



# Effect of pedal motion or motion inability on thermal expansion of organic crystals



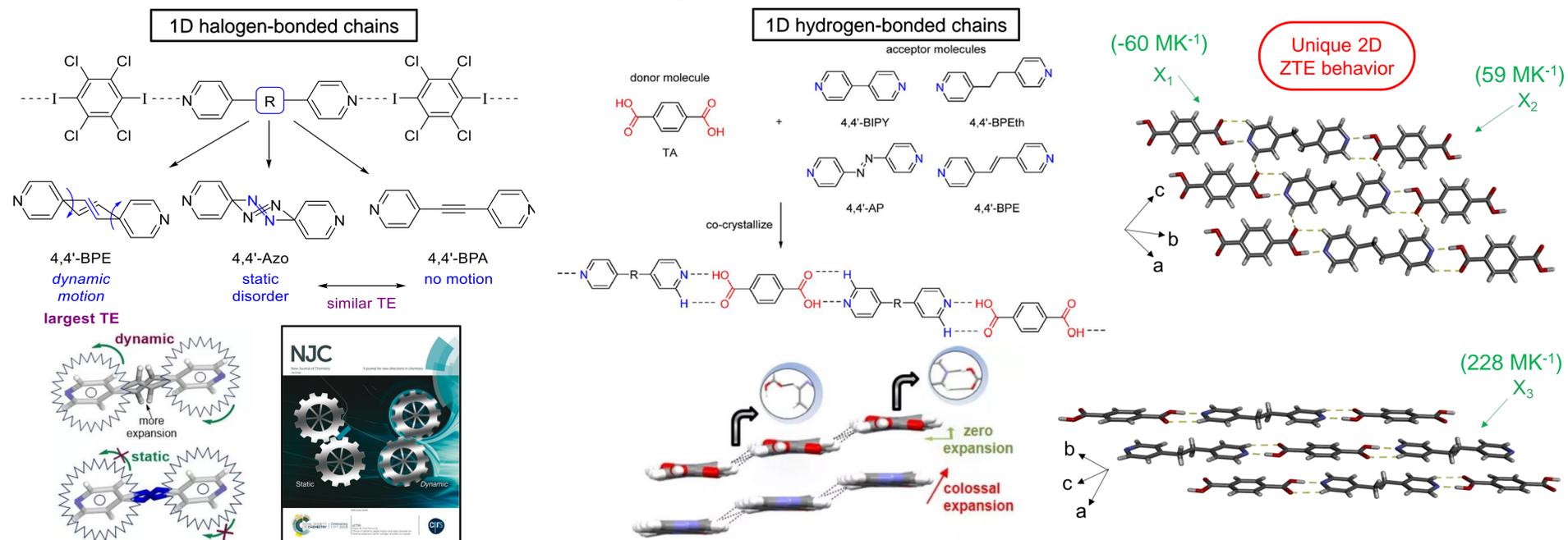
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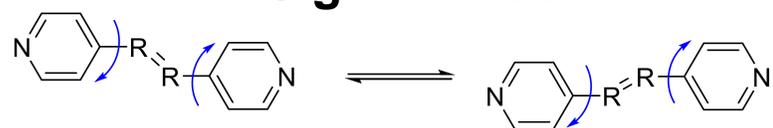
## Abstract

Thermal expansion of materials is mostly dependent on chemical composition and usually correlates with the crystal structure, electronic structure, and defects of the materials. Materials with desirable physical properties and controllable thermal expansion properties are useful in designing devices such as thermomechanical actuators, sensors, and composites. Atoms in molecules are not stationary and hence they undergo certain molecular motions depending upon the type of symmetry of the molecules. Here, we focus on molecules with a skeleton similar to that of azobenzenes and stilbenes, which are capable of undergoing pedal motion. Incorporating such molecules into a multi-component solid via co-crystallization can be a captivating way to design materials with movements or unique thermal expansion properties. The dynamic processes or motions in crystals can be investigated using variable temperature X-ray diffraction analysis of the crystal. In this presentation, we describe co-crystals sustained by halogen and hydrogen bonds and the role that molecular motion and bond type play on thermal expansion properties.

## Thermal expansion of halogen and hydrogen-bonded co-crystals

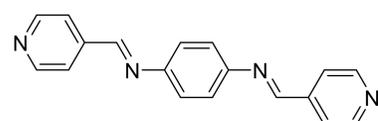


## Significance

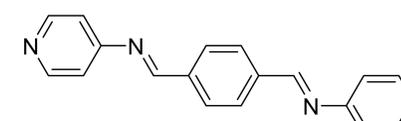


- Motion can occur in response to temperature changes
- Determined via variable temperature single-crystal X-ray diffraction
- Site occupancies are quantifiable
- Applications: thermomechanical actuators, sensors, and composites

## Thermal expansion of imine-based single component solids

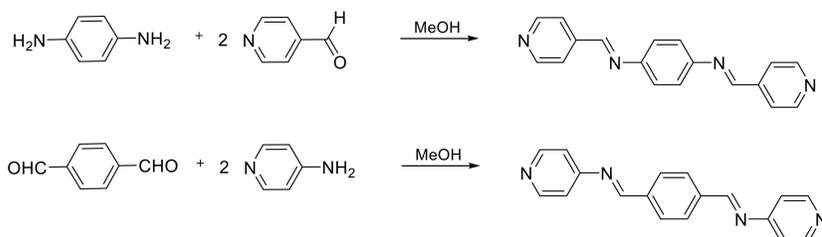


Principal axes	$\alpha_{xi} \text{ (MK}^{-1}\text{)}$
$X_1$	-0.2 (0)
$X_2$	40 (0)
$X_3$	152 (1)
V	192 (2)

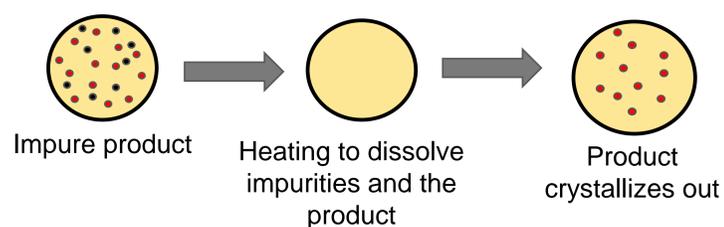


Principal axes	$\alpha_{xi} \text{ (MK}^{-1}\text{)}$
$X_1$	2.3 (2)
$X_2$	56 (4)
$X_3$	111 (2)
V	172 (8)

## Synthesis and purification



### Purification using recrystallization



## Conclusions and future work

- Pedal motion in co-crystals results in larger thermal expansion
- Presence of multiple hydrogen bonds influences the thermal expansion properties
- Thermal expansion is generally smaller along directions where stronger interactions dominate
- Large positive TE occurs along  $X_3$  and volumetrically for all crystals

### Future Work:

- Thermal expansion properties of co-crystals
- Molecular motion affecting chromic properties of solids

## References

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## Acknowledgements

