Catalytic Deracemization of Allenes

Significance: Bach and co-workers report an allene deracemization reaction catalyzed by an organic chiral sensitizer under visible light. By using this method, several racemic allenes were converted into enantiomers with yields of ≤100% and er values of ≤98.5:1.5. DFT calculations are also provided to support the proposed mechanistic description.

Comment: Light-driven deracemization of chiral compounds might be implicated in the origin of early-stage chirality. The present unprecedented discovery presents an example to support this hypothesis. With different substrate classes, solutions to generate chiral centers might be possible in cases where thermally controlled catalytic deracemizations are entropically disfavored.

Selected examples:

- 56% yield er = 95:5
- 89% yield er = 98:2
- 100% yield er = 97.5:2.5
- 100% yield er = 96.5:3.5

Mechanistic description on the basis of DFT calculations:

- d = 363 pm
- d = 510 pm