Poster

Identification of a metastable phase and an unstable phase in 1,1'- Binapthalene

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Temperature-dependent X-ray diffraction (XRD) is employed to study the phase transitions in axially chiral 1,1'-Binaphthalene at various heating and cooling rates. The known phases of 1,1'-Binaphthalene are monoclinic (racemate), a cisoid conformer with a melting temperature of 145°C, and tetragonal (enantiomers), a transoid conformer melting at 158°C[1-4]. Upon melting and recrystallization at 2°C/min, the system crystallizes in the monoclinic phase around 90°C and tetragonal phase at 60°C, whereas a metastable phase and an unstable phase are observed upon heating and cooling at 5°C/min and 10°C/min, respectively. The metastable phase occurs upon recrystallization from the melt around 125°C, and the recrystallization of the unstable phase starts at 58°C. The unstable phase isothermally transforms to the stable tetragonal phase over 6 hours. Quantification of the metastable and unstable phases is achieved by determining the lattice parameters and estimating the extent of the transformation. The metastable and unstable phases are also tetragonal, and the unstable phase undergoes an Avrami transformation to the stable tetragonal phase.

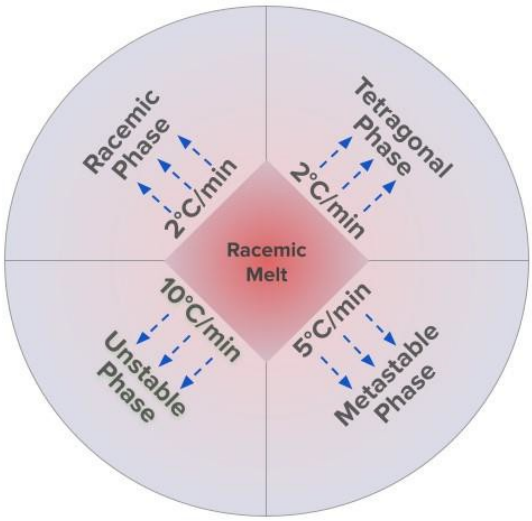

Figure 1. Schematic diagram representing recrystallization of 1,1'-Binapthalene from racemic melt at various cooling rates.

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