Organocatalytic Cycle — Experimental ΔG‡ = 20.8 kcal/mol = kcat/KM (rate-limiting step is turnover from deep intermediate)

Free Energy (kcal/mol)

Reaction coordinate

kcat barrier ≈ 38.8 kcal/mol

ΔG‡ = kcat/KM = 20.8 kcal/mol
(experimental activation barrier)

$Ea_3 = 20.8$

$Ea_1 = 16.5$

$Ea_2 = 9.0$

X_1

X_2

X_3

reactants

1

2

products

ΔG° ≈ –32 kcal/mol