MODEL PATHWAYS FOR HYDROGEN TRANSFER IN COAL LIQUEFACTION

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Hydrogen transfer from donor solvents to coal during liquefaction has been modelled by reactions between selected pure substrates. Model donors used were tetralin (control), Δ^1- and Δ^2-dialins, cyclohexanol and o-cyclohexylphenol, while anthracene and phenanthrene served as model acceptors. Experiments over the temperature range 250-450 C, at times from 0.1-10.0 hr, and donor/acceptor ratios of 0.12-16, revealed that, in general, three types of reactions occurred. In order of importance these were: (R1), the desired hydrogen transfer from donor to acceptor, (R2), the reversion of hydrogenated acceptor to original acceptor, either by elimination of molecular hydrogen or by disproportionation, and (R3), donor decomposition. Kinetic data showed that for every donor-acceptor pair (R1) was bimolecular, being of order one in each substrate. Also, Arrhenius parameters in all cases yielded activation entropies $\Delta S^{\dagger} \sim -30$ eu, indicative of a tight transition state. These accord with our earlier suggestion that the mechanism of hydrogen transfer might involve concerted pericyclic group-transfer reactions that are thermally-allowed by the Woodward-Hoffmann rules for orbital symmetry conservation. Detailed kinetic data were also obtained for each of (R2) and (R3), permitting fairly complete description of the present model pathways for hydrogen transfer.