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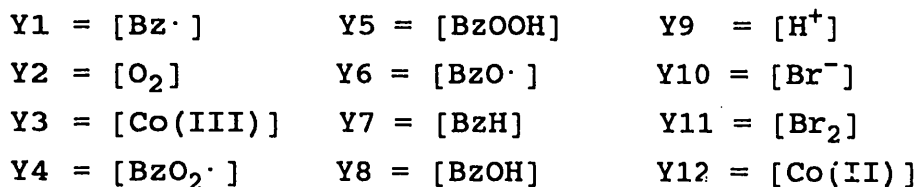
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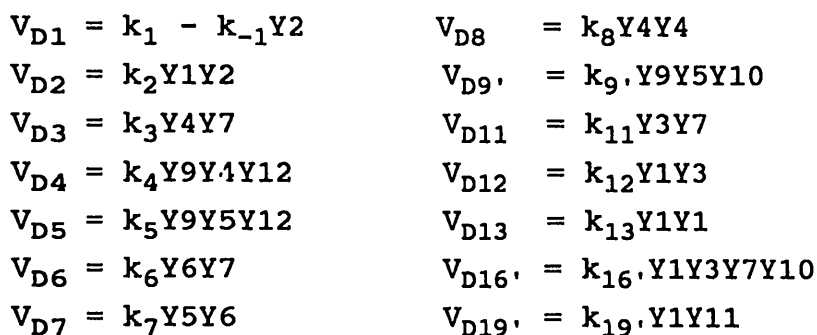
SUPPLEMENTARY MATERIAL FOR
COBALTOXALATOR. A SKELETON MODEL FOR THE
OSCILLATORY OXIDATION OF BENZALDEHYDE

The following material contains information for simulating the detailed model shown in Table II in order to reproduce the plot shown in Figure 5. First the variables and the velocities of each chemical step are defined. This is followed by the differential equations and the values for the rate constants and the initial conditions.

Variables for the D model



Velocities for the D model



Note that steps D9 and D10 were lumped together to get D9', likewise D14, D15 and D16 were lumped together to get D16'. Steps D17, D18 and D19 were also lumped together to get D19'.

Differential equations for the D model

$$dY1/dt = -V_{D2} + V_{D3} + V_{D6} + V_{D11} - V_{D12} - V_{D13} + V_{D16},$$

$$dY2/dt = V_{D1} - V_{D2} + V_{D8}$$

$$dY3/dt = V_{D4} + V_{D5} - V_{D11} - V_{D12} - V_{D16},$$

$$dY4/dt = V_{D2} - V_{D3} - V_{D4} + V_{D7} - V_{D8}$$

$$dY5/dt = V_{D3} + V_{D4} - V_{D5} - V_{D7} - V_{D9},$$

$$dY6/dt = V_{D5} - V_{D7} - V_{D6}$$

$$dY7/dt = -V_{D3} - V_{D6} - V_{D11} + V_{D13} - V_{D16} - V_{D19},$$

$$dY8/dt = V_{D7} + V_{D6} + V_{D9} + V_{D12} + V_{D13} + V_{D19},$$

$dY9/dt$ is by assumption set equal to 0 for this simulation

$$dY10/dt = -2V_{D9} + 2V_{D19},$$

$$dY11/dt = V_{D9} - V_{D19},$$

$$dY12/dt = -V_{D4} - V_{D5} + V_{D11} + V_{D12} + V_{D16},$$

Rate constants for the D model

$$k_{D1} = 4 \cdot 10^{-5}$$

$$k_{D8} = 10^5$$

$$k_{D-1} = .4$$

$$k_{D9, Y9} = 10^4$$

$$k_{D2} = 10^9$$

$$k_{D11} = 10^{-2}$$

$$k_{D3} = 10$$

$$k_{D12} = 10^6$$

$$k_{D4 Y9} = 10^5$$

$$k_{D13} = 10^8$$

$$k_{D5 Y9} = 10^4$$

$$k_{D16} = 10^8$$

$$k_{D6} = 10^2$$

$$k_{D19} = 10^9$$

$$k_{D7} = 10^8$$

Initial conditions for D model

$$Y1_0 = Y2_0 = Y4_0 = Y5_0 = Y6_0 = 10^{-7}M$$

$$Y3_0 = 10^{-3}M$$

$$Y7_0 = .75M$$

$$Y8_0 = Y11_0 = 10^{-12}M$$

$$Y9_0 = 10^{-2}M$$

$$Y10_0 = .04M$$

$$Y12_0 = 1.9 \cdot 10^{-2}M$$

Relative error tolerance = 10^{-5}

Absolute error tolerance = 10^{-20}