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Supporting Information Section

T.J. Strathmann and A.T. Stone. 2002. Reduction of Oxamyl and Related Pesticides by Fe^{II}: Influence of Organic Ligands and Natural Organic Matter, *Environmental Science and Technology*

Analysis of Kinetic Data

Calculating Pseudo First-Order Rate Constants

In aqueous solutions containing Fe^{II}, OCPs degrade by parallel reduction and elimination reactions (pathway for oxamyl and methomyl provided in Figure 1 of ref. 25). For batch reactions conducted in this study, Fe^{II} was present in considerable stoichiometric excess with respect to the OCPs. Consequently, the kinetics of OCP disappearance and reaction product formation can be described by the following pseudo first-order differential rate expressions:

$$-\frac{d[\text{OCP}]}{dt} = k_{obs}[\text{OCP}] = (k_{red} + k_{elim})[\text{OCP}] \quad \text{(SI-1)}$$

$$\frac{d[\text{Nitrile Reduction Product}]}{dt} = k_{red}[\text{OCP}] \quad \text{(SI-2)}$$

$$\frac{d[\text{Oxime Elimination Product}]}{dt} = k_{elim}[\text{OCP}] \quad \text{(SI-3)}$$

where k_{obs} (h^{-1}), k_{red} (h^{-1}), and k_{elim} (h^{-1}) are defined as pseudo first-order rate constants for overall OCP disappearance, OCP reduction by Fe^{II}, and base-catalyzed OCP elimination, respectively, and $[i]$ represents the concentration of parent OCP and selected degradation products that were monitored by HPLC.

The software package *Scientist for Windows* (*33*) was used to calculate values of k_{red} and k_{elim} for each batch reaction. Results of these calculations are provided in Table S1. *Scientist* calculates these parameters and the initial concentration of parent OCP by fitting numerically integrated solutions of the system of differential rate expressions shown above to experimental data for OCP disappearance and reaction product formation. Numerical integration was carried out using the Episode-stiff package (*33*). Data fitting was performed by method of least squared errors using a modified Powell algorithm, a hybrid of the Gauss-Newton and steepest descent techniques (*33*). Output and statistics from data fitting included the best fit estimate of each adjustable parameter, the standard deviation and 95 % confidence range of each parameter estimate, the sum of the squared deviations, the standard deviation of the data, the r-squared value, the coefficient of determination, the correlation coefficient, and the serial correlation. Only rate constants greater than 7.0×10^{-5} h^{-1} could be reliably calculated using the experimental approach and data analysis methods employed in this study.

In the absence of Fe^{II}, OCPs degrade solely by the elimination pathway, and the kinetic model used for data fitting can be simplified:

$$-\frac{d[\mathrm{OCP}]}{dt} = k_{obs}[\mathrm{OCP}] = k_{elim}[\mathrm{OCP}] \qquad \text{(SI-4)}$$

$$\frac{d[\text{Oxime Elimination Product}]}{dt} = k_{elim}[\mathrm{OCP}] \qquad \text{(SI-5)}$$

Control reactions carried out as part of this study and a prior study (*25*) demonstrate that k_{elim} (25 °C) depends solely on pH, and is independent of concentration and speciation of both Fe^{II} and organic ligands. Consequently, for data fitting in Fe^{II}-containing systems, values of k_{elim} were fixed at the values determined in Fe^{II}-free, organic ligand-free solutions of the same pH. This practice reduced the number of adjustable fitting parameters used when calculating k_{red} values. It should be noted, however, that fixing the values of k_{elim} did not significantly affect the final values of k_{red} obtained from data fitting.

Under selected conditions, OCP reduction is significantly faster than the parallel elimination reaction and no elimination products are observed on the time scale of reduction. Under these conditions, the kinetic model can be simplified to consider only reduction:

$$-\frac{d[\mathrm{OCP}]}{dt} = k_{obs}[\mathrm{OCP}] = k_{red}[\mathrm{OCP}] \qquad \text{(SI-6)}$$

$$\frac{d[\text{Nitrile Reduction Product}]}{dt} = k_{red}[\mathrm{OCP}] \qquad \text{(SI-7)}$$

For experiments conducted with aldicarb, only parent compound disappearance was followed in batch reactions; the formation of reaction products was not monitored. Consequently, the kinetic model was simplified to consider only first-order decay of the parent OCP:

$$-\frac{d[\mathrm{OCP}]}{dt} = k_{obs}[\mathrm{OCP}] \qquad \text{(SI-8)}$$

For purposes of data analysis, we then assumed that any increase in the value of k_{obs} obtained when Fe^{II} was added to solution was due solely to reactions involving electron transfer between Fe^{II} and aldicarb. Consequently, values of k_{red} for aldicarb were estimated by the difference between k_{obs} measured in the presence of Fe^{II} and k_{obs} measured in Fe^{II}-free solution at the same pH and temperature:

$$k_{red} = k_{obs}(Fe^{II}\ \text{present}) - k_{obs}(Fe^{II}\ \text{absent}) \qquad \text{(SI-9)}$$

It should be noted that this approach ignores the possible contribution of other aldicarb degradation pathways that might occur in solutions containing Fe^{II} and organic ligands (*e.g.*, metal-ion complex catalyzed hydrolysis). However, observed trends in the calculated values of k_{red} for aldicarb are similar to the trends observed for oxamyl and methomyl (Figure 11). This finding suggests that the assumption we invoked is valid.

Calculating Second-Order Rate Constants

Scientist was also used to calculate second-order rate constants (k_i ; $M^{-1} h^{-1}$) for oxamyl reduction by individual Fe^{II} species; results obtained from data fits are provided in Table 2. This was done by fitting an expanded form of eq 2 to experimentally measured values of k_{red}. For example, the following expression was used to fit kinetic data obtained in solutions containing Fe^{II} and the ligand EDTA:

$$k_{red} = [Fe^{II}](k_{Fe(2+)}\alpha_{Fe(2+)} + k_{Fe(OH)2}\alpha_{Fe(OH)2} + k_{Fe(HEDTA)}\alpha_{Fe(HEDTA)} + k_{Fe(EDTA)}\alpha_{Fe(EDTA)}) \quad \text{(SI-10)}$$

where $[Fe^{II}]$ and α_i represent the total Fe^{II} concentration and the fractional concentration of species *i*, respectively. According to eq SI-10, the overall reactivity of oxamyl with Fe^{II} is approximated by the sum of the contributions of parallel reactions with hexaquo Fe^{2+}, the second Fe^{II} hydrolysis species, and two different Fe^{II} complexes with EDTA. The kinetic contributions of all other Fe^{II} species were found to be negligible. Values of k_{red} were measured in batch reactions (Table S1) and values of α_i were calculated for the corresponding solution conditions using available equilibrium constants (Table S2). Consequently, the only unknown parameters in eq SI-10 were the values of k_i for each Fe^{II} species. Least-squares data fitting was then carried out using a modified Powell algorithm. Output and statistics obtained from data fitting was the same as that listed above for calculating first-order rate constants.

Model fitting was carried out in a stepwise fashion. Systems with the least number of Fe^{II} species were fit first (*e.g.*, solutions containing no organic ligands). Second-order rate constants derived from fitting data in these systems (*e.g.*, $k_{Fe(2+)}$, $k_{Fe(OH)2}$) were then fixed when fitting the data obtained for more complex systems that include additional Fe^{II} species (*e.g.*, Fe^{II}-EDTA species). This approach minimized the number of adjustable fitting parameters in complex systems that contain several different Fe^{II} species.

Data fits for individual systems (*e.g.*, solutions containing Fe^{II} + NTA) were carried out using the minimum number of "reactive" Fe^{II} species necessary. Species were considered to be "reactive" only if data fits were significantly improved when their k_i value was included as an adjustable fitting parameter. All other species were considered "unreactive" and their k_i values were fixed at zero during data fitting. It should be noted, however, that "unreactive" species still affected overall OCP reduction kinetics by reducing the α values for the "reactive" species present in the same system. Furthermore, the designation of individual Fe^{II} species as "unreactive" did not imply that oxamyl does not react with these species. Instead, it signified that their contribution to k_{red} (*i.e.*, $k_i\alpha_i$) is negligible compared with the contribution of other Fe^{II} species present in the same system.

Upper-limit estimates are also reported in Table 2 for selected Fe^{II} species that were considered "unreactive" during data fitting. Estimates were made by first calculating $k_{red}/[Fe^{II}_i]$ for each batch reaction in a given system (*e.g.*, all batch reactions containing Fe^{II} + NTA), where $[Fe^{II}_i]$ is the concentration of the "unreactive" species of interest (*e.g.*, $Fe(NTA)_2^{4-}$). This quotient would be equal to the second-order rate constant for species of interest if it were the only "reactive" species present. The minimum value obtained for $k_{red}/[Fe^{II}_i]$ in a given system was then taken to be a conservative upper-limit estimate for the k_i value of species *i*. Since we expect that the other "reactive" species are in fact responsible for the bulk of the observed reactivity, true values of k_i for the "unreactive" species are likely to be significantly lower than the upper-limit estimates calculated by this procedure.

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Table S1. Pseudo First-Order Rate Constants for OCP Degradation in the Presence of Selected Organic Ligands and Natural Organic Matter[a,b,c]

No Organic Ligand	
25 μM oxamyl, pH 2.07, 0.1 M NaCl	$k_{elim} < 7 \times 10^{-5}$ h^{-1} [d]
25 μM oxamyl, pH 3.08, 0.1 M NaCl	$k_{elim} < 7 \times 10^{-5}$ h^{-1} [d]
25 μM oxamyl, pH 4.66 (2 mM acetate), 0.1 M NaCl	$k_{elim} < 7 \times 10^{-5}$ h^{-1} [d]
25 μM oxamyl, pH 5.55 (25 mM MES), 0.1 M NaCl	$k_{elim} = 1.35(\pm0.041) \times 10^{-4}$ h^{-1}
25 μM oxamyl, pH 6.09 (25 mM MES), 0.1 M NaCl	$k_{elim} = 4.56(\pm0.051) \times 10^{-4}$ h^{-1}
25 μM oxamyl, pH 6.57 (25 mM MOPS), 0.1 M NaCl	$k_{elim} = 1.35(\pm0.014) \times 10^{-3}$ h^{-1}
25 μM oxamyl, pH 6.85 (25 mM MOPS), 0.1 M NaCl	$k_{elim} = 2.52(\pm0.020) \times 10^{-3}$ h^{-1}
25 μM oxamyl, pH 7.10 (25 mM MOPS), 0.1 M NaCl	$k_{elim} = 4.47(\pm0.026) \times 10^{-3}$ h^{-1}
25 μM oxamyl, pH 7.40 (25 mM MOPS), 0.1 M NaCl	$k_{elim} = 8.42(\pm0.062) \times 10^{-3}$ h^{-1}
25 μM oxamyl, pH 7.66 (25 mM MOPS), 0.1 M NaCl	$k_{elim} = 1.51(\pm0.007) \times 10^{-2}$ h^{-1}
25 μM oxamyl, pH 7.95 (25 mM TAPS), 0.1 M NaCl	$k_{elim} = 2.81(\pm0.025) \times 10^{-2}$ h^{-1}
0.5 mM Fe^{II}, 25 μM oxamyl, pH 2.02, 0.1 M NaCl	$k_{red} = 4.44(\pm0.040) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 3.04, 0.1 M NaCl	$k_{red} = 4.43(\pm0.031) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 3.93, 0.1 M NaCl	$k_{red} = 4.43(\pm0.026) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 4.56 (2 mM acetate), 0.1 M NaCl	$k_{red} = 4.72(\pm0.069) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 5.48 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.60(\pm0.046) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 6.11 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.85(\pm0.047) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 6.58 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 4.47(\pm0.47) \times 10^{-3}$ h^{-1}; $k_{elim} = 1.38 \times 10^{-3}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 6.87 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 5.58(\pm0.053) \times 10^{-3}$ h^{-1}; $k_{elim} = 2.62 \times 10^{-3}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 7.13 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 6.53(\pm0.075) \times 10^{-3}$ h^{-1}; $k_{elim} = 4.65 \times 10^{-3}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 7.40 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 8.94(\pm0.098) \times 10^{-3}$ h^{-1}; $k_{elim} = 8.43 \times 10^{-3}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 7.67 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.09(\pm0.020) \times 10^{-2}$ h^{-1}; $k_{elim} = 1.53 \times 10^{-2}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 7.80 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 6.46(\pm0.15) \times 10^{-2}$ h^{-1}; $k_{elim} = 2.04 \times 10^{-2}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 7.93 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 9.92(\pm0.19) \times 10^{-2}$ h^{-1}; $k_{elim} = 2.71 \times 10^{-2}$ h^{-1} [f]
0.5 mM Fe^{II}, 25 μM oxamyl, pH 8.19 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 2.47(\pm0.064) \times 10^{-1}$ h^{-1}; $k_{elim} = 4.81 \times 10^{-2}$ h^{-1} [f]

Table S1. Continued

Effect of Acetate	
0.5 mM Fe^{II}, 2 mM acetate, 25 μM oxamyl, pH 4.56, 0.1 M NaCl	$k_{red} = 4.72(\pm0.069) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 22 mM acetate, 25 μM oxamyl, pH 4.59, 0.1 M NaCl	$k_{red} = 6.20(\pm0.046) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 50 mM acetate, 25 μM oxamyl, pH 4.59, 0.1 M NaCl	$k_{red} = 7.64(\pm0.033) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 90 mM acetate, 25 μM oxamyl, pH 4.60, 0.1 M NaCl	$k_{red} = 9.77(\pm0.088) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 135 mM acetate, 25 μM oxamyl, pH 4.61, 0.1 M NaCl	$k_{red} = 1.20(\pm0.014) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 200 mM acetate, 25 μM oxamyl, pH 4.58, 0.1 M NaCl	$k_{red} = 1.54(\pm0.014) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 300 mM acetate, 25 μM oxamyl, pH 4.59, 0.1 M NaCl	$k_{red} = 2.01(\pm0.035) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 400 mM acetate, 25 μM oxamyl, pH 4.59, 0.1 M NaCl	$k_{red} = 2.60(\pm0.078) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 500 mM acetate, 25 μM oxamyl, pH 4.59, 0.1 M NaCl	$k_{red} = 3.38(\pm0.17) \times 10^{-2}$ h^{-1}; no elimination[e]
25 μM oxamyl, 10 mM acetate, pH 6.14, 0.1 M NaCl	$k_{elim} = 5.54(\pm0.16) \times 10^{-4}$ h^{-1}
Effect of Malonate	
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 3.01, 0.1 M NaCl	$k_{red} = 4.68(\pm0.053) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 4.20 (10 mM acetate), 0.1 M NaCl	$k_{red} = 6.52(\pm0.035) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 4.92 (10 mM acetate), 0.1 M NaCl	$k_{red} = 2.14(\pm0.013)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.05(\pm0.027)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 6.07 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.60(\pm0.031)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 25 mM malonate, 25 μM oxamyl, pH 6.98 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 4.99(\pm0.045)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 3 mM malonate, 25 μM oxamyl, pH 5.51 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.48(\pm0.070) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM malonate, 25 μM oxamyl, pH 5.51 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.95(\pm0.013)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 50 mM malonate, 25 μM oxamyl, pH 5.51 (25 mM MES)	$k_{red} = 6.31(\pm0.064)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 100 mM malonate, 25 μM oxamyl, pH 5.50 (25 mM MES)	$k_{red} = 8.97(\pm0.089)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 150 mM malonate, 25 μM oxamyl, pH 5.50 (25 mM MES)	$k_{red} = 1.09(\pm0.013) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 200 mM malonate, 25 μM oxamyl, pH 5.50 (25 mM MES)	$k_{red} = 1.18(\pm0.012) \times 10^{1}$ h^{-1}; no elimination[e]
25 μM oxamyl, 10 mM malonate, pH 6.20, 0.1 M NaCl	$k_{elim} = 6.34(\pm0.15) \times 10^{-4}$ h^{-1}

Table S1. Continued

Effect of Oxalate	
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 2.15, 0.1 M NaCl	$k_{red} = 6.38(\pm0.074) \times 10^{-1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 2.63, 0.1 M NaCl	$k_{red} = 2.04(\pm0.032)\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 2.98, 0.1 M NaCl	$k_{red} = 4.80(\pm0.010)\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 3.57, 0.1 M NaCl	$k_{red} = 1.02(\pm0.011) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 4.05, 0.1 M NaCl	$k_{red} = 1.91(\pm0.11) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 4.65, 0.1 M NaCl	$k_{red} = 1.98(\pm0.020) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 5.23, 0.1 M NaCl	$k_{red} = 2.10(\pm0.034) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 5.53 (25 mM MES), 0.1 M NaCl	$k_{red} = 2.20(\pm0.039) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 6.09 (25 mM MES), 0.1 M NaCl	$k_{red} = 2.16(\pm0.019) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 µM oxamyl, pH 7.13 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 2.25(\pm0.028) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 0.5 mM oxalate, 25 µM oxamyl, pH 5.55 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.61(\pm0.015)\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 1 mM oxalate, 25 µM oxamyl, pH 5.56 (25 mM MES), 0.1 M NaCl	$k_{red} = 3.86(\pm0.035)\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 2 mM oxalate, 25 µM oxamyl, pH 5.56 (25 mM MES), 0.1 M NaCl	$k_{red} = 8.58(\pm0.046)\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 4 mM oxalate, 25 µM oxamyl, pH 5.55 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.72(\pm0.013) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 8 mM oxalate, 25 µM oxamyl, pH 5.54 (25 mM MES), 0.1 M NaCl	$k_{red} = 2.72(\pm0.025) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 16 mM oxalate, 25 µM oxamyl, pH 5.54 (25 mM MES), 0.1 M NaCl	$k_{red} = 3.84(\pm0.031) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 32 mM oxalate, 25 µM oxamyl, pH 5.55 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.47(\pm0.024) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 50 mM oxalate, 25 µM oxamyl, pH 5.56 (25 mM MES)	$k_{red} = 4.62(\pm0.031) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 75 mM oxalate, 25 µM oxamyl, pH 5.60 (25 mM MES)	$k_{red} = 4.51(\pm0.026) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 100 mM oxalate, 25 µM oxamyl, pH 5.55 (25 mM MES)	$k_{red} = 3.91(\pm0.027) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 125 mM oxalate, 25 µM oxamyl, pH 5.59 (25 mM MES)	$k_{red} = 3.61(\pm0.036) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 150 mM oxalate, 25 µM oxamyl, pH 5.63 (25 mM MES)	$k_{red} = 3.23(\pm0.046) \times 10^{1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 200 mM oxalate, 25 µM oxamyl, pH 5.61 (25 mM MES)	$k_{red} = 2.60(\pm0.024) \times 10^{1}\ h^{-1}$; no elimination[e]
25 µM oxamyl, 10 mM oxalate, pH 6.12, 0.1 M NaCl	$k_{elim} = 5.44(\pm0.096) \times 10^{-4}\ h^{-1}$
Effect of Citrate	
0.5 mM Fe^{II}, 5 mM citrate, 25 µM oxamyl, pH 2.14, 0.1 M NaCl	$k_{red} = 5.78(\pm0.060) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 µM oxamyl, pH 2.55, 0.1 M NaCl	$k_{red} = 1.26(\pm0.075) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 µM oxamyl, pH 2.99, 0.1 M NaCl	$k_{red} = 2.94(\pm0.033) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 µM oxamyl, pH 3.48, 0.1 M NaCl	$k_{red} = 1.35(\pm0.098) \times 10^{-1}\ h^{-1}$; no elimination[e]

Table S1. Continued

0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 3.93, 0.1 M NaCl	$k_{red} = 4.64(\pm0.046) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 4.51, 0.1 M NaCl	$k_{red} = 9.68(\pm0.012) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 5.30 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.19(\pm0.018)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 5.49 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.04(\pm0.016)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 5.87 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.20(\pm0.020)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM oxamyl, pH 7.12 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.14(\pm0.020)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM citrate, 25 μM oxamyl, pH 4.04, 0.1 M NaCl	$k_{red} = 6.98(\pm0.097) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 20 mM citrate, 25 μM oxamyl, pH 4.04, 0.1 M NaCl	$k_{red} = 7.99(\pm0.15) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 30 mM citrate, 25 μM oxamyl, pH 4.00, 0.1 M NaCl	$k_{red} = 7.83(\pm0.11) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 40 mM citrate, 25 μM oxamyl, pH 4.02, 0.1 M NaCl	$k_{red} = 7.96(\pm0.11) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.5 mM citrate, 25 μM oxamyl, pH 5.47 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.97(\pm0.081) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.75 mM citrate, 25 μM oxamyl, pH 5.49 (25 mM MES), 0.1 M NaCl	$k_{red} = 8.28(\pm0.12) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 1 mM citrate, 25 μM oxamyl, pH 5.49 (25 mM MES), 0.1 M NaCl	$k_{red} = 9.00(\pm0.12) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 2 mM citrate, 25 μM oxamyl, pH 5.48 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.02(\pm0.013)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM citrate, 25 μM oxamyl, pH 5.49 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.05(\pm0.012)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 20 mM citrate, 25 μM oxamyl, pH 5.48 (25 mM MES), 0.1 M NaCl	$k_{red} = 9.06(\pm0.013) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 50 mM citrate, 25 μM oxamyl, pH 5.51 (25 mM MES)	$k_{red} = 7.98(\pm0.16) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 100 mM citrate, 25 μM oxamyl, pH 5.49 (25 mM MES)	$k_{red} = 4.61(\pm0.036) \times 10^{-1}$ h^{-1}; no elimination[e]
25 μM oxamyl, 10 mM citrate, pH 6.13, 0.1 M NaCl	$k_{elim} = 5.45(\pm0.13) \times 10^{-4}$ h^{-1}
Effect of IDA	
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 2.09, 0.1 M NaCl	$k_{red} = 5.12(\pm0.051) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 3.02, 0.1 M NaCl	$k_{red} = 1.10(\pm0.011) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 4.58 (10 mM acetate), 0.1 M NaCl	$k_{red} = 2.30(\pm0.028) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 5.51 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.01(\pm0.012)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 6.03 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.51(\pm0.016)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 6.49 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.65(\pm0.020)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 7.09 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.25(\pm0.012)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 7.52 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 7.96(\pm0.094) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM oxamyl, pH 8.09 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 3.45(\pm0.064) \times 10^{-1}$ h^{-1}; $k_{elim} = 3.86 \times 10^{-2}$ h^{-1}[f]
0.5 mM Fe^{II}, 0.25 mM IDA, 25 μM oxamyl, pH 7.10 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 7.49(\pm0.14) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.50 mM IDA, 25 μM oxamyl, pH 7.11 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.28(\pm0.017)$ h^{-1}; no elimination[e]

Table S1. Continued

0.5 mM Fe^{II}, 0.75 mM IDA, 25 µM oxamyl, pH 7.08 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.31(\pm0.0091)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 1 mM IDA, 25 µM oxamyl, pH 7.08 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.49(\pm0.015)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 2 mM IDA, 25 µM oxamyl, pH 7.07 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.75(\pm0.012)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 4 mM IDA, 25 µM oxamyl, pH 7.06 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.65(\pm0.019)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 20 mM IDA, 25 µM oxamyl, pH 7.10 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 8.43(\pm0.098) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 40 mM IDA, 25 µM oxamyl, pH 7.09 (25 mM MOPS)	$k_{red} = 5.33(\pm0.051) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 100 mM IDA, 25 µM oxamyl, pH 7.11 (25 mM MOPS)	$k_{red} = 2.50(\pm0.024) \times 10^{-1}$ h^{-1}; no elimination[e]
25 µM oxamyl, 10 mM IDA, pH 6.13, 0.1 M NaCl	$k_{elim} = 5.82(\pm0.12) \times 10^{-4}$ h^{-1}
Effect of NTA	
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 1.99, 0.1 M NaCl	$k_{red} = 1.92(\pm0.060) \times 10^{-1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 2.45, 0.1 M NaCl	$k_{red} = 1.24(\pm0.012)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 2.99, 0.1 M NaCl	$k_{red} = 4.12(\pm0.030)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 3.45, 0.1 M NaCl	$k_{red} = 7.24(\pm0.068)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 4.64 (25 mM acetate), 0.1 M NaCl	$k_{red} = 1.07(\pm0.087) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.15(\pm0.047) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 6.14 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.15(\pm0.011) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 7.12 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.16(\pm0.044) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 7.37 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.16(\pm0.018) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 8.42 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 8.55(\pm0.11)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 µM oxamyl, pH 8.89 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 6.27(\pm0.092)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.2 mM NTA, 25 µM oxamyl, pH 7.41 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 5.27(\pm0.043)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.35 mM NTA, 25 µM oxamyl, pH 7.38 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 9.63(\pm0.048)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 0.5 mM NTA, 25 µM oxamyl, pH 7.40 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.10(\pm0.035) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 1 mM NTA, 25 µM oxamyl, pH 7.40 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.07(\pm0.018) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 2 mM NTA, 25 µM oxamyl, pH 7.39 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.09(\pm0.011) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM NTA, 25 µM oxamyl, pH 7.39 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.00(\pm0.010) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 20 mM NTA, 25 µM oxamyl, pH 7.38 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 8.97(\pm0.11)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 50 mM NTA, 25 µM oxamyl, pH 7.39 (25 mM MOPS)	$k_{red} = 7.46(\pm0.070)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 100 mM NTA, 25 µM oxamyl, pH 7.37 (25 mM MOPS)	$k_{red} = 4.87(\pm0.031)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 1 mM NTA, 25 µM oxamyl, pH 8.87 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 1.15(\pm0.0085) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 15 mM NTA, 25 µM oxamyl, pH 8.87 (25 mM TAPS), 0.1 M NaCl	$k_{red} = 3.41(\pm0.036)$ h^{-1}; no elimination[e]

Table S1. Continued

0.5 mM Fe^{II}, 50 mM NTA, 25 μM oxamyl, pH 8.89 (25 mM TAPS)	$k_{red} = 1.31(\pm0.016)\ h^{-1}$; $k_{elim} = 2.25 \times 10^{-1}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 75 mM NTA, 25 μM oxamyl, pH 8.90 (25 mM TAPS)	$k_{red} = 8.08(\pm0.29) \times 10^{-1}\ h^{-1}$; $k_{elim} = 2.30 \times 10^{-1}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 100 mM NTA, 25 μM oxamyl, pH 8.87 (25 mM TAPS)	$k_{red} = 6.20(\pm0.26) \times 10^{-1}\ h^{-1}$; $k_{elim} = 2.15 \times 10^{-1}\ h^{-1}$ [f]
25 μM oxamyl, 10 mM NTA, pH 6.16, 0.1 M NaCl	$k_{elim} = 5.98(\pm0.12) \times 10^{-4}\ h^{-1}$
Effect of EDTA	
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 2.84, 0.1 M NaCl	$k_{red} = 1.65(\pm0.024) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 3.39, 0.1 M NaCl	$k_{red} = 9.02(\pm0.13) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 3.99 (5 mM acetate), 0.1 M NaCl	$k_{red} = 5.52(\pm0.084) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 4.46 (5 mM acetate), 0.1 M NaCl	$k_{red} = 4.91(\pm0.044) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 5.01 (5 mM acetate), 0.1 M NaCl	$k_{red} = 4.71(\pm0.044) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 5.42 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.55(\pm0.033) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 6.04 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.40(\pm0.033) \times 10^{-3}\ h^{-1}$; $k_{elim} = 4.20 \times 10^{-4}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 7.09 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 4.86(\pm0.12) \times 10^{-3}\ h^{-1}$; $k_{elim} = 4.25 \times 10^{-3}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 0.5 mM EDTA, 25 μM oxamyl, pH 5.41 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.80(\pm0.14) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 1 mM EDTA, 25 μM oxamyl, pH 5.40 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.52(\pm0.14) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM oxamyl, pH 5.41 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.34(\pm0.056) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 20 mM EDTA, 25 μM oxamyl, pH 5.39 (25 mM MES), 0.1 M NaCl	$k_{red} = 4.31(\pm0.098) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 50 mM EDTA, 25 μM oxamyl, pH 5.55 (25 mM MES)	$k_{red} = 4.41(\pm0.027) \times 10^{-3}\ h^{-1}$; no elimination[e]
25 μM oxamyl, 10 mM EDTA, pH 6.14, 0.1 M NaCl	$k_{elim} = 5.75(\pm0.12) \times 10^{-4}\ h^{-1}$
Effect of TMDTA	
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 2.05, 0.1 M NaCl	$k_{red} = 8.29(\pm0.078) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 2.50, 0.1 M NaCl	$k_{red} = 2.14(\pm0.027) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 3.02, 0.1 M NaCl	$k_{red} = 6.97(\pm0.096) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 3.81 (25 mM acetate), 0.1 M NaCl	$k_{red} = 1.26(\pm0.021) \times 10^{-1}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 4.32 (25 mM acetate), 0.1 M NaCl	$k_{red} = 6.19(\pm0.071) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 4.86 (25 mM acetate), 0.1 M NaCl	$k_{red} = 2.14(\pm0.022) \times 10^{-2}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.00(\pm0.053) \times 10^{-3}\ h^{-1}$; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 5.99 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.76(\pm0.019) \times 10^{-3}\ h^{-1}$; $k_{elim} = 3.76 \times 10^{-4}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 6.42 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 7.10(\pm0.082) \times 10^{-4}\ h^{-1}$; $k_{elim} = 9.71 \times 10^{-4}\ h^{-1}$ [f]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 6.98 (25 mM MOPS), 0.1 M NaCl	$k_{red} = 1.91(\pm0.34) \times 10^{-4}\ h^{-1}$; $k_{elim} = 3.34 \times 10^{-3}\ h^{-1}$ [f]

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Table S1. Continued

0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM oxamyl, pH 7.59 (25 mM MES), 0.1 M NaCl	$k_{elim} = 1.29(\pm0.028) \times 10^{-2}$ h^{-1}; no reduction[g]
0.5 mM Fe^{II}, 0.5 mM TMDTA, 25 μM oxamyl, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.65(\pm0.064) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 1 mM TMDTA, 25 μM oxamyl, pH 5.41 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.17(\pm0.051) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 2 mM TMDTA, 25 μM oxamyl, pH 5.42 (25 mM MES), 0.1 M NaCl	$k_{red} = 6.11(\pm0.044) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM TMDTA, 25 μM oxamyl, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{red} = 5.91(\pm0.044) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 20 mM TMDTA, 25 μM oxamyl, pH 5.44 (25 mM MES), 0.1 M NaCl	$k_{red} = 5.74(\pm0.037) \times 10^{-3}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 50 mM TMDTA, 25 μM oxamyl, pH 5.45 (25 mM MES)	$k_{red} = 6.21(\pm0.019) \times 10^{-3}$ h^{-1}; no elimination[e]
25 μM oxamyl, 10 mM TMDTA, pH 6.14, 0.1 M NaCl	$k_{elim} = 5.59(\pm0.087) \times 10^{-4}$ h^{-1}
Reactions in Reconstituted Great Dismal Swamp Water [h]	
0.25 mM Fe^{II}, 0 mg TOC/L, 12.5 μM oxamyl, pH 5.53 (10 mM MES)	$k_{red} = 2.45(\pm0.17) \times 10^{-3}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 18.75 mg TOC/L, 12.5 μM oxamyl, pH 5.50 (10 mM MES)	$k_{red} = 3.82(\pm0.056) \times 10^{-2}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 37.5 mg TOC/L, 12.5 μM oxamyl, pH 5.51 (10 mM MES)	$k_{red} = 8.03(\pm0.073) \times 10^{-2}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 75 mg TOC/L, 12.5 μM oxamyl, pH 5.53 (10 mM MES)	$k_{red} = 1.55(\pm0.021) \times 10^{-1}$ h^{-1}; no elimination[e]
12.5 μM oxamyl, 37.5 mg TOC/L, pH 5.52 (10 mM MES)	$k_{red} = 1.58(\pm0.021) \times 10^{-2}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 37.5 mg TOC/L, 10 mM EDTA, 12.5 μM oxamyl, pH 5.53 (10 mM MES)	$k_{red} = 2.06(\pm0.14) \times 10^{-3}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 10 mM EDTA, 12.5 μM oxamyl, pH 5.51 (10 mM MES)	$k_{red} = 2.12(\pm0.09) \times 10^{-3}$ h^{-1}; no elimination[e]
Survey of Ligand Effects on Methomyl Reduction	
0.5 mM Fe^{II}, 25 μM methomyl, pH 5.52 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.31(\pm0.037) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 200 mM acetate, 25 μM methomyl, pH 4.57, 0.1 M NaCl	$k_{red} = 3.21(\pm0.013) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM malonate, 25 μM methomyl, pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.25(\pm0.020)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM oxalate, 25 μM methomyl, pH 5.53 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.02(\pm0.008) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM citrate, 25 μM methomyl, pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.77(\pm0.025)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 10 mM IDA, 25 μM methomyl, pH 5.51 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.77(\pm0.026)$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM NTA, 25 μM methomyl; pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{red} = 2.36(\pm0.015) \times 10^{1}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM methomyl, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.89(\pm0.031) \times 10^{-2}$ h^{-1}; no elimination[e]
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM methomyl, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{red} = 1.22(\pm0.017) \times 10^{-2}$ h^{-1}; no elimination[e]
0.25 mM Fe^{II}, 37.5 mg TOC/L, 12.5 μM methomyl, pH 5.54 (10 mM MES)	$k_{red} = 9.07(\pm0.28) \times 10^{-2}$ h^{-1}; no elimination[e]

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Table S1. Continued

Survey of Ligand Effects on Aldicarb Reduction[i]	
0.5 mM Fe^{II}, 25 μM aldicarb, pH 5.52 (25 mM MES), 0.1 M NaCl	$k_{obs} = 8.04(\pm0.21) \times 10^{-4}\ h^{-1}$
0.5 mM Fe^{II}, 200 mM acetate, 25 μM aldicarb, pH 4.57, 0.1 M NaCl	$k_{obs} = 1.33(\pm0.045) \times 10^{-3}\ h^{-1}$
0.5 mM Fe^{II}, 10 mM malonate, 25 μM aldicarb, pH 5.50 (25 mM MES), 0.1 M NaCl	$k_{obs} = 5.75(\pm0.031) \times 10^{-2}\ h^{-1}$
0.5 mM Fe^{II}, 5 mM oxalate, 25 μM aldicarb, pH 5.53 (25 mM MES), 0.1 M NaCl	$k_{obs} = 7.50(\pm0.065) \times 10^{-1}\ h^{-1}$
0.5 mM Fe^{II}, 5 mM citrate, 25 μM aldicarb, pH 5.46 (25 mM MES), 0.1 M NaCl	$k_{obs} = 1.42(\pm0.011) \times 10^{-1}\ h^{-1}$
0.5 mM Fe^{II}, 10 mM IDA, 25 μM aldicarb, pH 5.51 (25 mM MES), 0.1 M NaCl	$k_{obs} = 7.73(\pm0.028) \times 10^{-2}\ h^{-1}$
0.5 mM Fe^{II}, 5 mM NTA, 25 μM aldicarb, pH 5.46 (25 mM MES), 0.1 M NaCl	$k_{obs} = 4.07(\pm0.074) \times 10^{-1}\ h^{-1}$
0.5 mM Fe^{II}, 5 mM EDTA, 25 μM aldicarb, pH 5.43 (25 mM MES), 0.1 M NaCl	$k_{obs} = 6.03(\pm0.16) \times 10^{-4}\ h^{-1}$
0.5 mM Fe^{II}, 5 mM TMDTA, 25 μM aldicarb, pH 5.40 (25 mM MES), 0.1 M NaCl	$k_{obs} = 8.38(\pm0.20) \times 10^{-4}\ h^{-1}$
0.25 mM Fe^{II}, 37.5 mg TOC/L, 25 μM aldicarb, pH 5.49 (10 mM MES)	$k_{obs} = 5.57(\pm0.10) \times 10^{-3}\ h^{-1}$
25 μM aldicarb, pH 4.57 (25 mM acetate), 0.1 M NaCl	$k_{obs} = 1.83(\pm0.18) \times 10^{-4}\ h^{-1}$
25 μM aldicarb, pH 5.52 (25 mM MES), 0.1 M NaCl	$k_{obs} = 7.09(\pm2.06) \times 10^{-5}\ h^{-1}$

[a]All reactions continuously mixed under darkness at 25.0 ± 0.1 °C (constant temperature water bath) within a glove box (95 % N_2, 5 % H_2). [b]Fe^{II} added as $FeCl_2 \bullet 6H_2O$. [c]Numbers in parenthesis indicate standard deviation of best-fit values determined from model fits. [d]Elimination is too slow to accurately calculate k_{elim}. [e]No significant formation of OCP elimination product observed during OCP degradation (*i.e.*, $k_{red} >> k_{elim}$); data fitting only considers OCP reduction. [f]k_{elim} calculated using eq 12 in Ref. *25*; this value is then fixed when calculating k_{red}. [g]No significant formation of nitrile reduction product observed during OCP degradation (*i.e.*, $k_{elim} >> k_{red}$); data fitting only considers OCP elimination. [h]Concentration of Fe^{II} listed for NOM reactions represents the concentration spiked into solution. The NOM isolate itself contains 0.21 μM Fe^{II}/mg TOC. [i]For aldicarb, k_{red} values shown in Figure 11 are calculated as the difference between k_{obs} measured in the presence of Fe^{II} and k_{obs} measured in Fe^{II}-free solution at the same pH.

Table S2. Equilibrium Expressions and Stability Constants Used for Calculating the Fe^{II} Speciation and Standard One-Electron Reduction Potentials of Selected Fe^{III}/Fe^{II} Redox Couples

Reaction	log *K* [a]
Iron Hydrolysis Reactions	
$Fe^{2+} + H_2O - H^+ = FeOH^+$	-9.397
$Fe^{2+} + 2\,H_2O - 2\,H^+ = Fe(OH)_2^0$	-20.494
$Fe^{2+} + 3\,H_2O - 3\,H^+ = Fe(OH)_3^-$	-28.991
$Fe^{2+} + 4\,H_2O - 4\,H^+ = Fe(OH)_4^{2-}$	-45.988
$Fe^{3+} + H_2O - H^+ = FeOH^{2+}$	-2.187
$Fe^{3+} + 2\,H_2O - 2\,H^+ = Fe(OH)_2^+$	-4.594
$Fe^{3+} + 3\,H_2O - 3\,H^+ = Fe(OH)_3^0$	-13.600[b]
$Fe^{3+} + 4\,H_2O - 4\,H^+ = Fe(OH)_4^-$	-21.588
$2\,Fe^{3+} + 2\,H_2O - 2\,H^+ = Fe_2(OH)_2^{4+}$	-2.854
$3\,Fe^{3+} + 4\,H_2O - 4\,H^+ = Fe_3(OH)_4^{5+}$	-6.288
Iron Oxide Solubility-Controlling Phases	
$Fe^{2+} + 2\,H_2O - 2\,H^+ = Fe(OH)_2(s)$ (amorphous)	-12.844[c]
$Fe^{3+} + 3\,H_2O - 3\,H^+ = Fe(OH)_3(s)$ (amorphous)	-3.00[d]
Reactions Involving Chloride	
$Fe^{2+} + Cl^- = FeCl^+$	-0.200
$Fe^{3+} + Cl^- = FeCl^{2+}$	1.480
$Fe^{3+} + 2\,Cl^- = FeCl_2^+$	2.130
$Fe^{3+} + 3\,Cl^- = FeCl_3^0$	1.13[b]
$Na^+ + Cl^- = NaCl^0$	-0.500
Reactions Involving Acetate	
$H^+ + L^- = HL^0$	4.757
$Fe^{2+} + L^- = FeL^+$	1.400
$Fe^{3+} + L^- = FeL^{2+}$	4.023[e]
$Fe^{3+} + 2\,L^- = FeL_2^+$	7.571[e]
$Fe^{3+} + 3\,L^- = FeL_3^0$	9.586[e]
$Na^+ + L^- = NaL^0$	-0.180
Reactions Involving Malonate	
$H^+ + L^{2-} = HL^-$	5.696
$2\,H^+ + L^{2-} = H_2L^0$	8.543
$Fe^{2+} + L^{2-} = FeL^0$	2.985
$Fe^{2+} + 2\,L^{2-} = FeL_2^{2-}$	4.025
$Fe^{3+} + L^{2-} = FeL^+$	9.136
$Fe^{3+} + 2\,L^{2-} = FeL_2^-$	15.444
$Fe^{3+} + 3\,L^{2-} = FeL_3^{3-}$	1.616
$Na^+ + L^{2-} = NaL^-$	0.800
Reactions Involving Oxalate	
$H^+ + L^{2-} = HL^-$	4.266
$2\,H^+ + L^{2-} = H_2L^0$	5.518
$Fe^{2+} + L^{2-} = FeL^0$	3.865
$Fe^{2+} + 2\,L^{2-} = FeL_2^{2-}$	5.895

Table S2. Continued

$Fe^{2+} + 3\,L^{2-} = FeL_3^{4-}$	5.220[f]
$Fe^{3+} + L^{2-} = FeL^{+}$	8.803
$Fe^{3+} + 2\,L^{2-} = FeL_2^{-}$	15.441
$Fe^{3+} + 3\,L^{2-} = FeL_3^{3-}$	19.823
$Na^{+} + L^{2-} = NaL^{-}$	0.900
Reactions Involving Citrate	
$H^{+} + L^{3-} = HL^{2-}$	6.396
$2\,H^{+} + L^{3-} = H_2L^{-}$	11.157
$3\,H^{+} + L^{3-} = H_3L^{0}$	14.285
$Fe^{2+} + L^{3-} = FeL^{-}$	6.086
$Fe^{2+} + L^{3-} + H^{+} = FeHL^{0}$	10.153
$Fe^{2+} + L^{3-} + 2\,H^{+} = FeH_2L^{+}$	12.734[g]
$Fe^{2+} + 2\,L^{3-} + H^{+} = FeHL_2^{3-}$	13.343[g]
$2\,Fe^{2+} + 2\,L^{3-} + 2\,H_2O - 2\,H^{+} = Fe_2(OH)_2L_2^{4-}$	-4.583[g]
$Fe^{3+} + L^{3-} = FeL^{0}$	13.129
$Fe^{3+} + L^{3-} + H^{+} = FeHL^{+}$	14.382
$Fe^{3+} + L^{3-} + H_2O - H^{+} = Fe(OH)L^{-}$	10.214
$2\,Fe^{3+} + 2L^{3-} + 2\,H_2O - 2\,H^{+} = Fe_2(OH)_2L_2^{2-}$	24.414[e]
$Na^{+} + L^{3-} = NaL^{2-}$	1.393
Reactions Involving IDA	
$H^{+} + L^{2-} = HL^{-}$	9.790
$2\,H^{+} + L^{2-} = H_2L^{0}$	12.630
$3\,H^{+} + L^{2-} = H_3L^{+}$	14.480
$Fe^{2+} + L^{2-} = FeL^{0}$	6.657[e]
$Fe^{2+} + 2\,L^{2-} = FeL_2^{2-}$	10.957[e]
$Fe^{3+} + L^{2-} = FeL^{+}$	12.336
$Fe^{3+} + 2\,L^{2-} = FeL_2^{-}$	22.184
$Fe^{3+} + H^{+} + L^{2-} = FeHL^{2+}$	13.102
$Fe^{3+} + L^{2-} + H_2O - H^{+} = Fe(OH)L^{0}$	9.440
$Na^{+} + L^{2-} = NaL^{-}$	0.789[e]
Reactions Involving NTA	
$H^{+} + L^{3-} = HL^{2-}$	10.103
$2\,H^{+} + L^{3-} = H_2L^{-}$	13.051
$3\,H^{+} + L^{3-} = H_3L^{0}$	15.076
$4\,H^{+} + L^{3-} = H_4L^{+}$	16.076
$Fe^{2+} + L^{3-} = FeL^{-}$	10.186
$Fe^{2+} + 2\,L^{3-} = FeL_2^{4-}$	12.623
$Fe^{2+} + L^{3-} + H_2O - H^{+} = Fe(OH)L^{2-}$	-1.063
$Fe^{3+} + L^{3-} = FeL^{0}$	17.829
$Fe^{3+} + 2\,L^{3-} = FeL^{3-}$	25.929
$Fe^{3+} + L^{3-} + H^{+} = FeHL^{+}$	18.729
$Fe^{3+} + L^{3-} + H_2O - H^{+} = Fe(OH)L^{-}$	13.254
$Fe^{3+} + L^{3-} + 2\,H_2O - 2\,H^{+} = Fe(OH)_2L^{2-}$	5.246
$Fe^{3+} + L^{3-} + 3\,H_2O - 3\,H^{+} = Fe(OH)_3L^{3-}$	-6.117
$Na^{+} + L^{3-} = NaL^{2-}$	1.843

Table S2. Continued

Reactions Involving EDTA	
$H^+ + L^{4-} = HL^{3-}$	10.948
$2\,H^+ + L^{4-} = H_2L^{2-}$	17.221
$3\,H^+ + L^{4-} = H_3L^-$	20.340
$4\,H^+ + L^{4-} = H_4L^0$	22.554
$5\,H^+ + L^{4-} = H_5L^+$	24.054
$6\,H^+ + L^{4-} = H_6L^{2+}$	23.840
$Fe^{2+} + L^{4-} = FeL^{2-}$	16.014
$Fe^{2+} + L^{4-} + H^+ = FeHL^-$	19.054
$Fe^{3+} + L^{4-} = FeL^-$	27.671
$Fe^{3+} + L^{4-} + H^+ = FeHL^0$	29.186
$Fe^{3+} + L^{4-} + H_2O - H^+ = Fe(OH)L^{2-}$	19.873
$Na^+ + L^{4-} = NaL^{3-}$	2.717
Reactions Involving TMDTA	
$H^+ + L^{4-} = HL^{3-}$	11.157
$2\,H^+ + L^{4-} = H_2L^{2-}$	19.700
$3\,H^+ + L^{4-} = H_3L^-$	22.759
$4\,H^+ + L^{4-} = H_4L^0$	25.063
$Fe^{2+} + L^{4-} = FeL^{2-}$	15.134[e]
$Fe^{2+} + L^{4-} + H^+ = FeHL^-$	18.903[e]
$Fe^{3+} + L^{4-} = FeL^-$	23.971[e]
$Fe^{3+} + L^{4-} + H^+ = FeHL^0$	26.636[e]

[a]All equilibrium constants reported are corrected to zero ionic strength conditions using the Davies equation (*36*). Unless otherwise noted, equilibrium constants obtained from the computer program Critical (*35*) and are valid for 25 °C. [b]Ref *34*. [c]Ref *37*. [d]Ref *36*. [e]Valid for 20 °C. [f]Ref. *38*. [g]Valid for 37 °C.