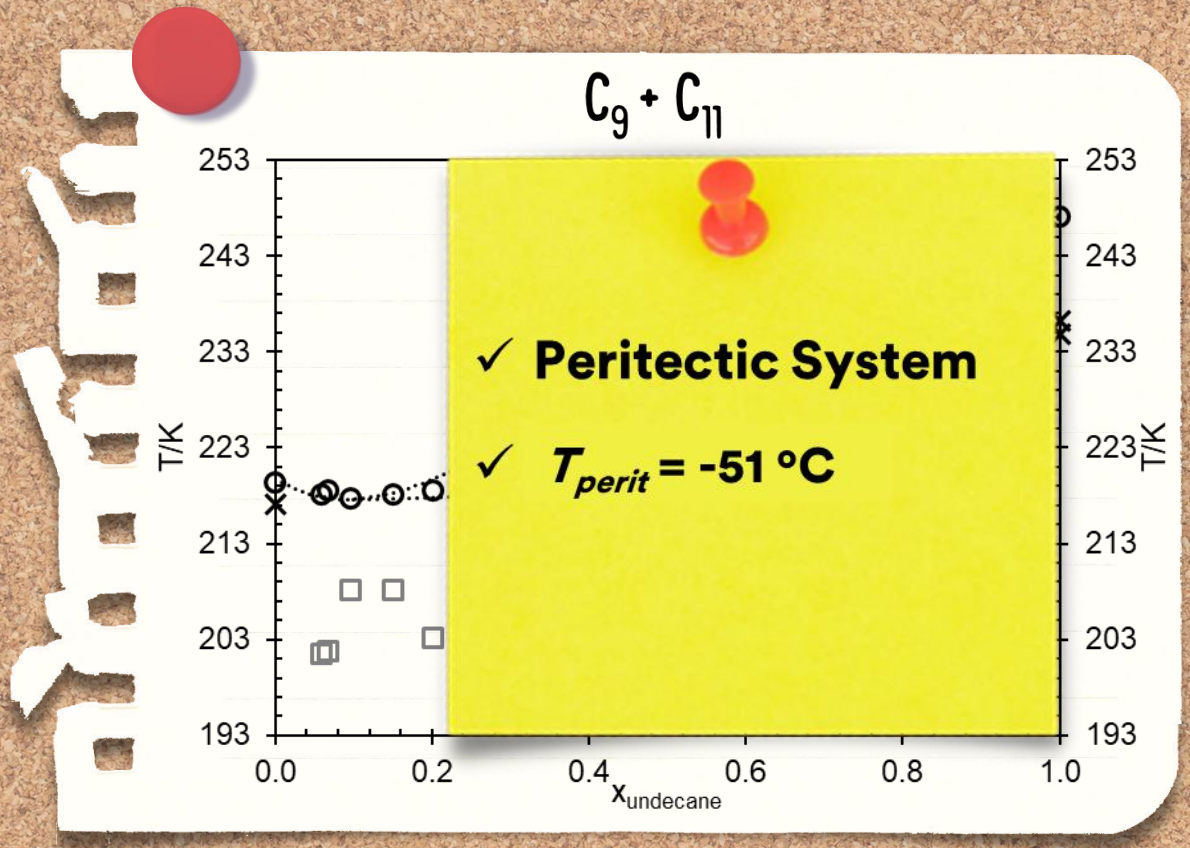


Fig. 11 – Binary solid-liquid phase diagram of *n*-C_9 and *n*-C_{11} (submitted to the International Journal of Thermophysics)

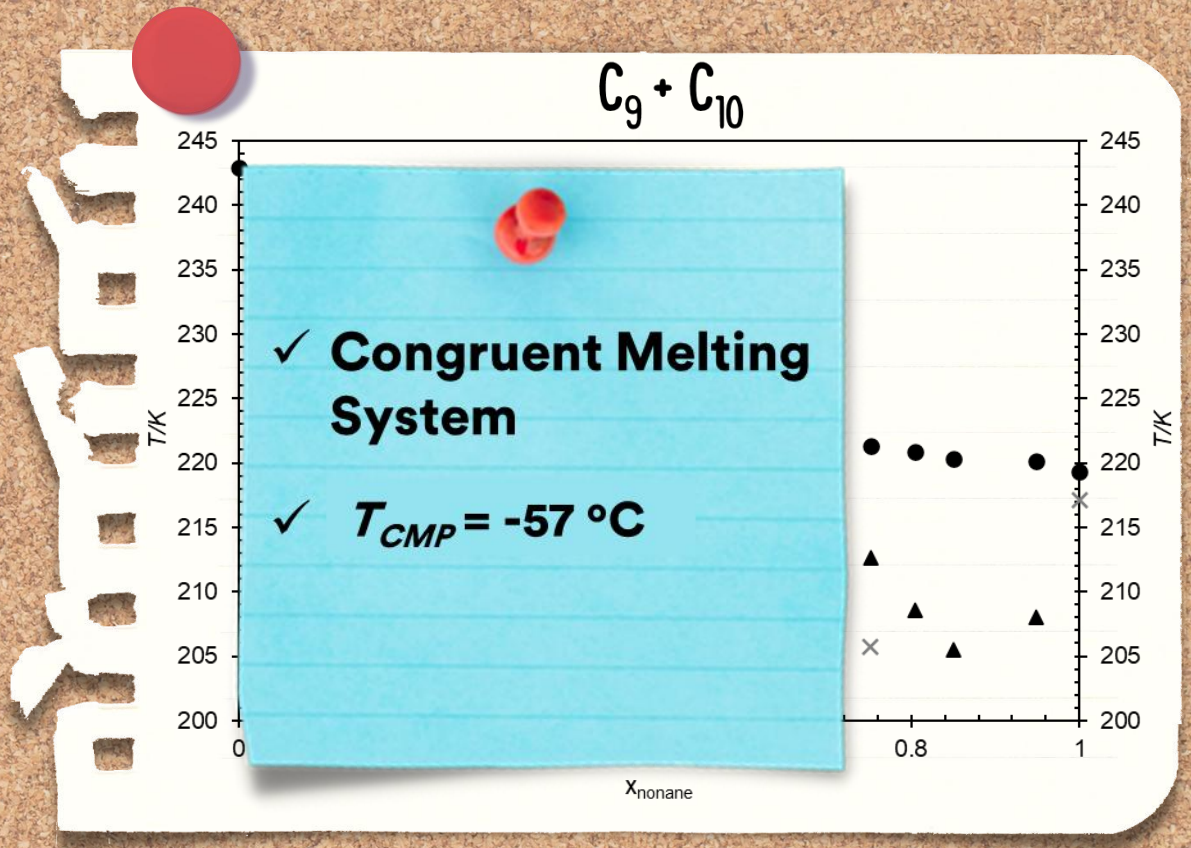


Fig. 12 – Preliminary binary solid-liquid phase diagram of *n*-C_9 and *n*-C_{10}.


Odd-even effects
Grouping of characteristics
Polymorphism
n - Alkanes
Chain size
Phase Equilibrium
Predict the potential as PCMs

Conclusions

Odd-Even effects identified and analyzed

Phase equilibrium studies for odd and even alkanes

3/4 alkane systems with good potential as PCMs for low T

Prediction of the phase equilibrium characteristics

Fulfill the lack of available data on low T PCM systems

Acknowledgements

This work was supported by Fundação para a Ciência e a Tecnologia (FCT), Portugal, Projects UIDB/00100/2020 (https:// doi. org/ 10. 54499/ UIDB/ 00100/ 2020), UIDP/00100/2020 (https://doi. org/ 10. 54499/ UIDP/ 00100/ 2020), and IMS-LA/P/0056/2020UIDB/00100/2020 (https:// doi. org/ 10. 54499/ LA/P/ 0056/ 2020).

M.C.M. Sequeira acknowledges the PhD grant funded by FCT ref. UI/BD/152239/2021 (https://doi.org/10.54499/UI/BD/152239/2021) and the FLAD grant "Papers@USA".

Literature vs Our Results

Even + Even

↓

Eutectic

$C_8 + C_{10}$ / $C_{10} + C_{12}$

Odd + Odd

↓

Congruent Melting

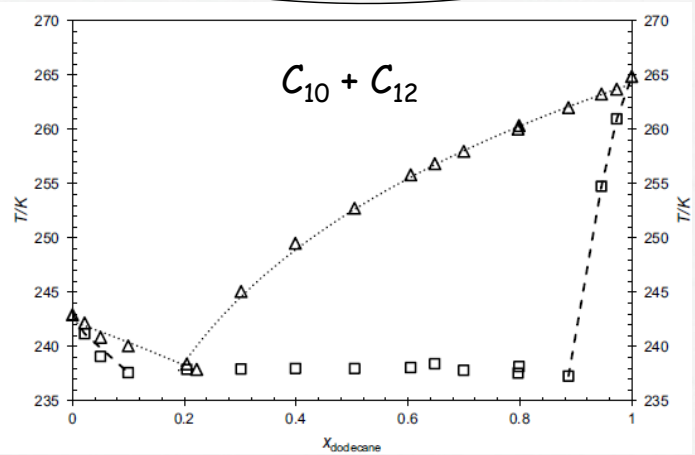
$C_9 + C_{11}$

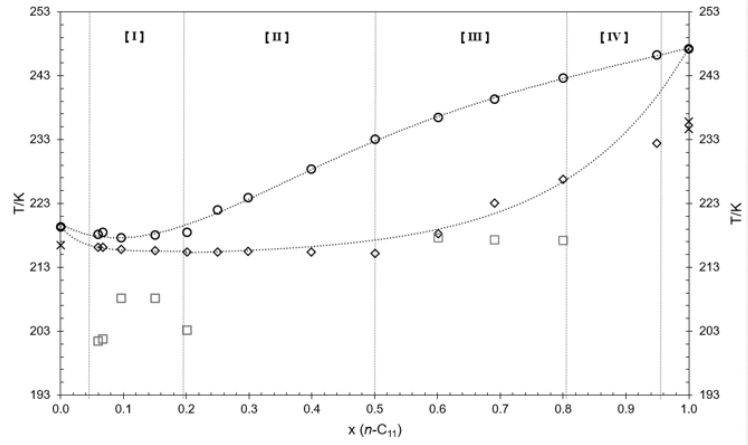
Even + Odd

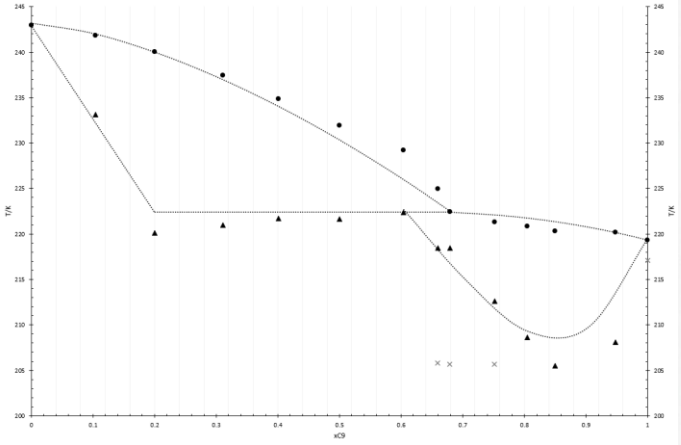
↓

Peritectic

$C_9 + C_{10}$

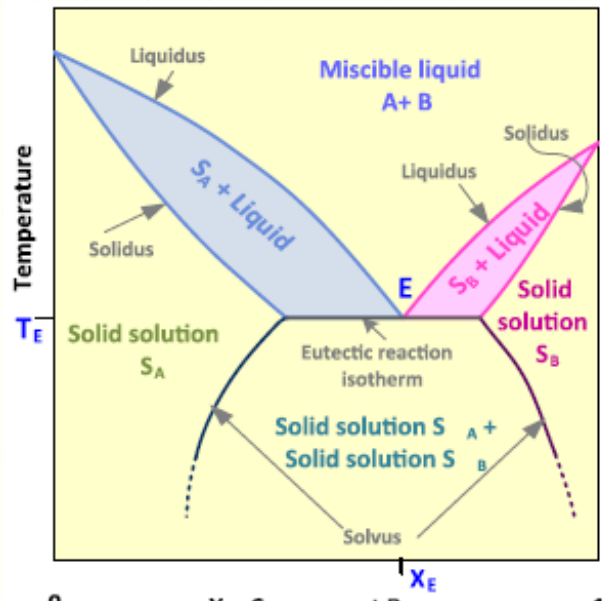




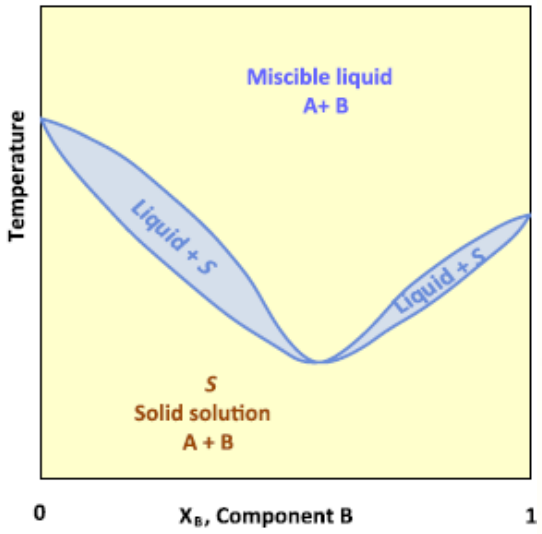


Phase Equilibrium in TES

Eutectic Systems



Congruent Melting Systems



Peritectic Systems