

Cloud-point behavior of polyethylene-butene copolymer in pentane isomers

A. F. Kostko* and A. M. McHugh**

* Department of Physics,
Saint Petersburg National Research University of Information Technologies, Mechanics and
Optics
St. Petersburg 191002, Russia

** Department of Chemical and Life Science Engineering
Virginia Commonwealth University, Richmond, Virginia 23284, USA

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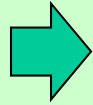
Moscow

Outline

- Motivation: what is the effect of molecular structure of hydrocarbons on their solvent quality in polymer solution?
- Pentane isomers
- High-pressure setup for cloud-point experiment in polymer solutions
- Polyethylene-butene copolymer in pentanes. P - T phase diagram. Solvent quality comparison.
- Conclusion

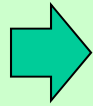
Motivation

Hydrocarbons



conventional
solvents

Hydrocarbon's
properties



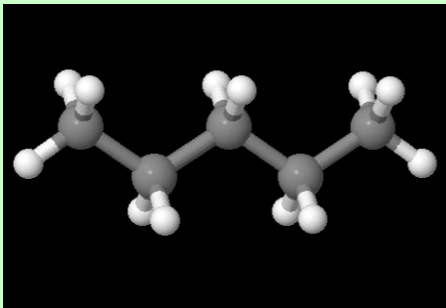
solvent
quality



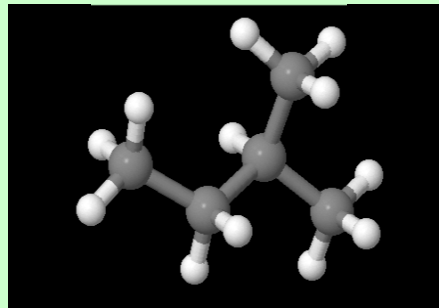
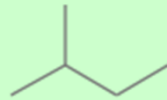
What is the effect of molecular structure on solvent quality in polymer solution?

Pentane isomers

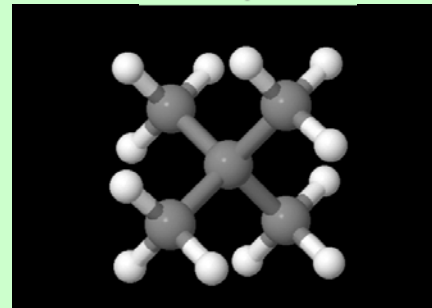
C_5H_{12}
Pentane;
 n-Pentane



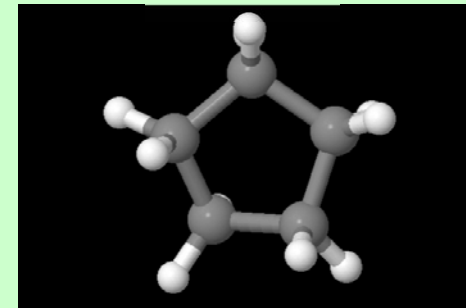
C_5H_{12}
iso-Pentane;
 2-Methylbutane



C_5H_{12}
Neopentane;
 2,2- Dimethylpropane

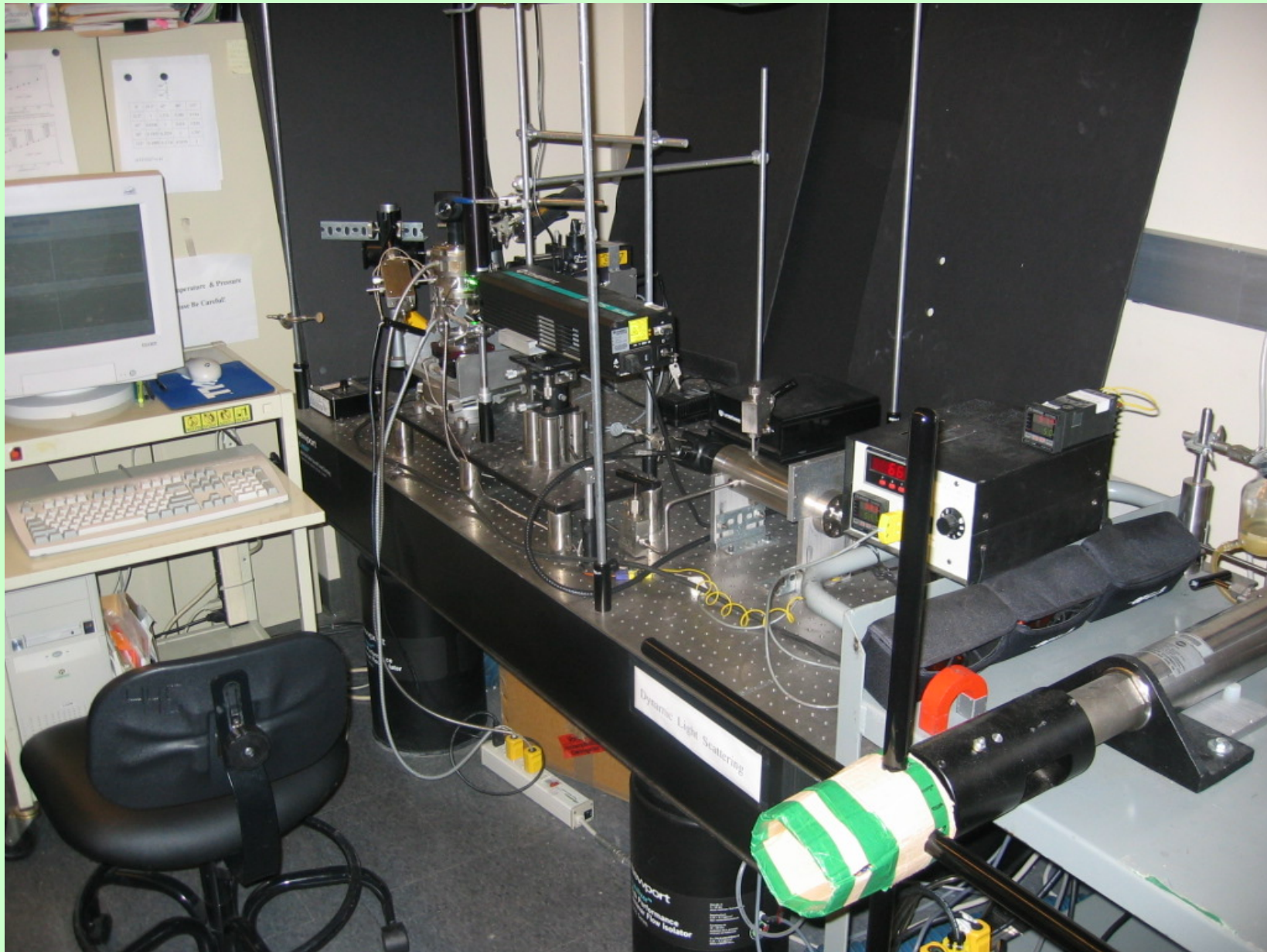


C_5H_{10}
Cyclopentane



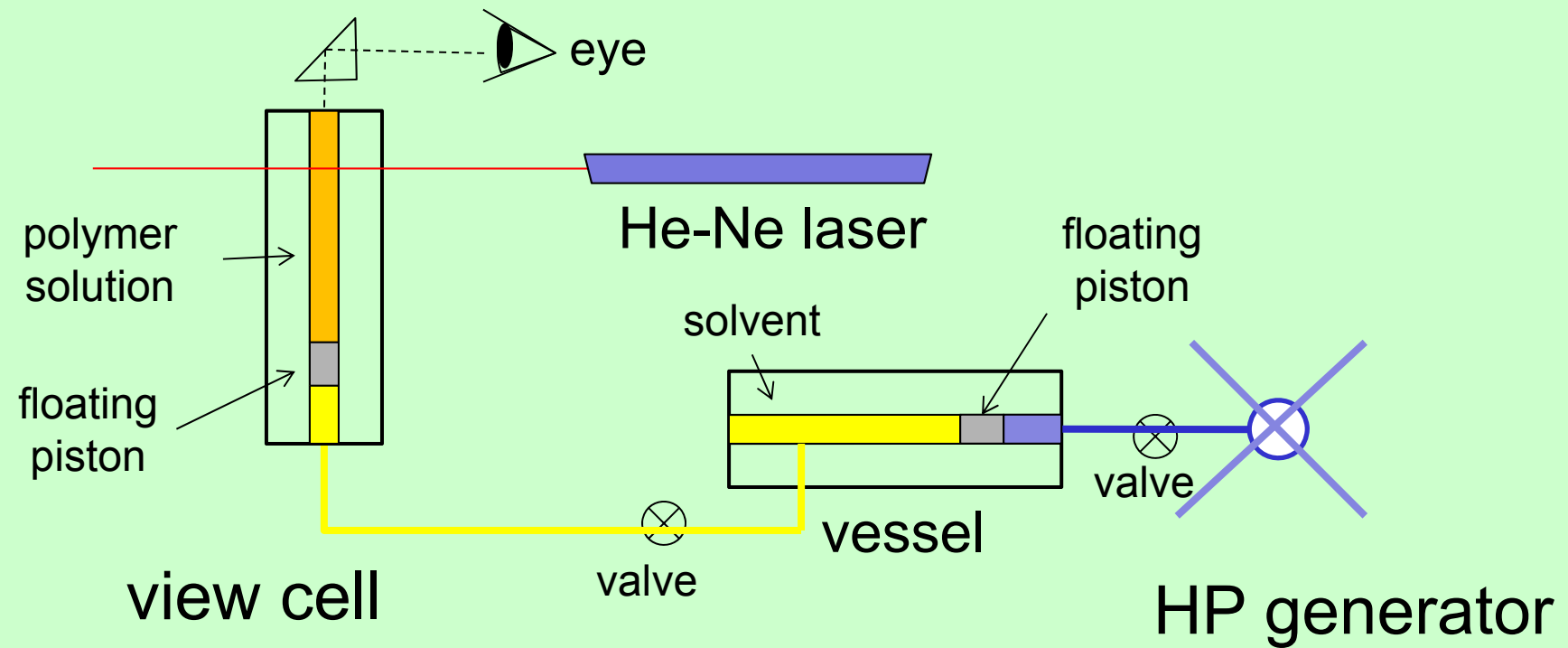
M	72.1488	72.1488	72.1488	70.1329
T_{boil} (K)	309.2	301.1	282.6	322.4
T_{fus} (K)	143.4	113.0	255.0	179.2
T_c (K)	469.8	461.0	433.8	511.7
P_c (bar)	33.6	33.8	32.0	45.1
V_c (l/mol)	0.311	0.306	0.307	0.259
$\Delta_{\text{vap}}H^\circ$ (kJ/mol)	26,50	25,00	22,40	28,80

obtained from the NIST WebBook

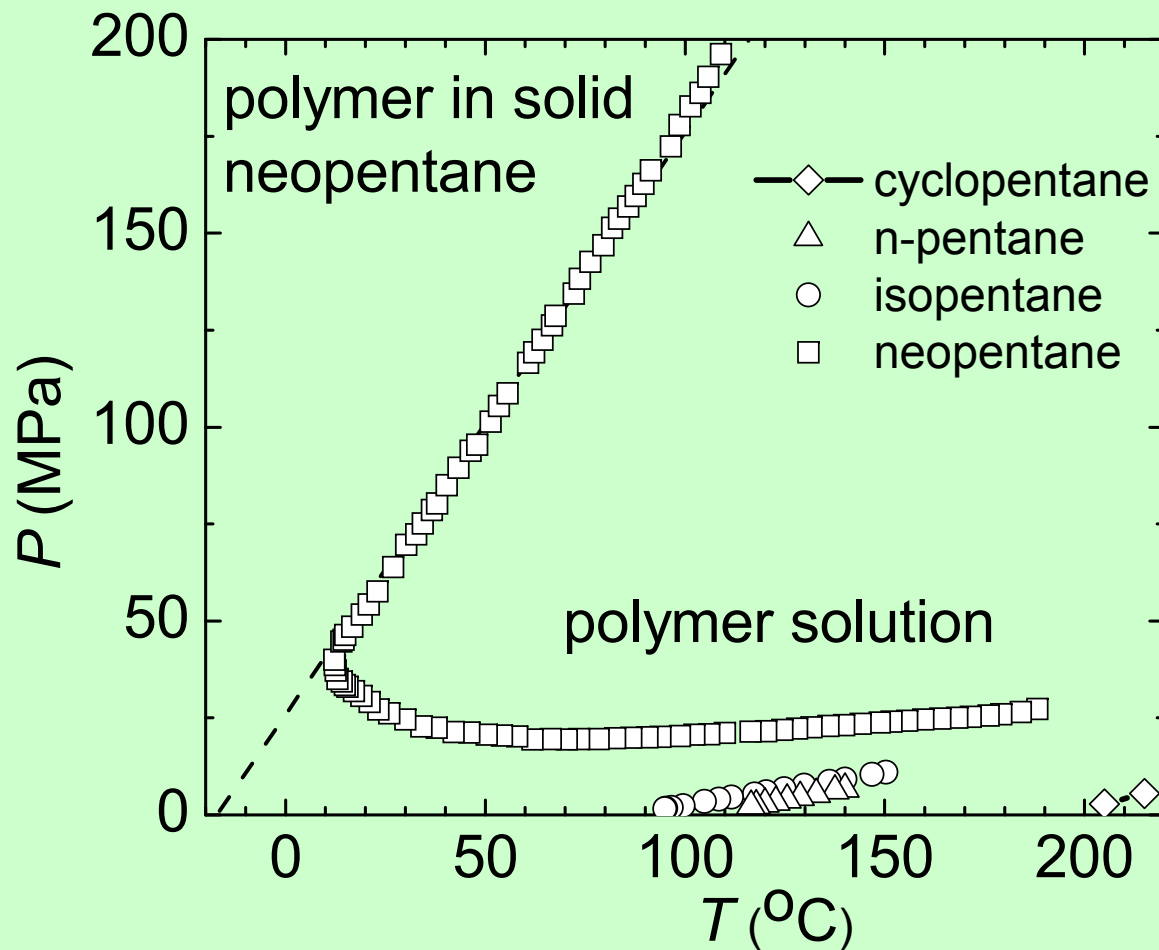


High-pressure DLS setup (up to 250 MPa, 250 °C)
at Virginia Commonwealth University

High-pressure setup



P-T diagram: polymer in pentanes



Polymer: deuterated poly(ethylene-co-20.2 mol %-1-butene)

Polymer concentration: 0.15 wt % - in cyclopentane,

0.5 wt % - in n-pentane and isopentane,

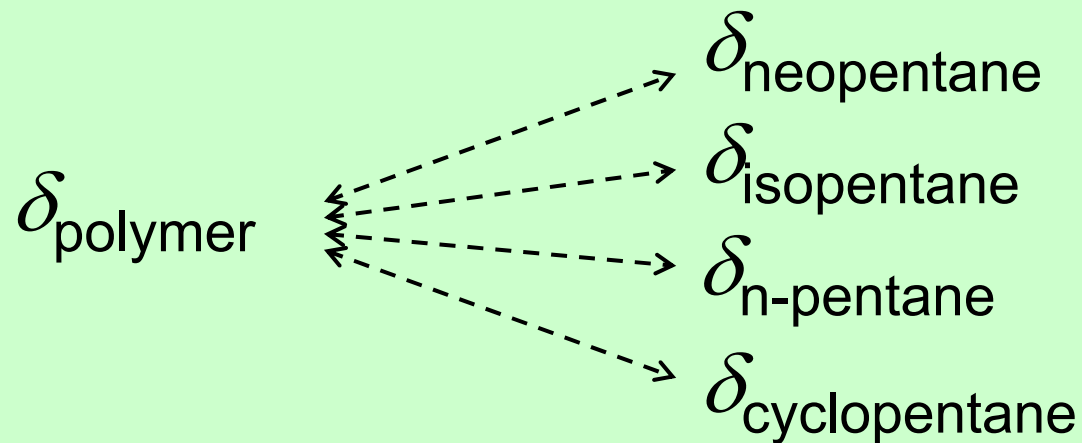
0.3 wt % - in neopentane,

Solubility Parameter (Hildebrand / Hansen*)

for non-polar and non-hydrogen-bonding solvents:

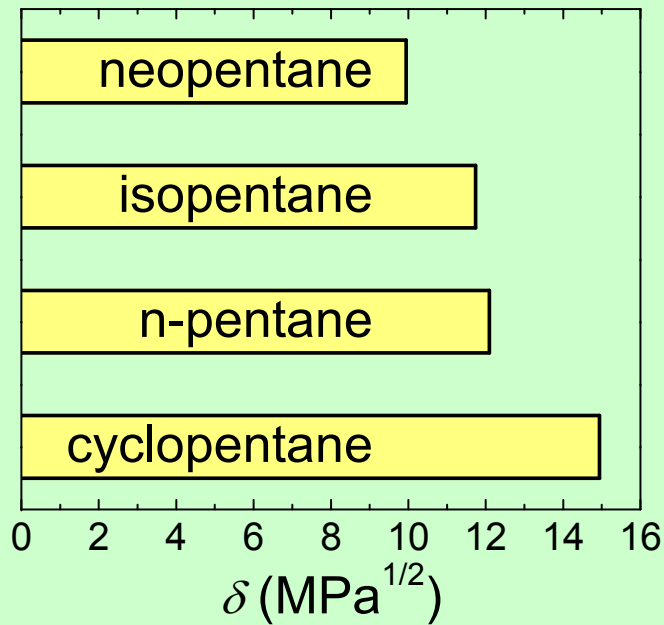
$$\delta = \sqrt{\frac{\Delta H_v - RT}{V_m}}$$

$\delta_1 \approx \delta_2 \quad \rightarrow \quad (1) \text{ will dissolve in } (2)$

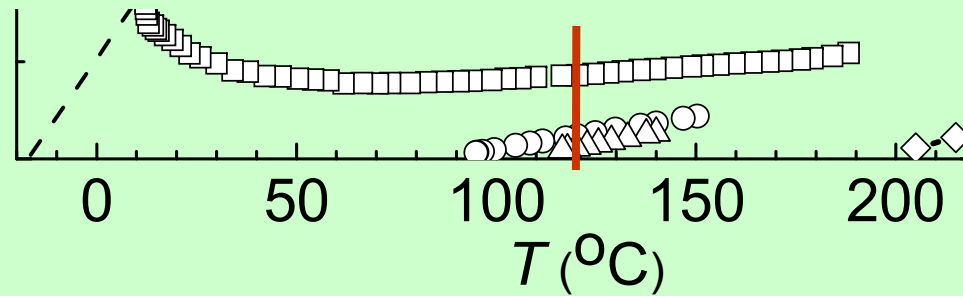
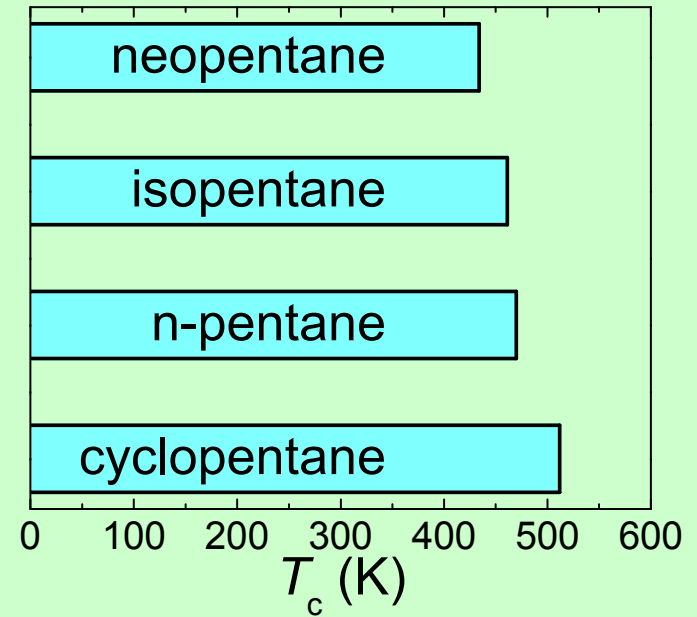


* Hansen parameter for non-polar and non-hydrogen-bonding solvents is analogous to the Hildebrand value (www.hansen-solubility.com)

Solubility Parameter (Hildebrand / Hansen)



qualitative



$$\left. \frac{\delta_{\text{iso}} - \delta_{\text{neo}}}{\delta_{\text{n}} - \delta_{\text{iso}}} \right|_{T=120^\circ\text{C}} = 5,3$$

quantitative

$$\left. \frac{P_{\text{neo}} - P_{\text{iso}}}{P_{\text{iso}} - P_{\text{n}}} \right|_{T=120^\circ\text{C}} = 4,8$$

Conclusion

- Molecular structure of pentane isomers affects their high-pressure solubility quality in accordance with δ and T_c
- $\Delta P_{\text{cloud}} \sim \Delta \delta$

THANK YOU!