THE MECHANISM OF HYDROGEN TRANSFER FROM DIALIN DONORS, D.H. Bass and P.S. Virk, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02181

We report experiments concerning the transfer of hydrogen from the two dihydronaphthalene isomers, namely Δ^1-dialin and Δ^2-dialin, to two polynuclear hydrocarbon acceptors, namely anthracene and phenanthrene. These substrates were chosen both to model some of the hydrocarbon moieties involved in coal liquefaction as well as to test our hypothesis that the hydrogen transfer occurs by a concerted pericyclic reaction. The Woodward-Hoffmann rules for orbital symmetry conservation then suggest that hydrogen transfer to anthracene should be thermally-allowed from Δ^2-dialin but forbidden from Δ^1-dialin; however hydrogen transfer to phenanthrene should be thermally-allowed from Δ^1-dialin but forbidden from Δ^2-dialin. The experiments were conducted in tubing bomb reactors in the temperature range 240 C to 430 C, at times from 5 to 960 minutes and donor-to-acceptor mol ratios from 0.25 to 16. Reactions were essentially first order in each of donor and acceptor, with second order rate constants, $\log_{10}k$ (liter/mol s) tabulated below:

Donor →	Δ^1-dialin	Δ^2-dialin	tetralin
Acceptor ↓			
Anthracene 300 C	-5.1	-3.0	-6.1
Phenanthrene 400 C	-4.0	-5.5	-5.7

The experimental results evidently accord with the theoretical predictions for a pericyclic hydrogen-transfer.