

# Controlling Thermal Expansion within Mixed Co-crystals by Tuning Molecular Motion Capability

TEXAS TECH UNIVERSITY®

Xiaodan Ding,<sup>a</sup> Daniel K. Unruh,<sup>a</sup> Ryan H. Groeneman,<sup>b</sup> and Kristin M. Hutchins<sup>a</sup>

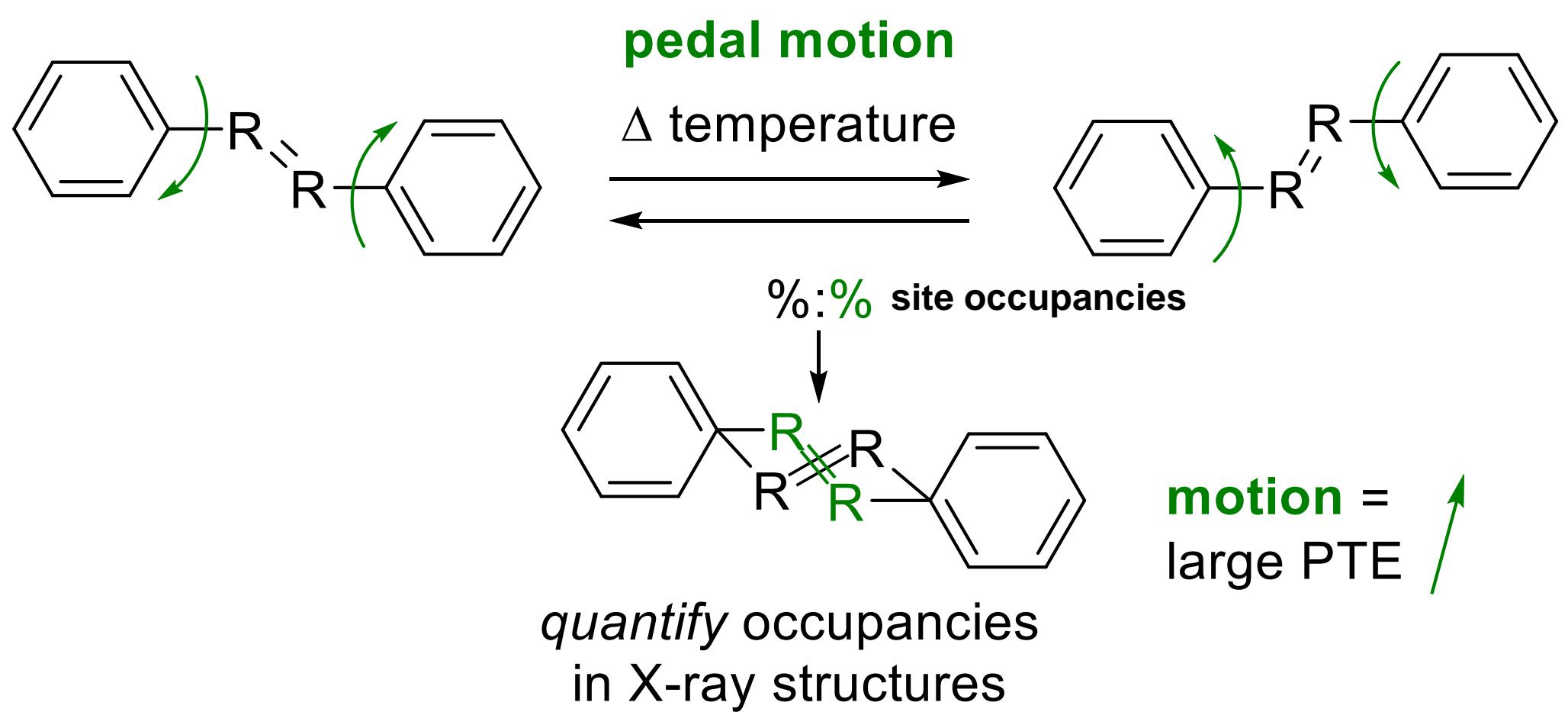
<sup>a</sup>Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX 79409 USA

<sup>b</sup>Department of Biological Sciences, Webster University, St. Louis, MO 63119, USA

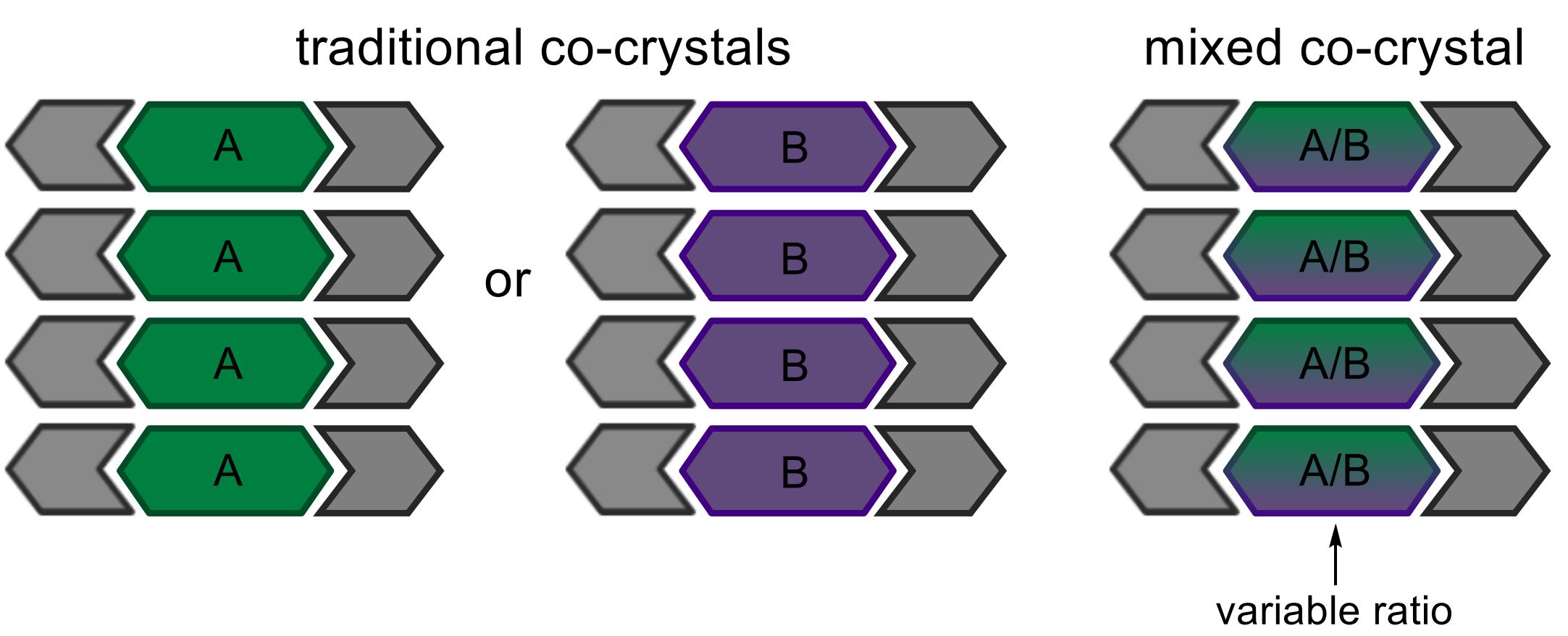


## Background

- Thermal expansion (TE)
  - Response of a material to changes in temperature.
  - Classification: Positive TE (PTE), negative TE (NTE), and zero TE (ZTE).
  - Potential applications in thermal sensors and actuators.
  - Dynamic pedal motion can give rise to large PTE along the direction where motion happens.



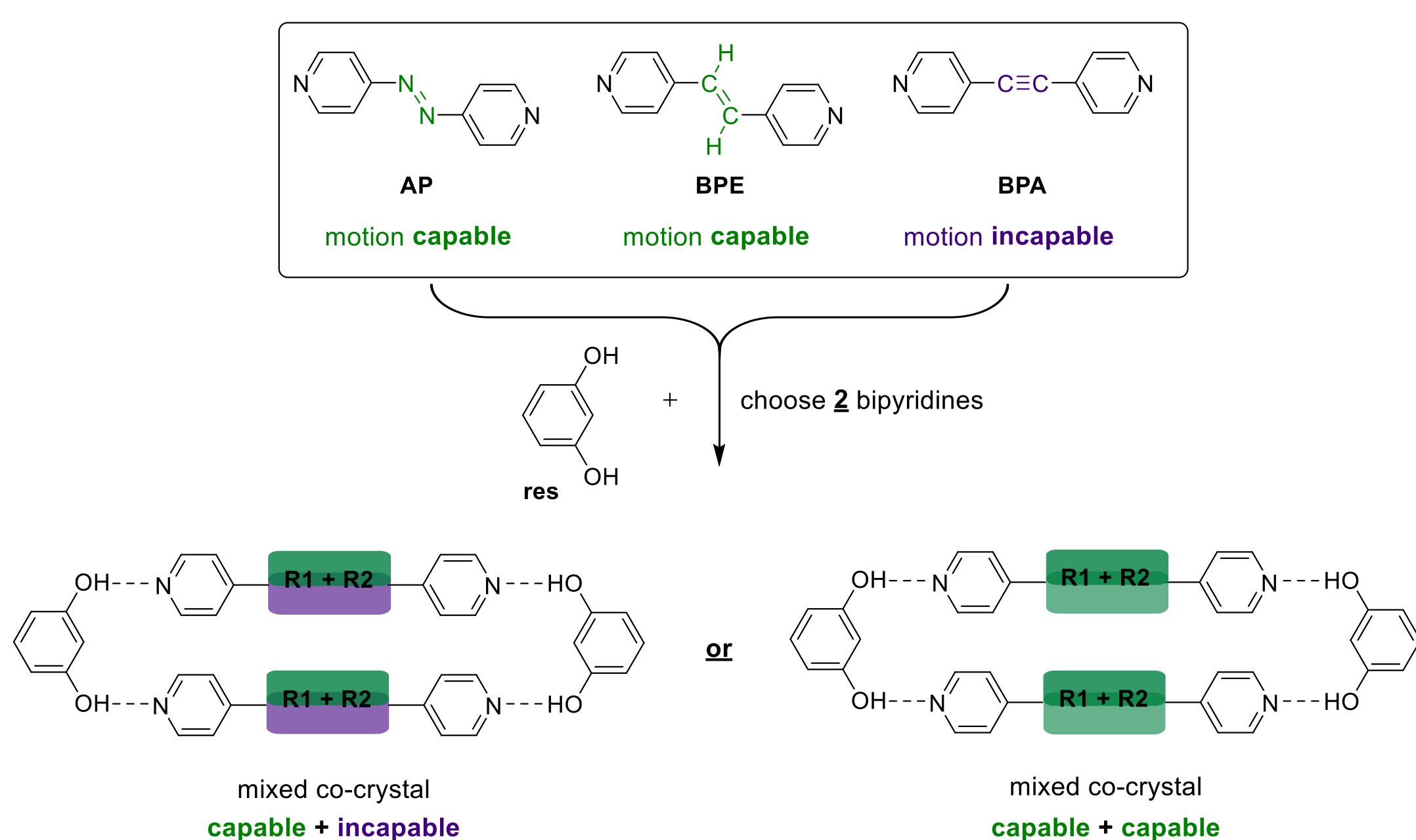
- Mixed co-crystals
  - Multiple components are incorporated at one molecule site.
  - Similarly shaped molecules are used to replace each other at equivalent crystallographic site.
  - Mixed co-crystals could provide a strategy to tune TE behaviors in organic solids.



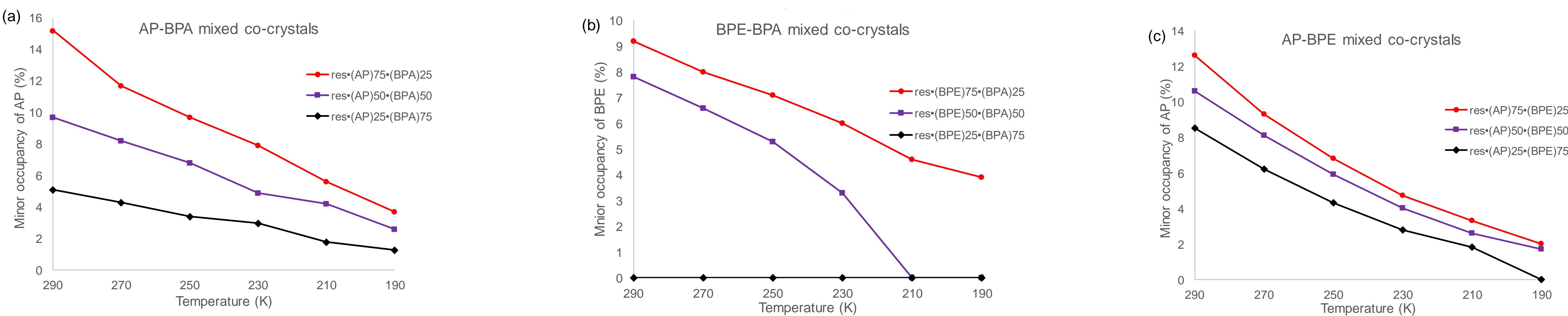
## References

- (1) Saha, B. K. *J. Indian Inst. Sci.* **2017**, *97*, 177-191.
- (2) Harada, J.; Ogawa, K. *Chem. Soc. Rev.* **2009**, *38*, 2244-2252.
- (3) Lusi, M. *CrystEngComm*, **2018**, *20*, 7042-7052.
- (4) Cliffe, M. J.; Goodwin, A. L. *J. Appl. Cryst.* **2012**, *45*, 1321-1329.
- (5) Hutchins, K. M.; Unruh, D. K.; Verdu, F. A.; Groeneman, R. H. *Cryst. Growth Des.* **2018**, *18*, 566-570.
- (6) Ding, X.; Unruh, D. K.; Groeneman, R. H.; Hutchins, K. M. *Chem. Sci.* **2020**, *11*, 7701-7707.

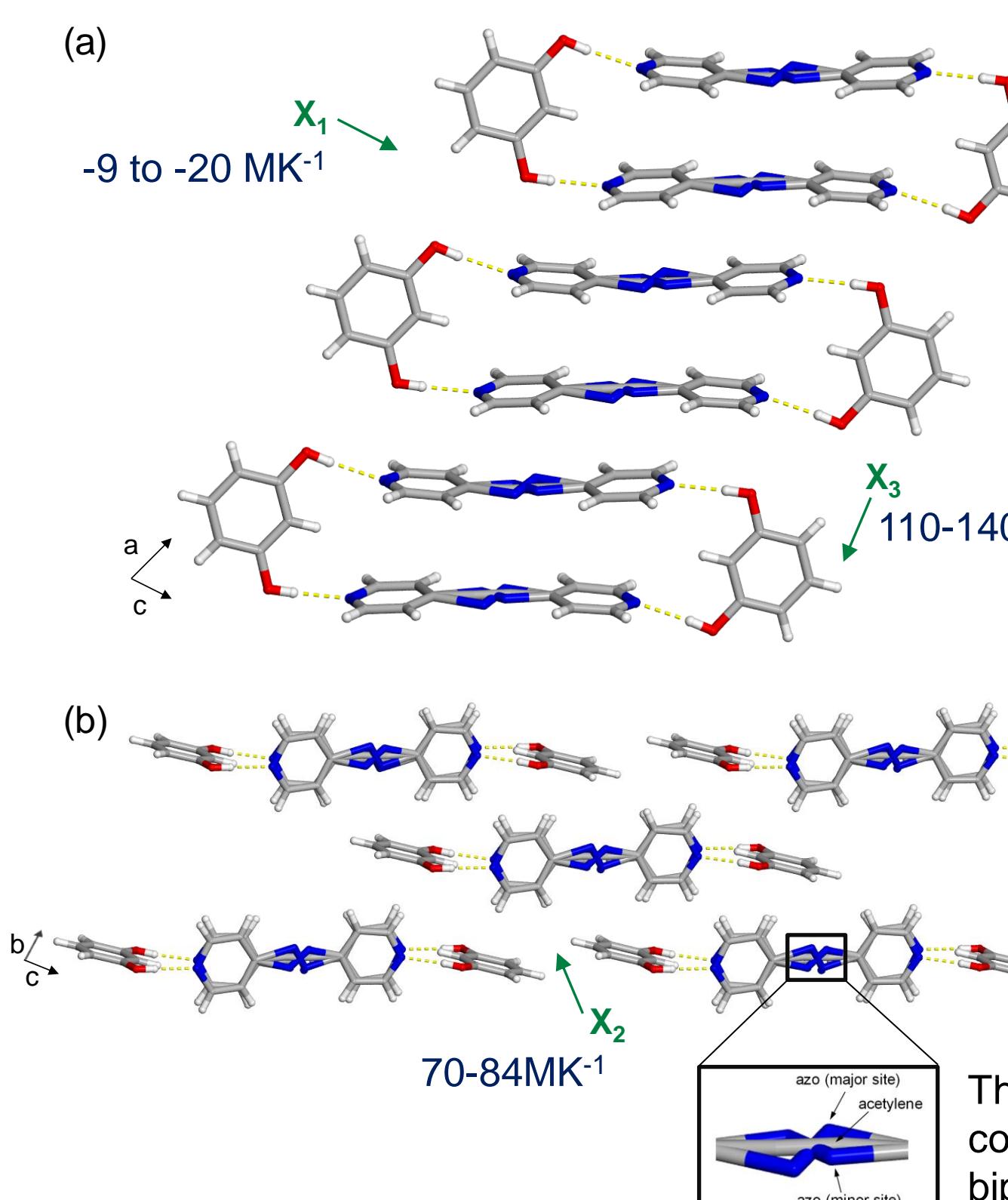
## Synthesis of mixed co-crystals



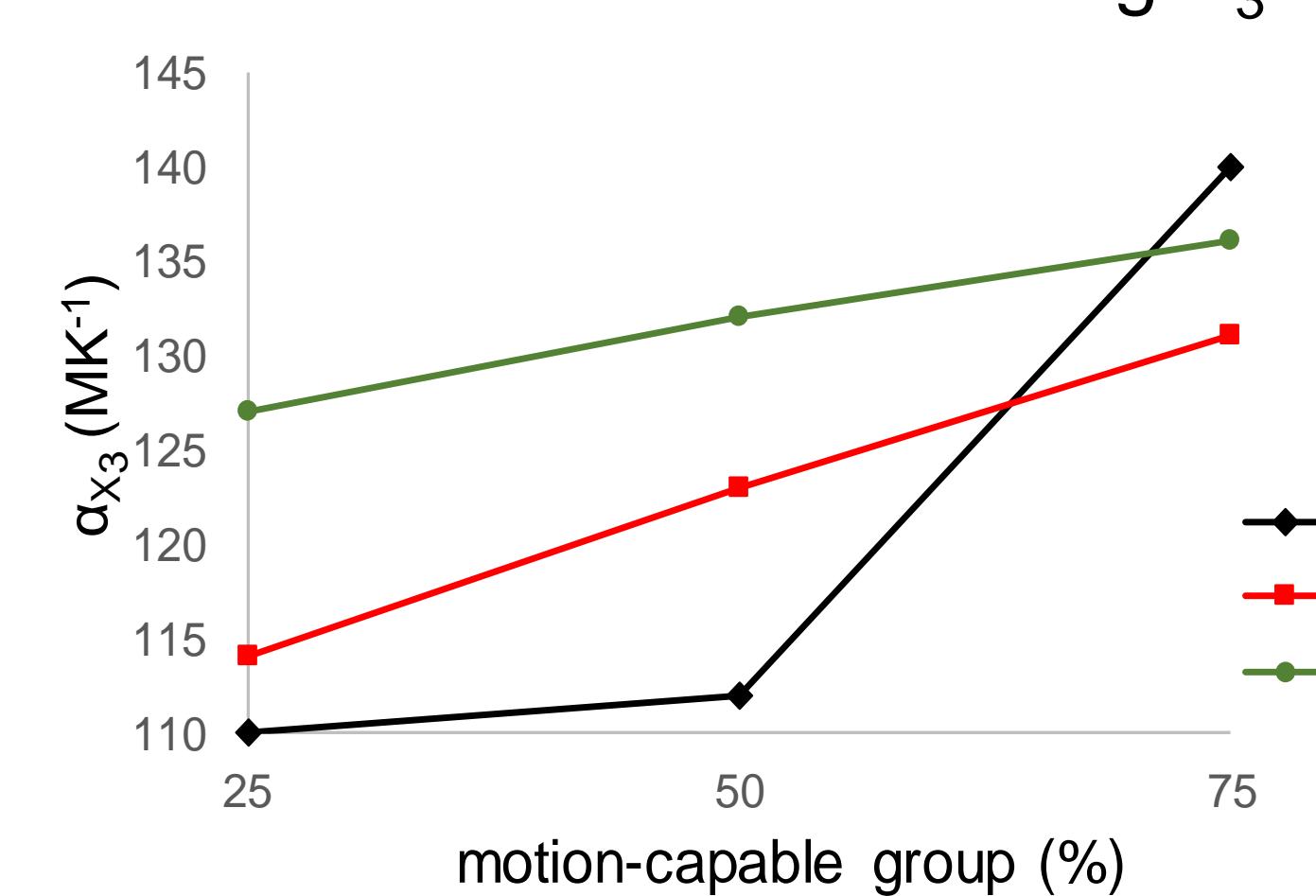
## Pedal motion in mixed co-crystals



## Mixed Co-crystals



## TE coefficients along $X_3$



## Halogen-Bond Donors

### Motion-capable groups olefin (C=C), azo (N=N), imine (C=N)

