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Item title: Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination

Link back to the item: https://hdl.handle.net/1721.1/123827
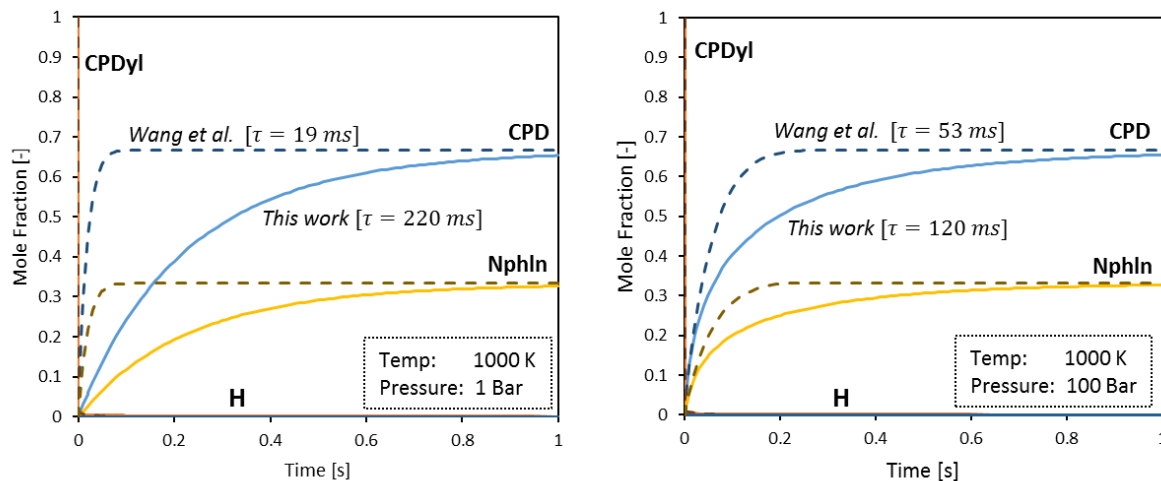
Supporting Figures:

Fig. S1: Comparative analysis between the pressure dependent reaction network calculated in this work and that which was estimated by Wang et al. [48]. Comparison was achieved by simulating the behavior of each sub-mechanism using a Chemkin homogenous reactor module and starting the simulation entirely with CPDyl. The CPD = CPDyl + H reaction was included to allow for consumption of H and a reasonable formation of naphthalene. The network presented in this work is roughly an order of magnitude slower than that of Wang et al at atmospheric pressure and roughly a factor of 2 slower at 100 bar. The opposing pressure trends are attributed to the importance of CPDyl H-abstraction discussed in this work which was not included in the Wang model.
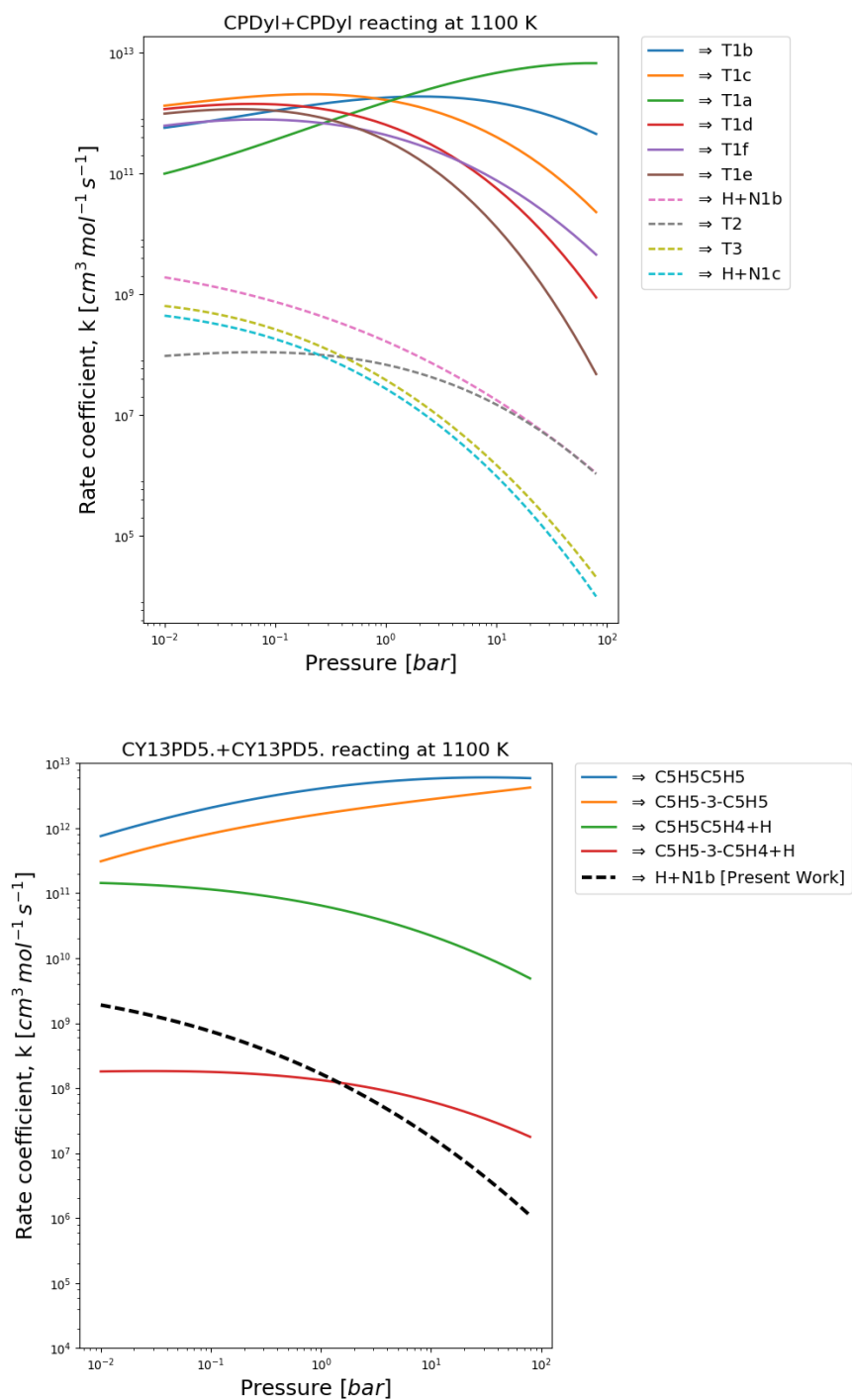
Fig. S2: Reproduction of Figure 5A from this paper (TOP) compared with an analogous figure created from the Wang et al. [48] estimated pressure dependent network rates (BOTTOM). The two networks are observed to be consistent in their high pressure limit rate for CPDyl + CPDyl, but the estimated Wang et al. network shows a significantly higher rate for the chemically activated pathway to $C_{10}H_9 + H$.
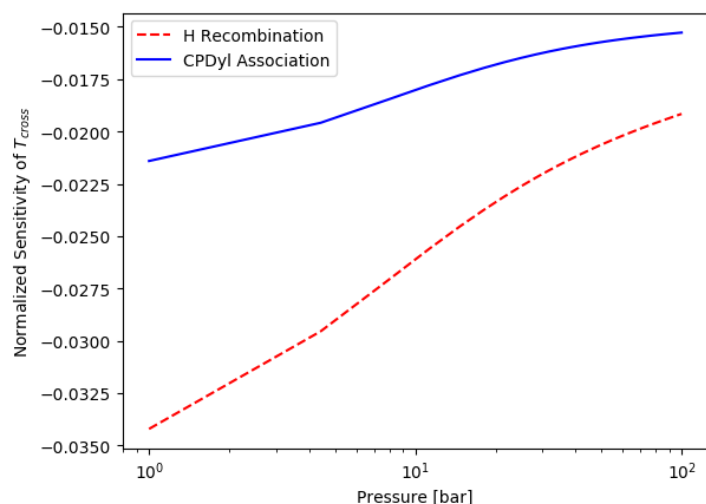
Fig. S3: Brute force sensitivity analysis $\left(s = \dfrac{A_i}{T_{cross,i}} \dfrac{\Delta T_{cross}}{\Delta A} \right)$ for the crossover temperature at which the chemically activated rate, 2 CPDyl = $C_{10}H_9$ + H becomes the dominant route to the $C_{10}H_9$ surface. An increase in either rate will lead to a lower T_{cross} with the hydrogen recombination rate having the stronger effect. Both sensitivities are low.
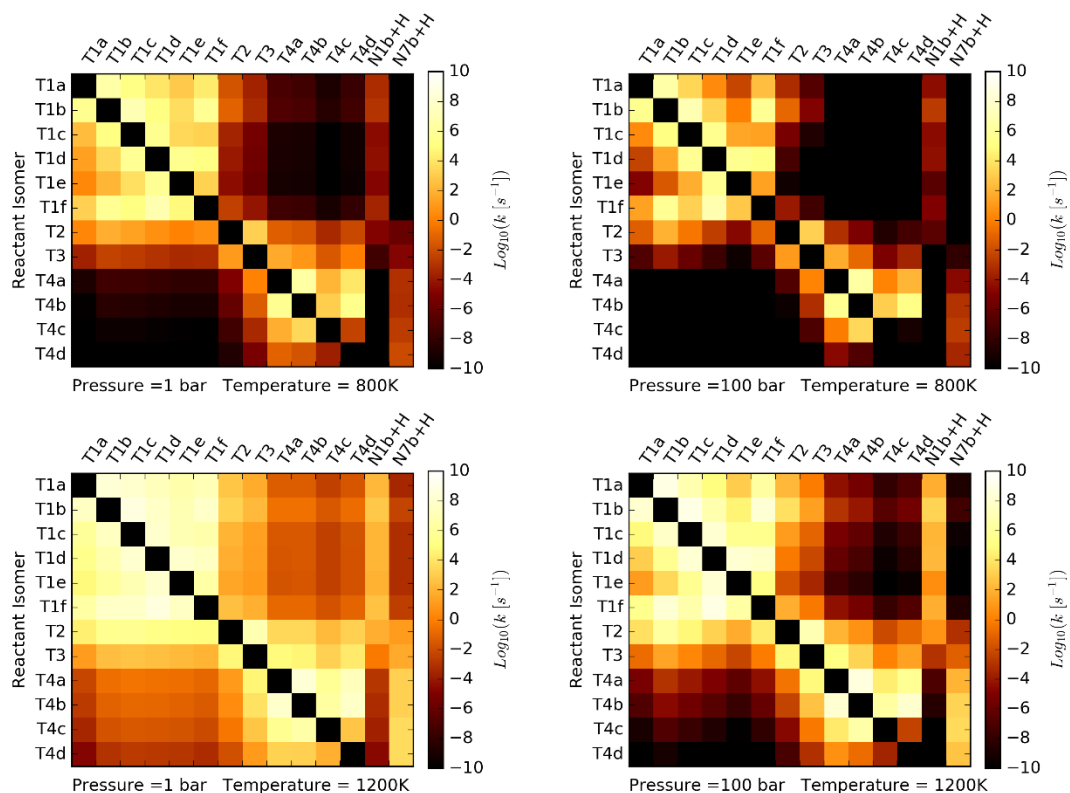

Fig. S4: Isomerization rate constant matrices for the $C_{10}H_{10}$ surface at varying temperature and pressure.
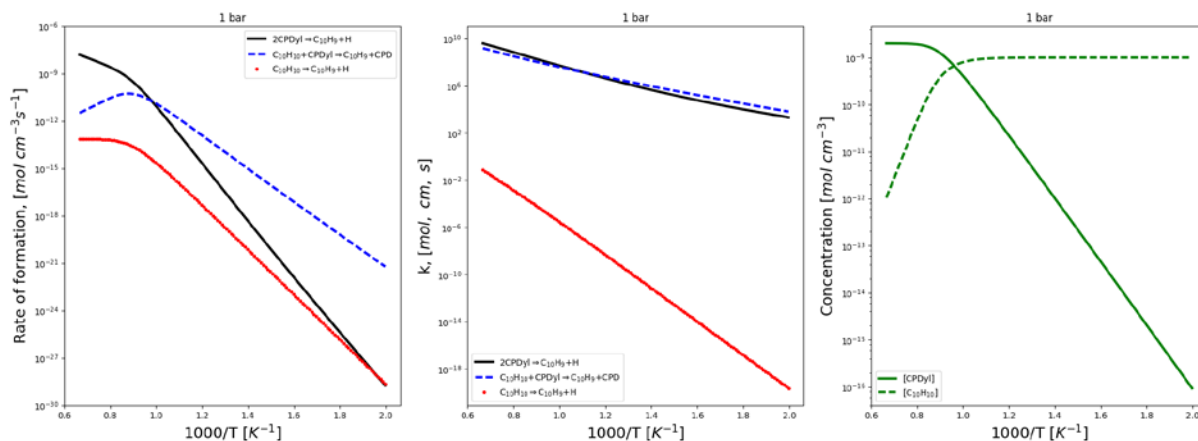
Fig. S5: Factor breakdown of the $C_{10}H_9$ rate of formation plot shown in Figure 6. Changes in slopes for the left most plot are attributed to a shift in the assumed equilibrium between the $C_{10}H_{10}$ species and CPDyl shown in the right most concentration plot.
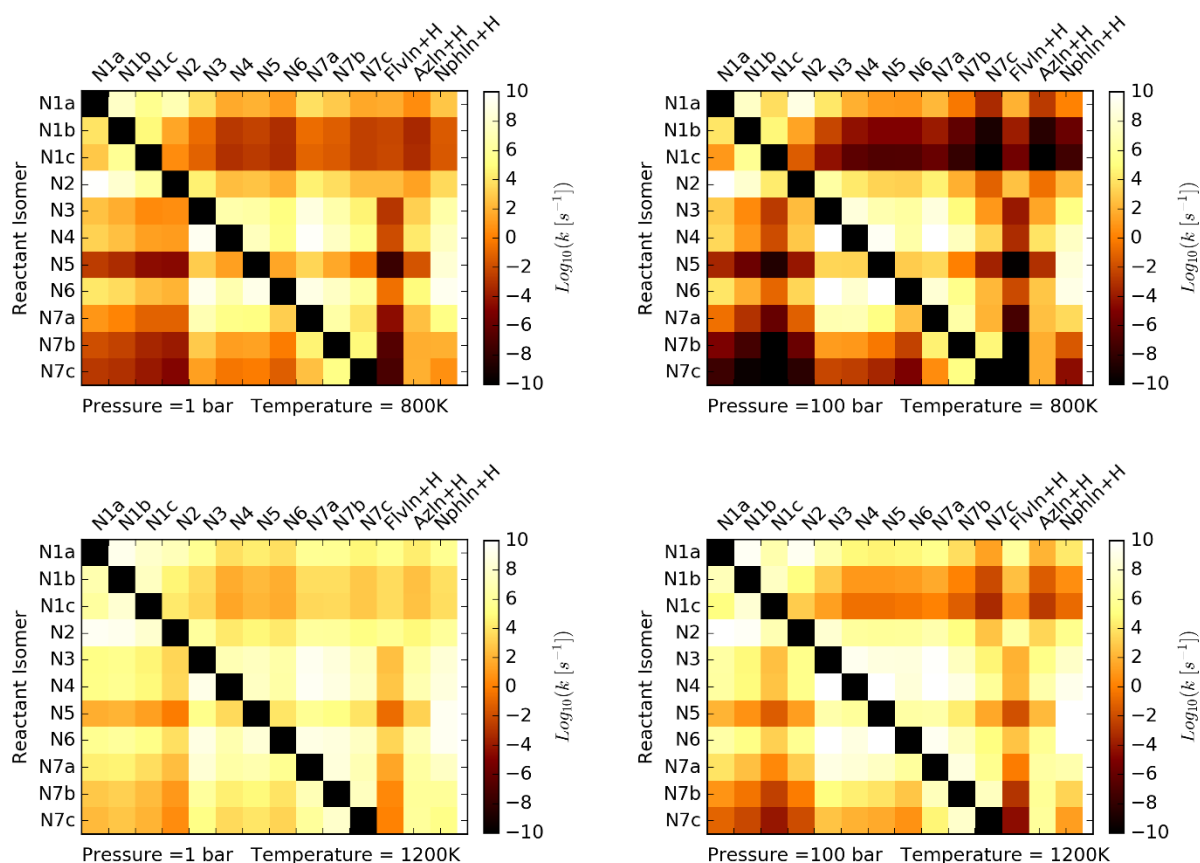

Fig. S6: Isomerization rate constant matrices for the $C_{10}H_9$ surface at varying temperature and pressure.