

Supporting Information

Fig. S1. Quantitative analysis of the Mössbauer spectrum of the initial brown product from the reaction at 5 °C of apo R2-W48F/D84E with Fe(II) (3.1 equiv) and O₂. The sample is the same as that used to acquire Fig. 10, spectrum A. The spectrum was acquired at 4.2 K with a field of 50 mT applied parallel to the γ -beam. The solid line in A is the summation of the five quadrupole doublets determined to make up the diamagnetic portion of the spectrum. The parameters of these doublets are given in Table S1. B shows the spectrum of the same sample taken under identical conditions but with a narrower velocity range. The solid lines above the data are the constituent sub-spectra of the diamagnetic region, and the solid line plotted over the data is again the summation of these sub-spectra.

Fig. S2. Subtraction result of the high-field Mössbauer spectra of the brown and purple products of the R2-W48F/D84E reaction. The samples were the same as those used to acquire Fig. 10, spectra A and B. The experimental spectra of these samples were acquired at 4.2 K with a magnetic field of 8 T applied parallel to the γ -beam. The data shown is the result of subtracting the spectrum of the purple sample from that of the brown sample. The solid line plotted over the data is the summation of the simulated high-field sub-spectra of the decaying quadrupole doublets. These spectra were generated with the assumption that the associated species are diamagnetic.

Table S1. Mössbauer parameters for the diamagnetic early products of the reaction of apo R2-W48F/D84E with Fe(II) (3.1 equiv) and O₂.

Product	δ (mm/s)	ΔE_Q (mm/s)	Absorption (%)
1	0.50	0.57	20
2	0.48	1.24	10
3	0.49	2.17	16
4	0.53	1.73	16
5	0.46	2.47	5



