

Master Equation Rate Coefficients

The Excel file in the Supporting Information contains rate coefficients from a master equation solution based on the adjusted final stationary points for the cyclohexyl + O₂ system. There are three sheets; one gives rate coefficients for several temperatures at a total density, rho, of $8.5 \times 10^{17} \text{ cm}^{-3}$, the second gives rate coefficients at 638 K for several pressures, and the final sheet gives rate coefficients at a total density of $3.65 \times 10^{17} \text{ cm}^{-3}$. Each sheet is arranged as a set of tables, where the column headings give the product of the reaction, and the first column lists a reaction condition (temperature or pressure). Each table is filled with the set of rate coefficients from a particular reactant to the products in the columns. For example, the first sheet lists rate coefficients for 24 temperatures at a total density of $8.5 \times 10^{17} \text{ cm}^{-3}$. The first table in this sheet lists the rate coefficients for the original reactants (cyclohexyl + O₂), r , proceeding to each of the products listed in the various columns. The second table lists the rate coefficients for the first well (the RO₂ radical), w1, proceeding to the same set of products, and so on. Question marks are used to denote reactions where either reactant or product is above its stabilization limit.

Units for second-order rate coefficients (i.e., those from reactants r) are $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and first order rate coefficients (all the rest) are in s^{-1} .