Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Probing the Ligand Recognition and Discrimination Environment of the Globin-Coupled Oxygen Sensor Protein YddV by FTIR and Time-Resolved Step-Scan FTIR Spectroscopy

Andrea Pavlou,[a] Markéta Martínková,[b] Toru Shimizu,[b] Kenichi Kitanishi,[b] Martin Stranava,[b] Andreas Loullis,[a] Eftychia Pinakoulaki[a,*]

[a] Department of Chemistry, University of Cyprus, PO Box 2037, 1678 Nicosia, Cyprus.

[b] Department of Biochemistry, Faculty of Science, Charles University in Prague, 128 43 Prague 2, Czech Republic.

Supplementary Figures

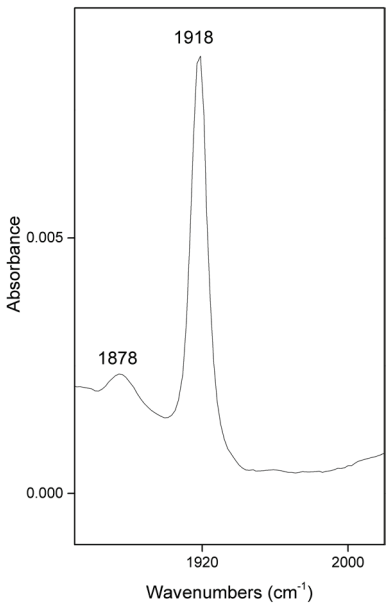

Fig. S1. FTIR spectrum of the YddV-heme-$^{13}C^{16}O$ adduct at pH 8. No baseline correction was performed in the FTIR spectrum.

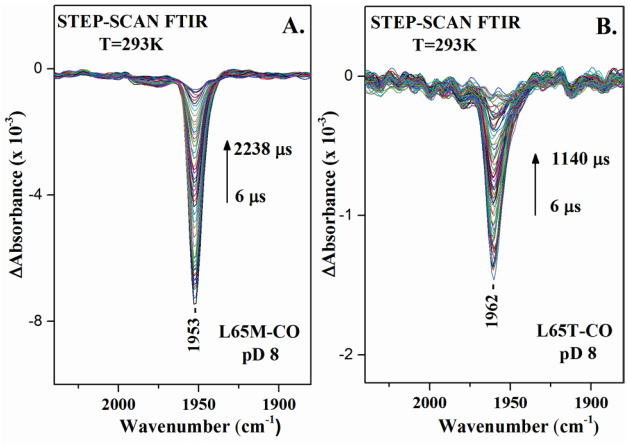

Fig. S2. Time-resolved step-scan FTIR difference spectra of the L65M **(A)** and L65T **(B)** YddV-heme-CO adducts at pD 8 subsequent to CO photolysis.

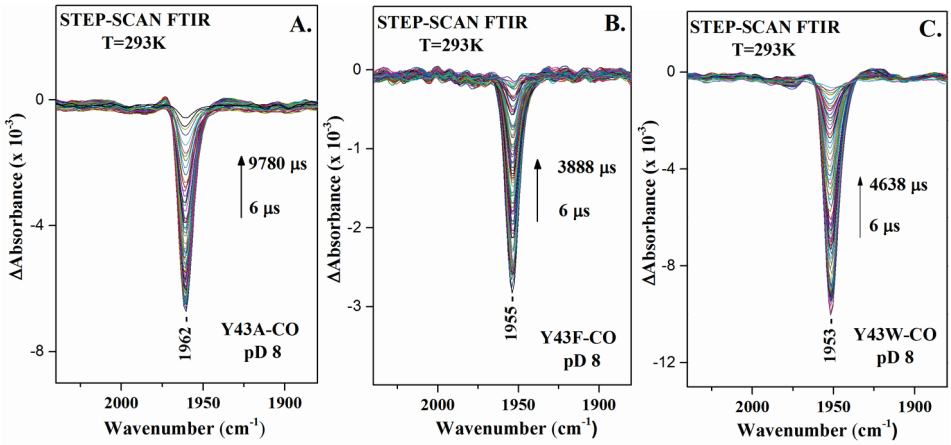

Fig. S3. Time-resolved step-scan FTIR difference spectra of the Y43A **(A)**, Y43F **(B)** and Y43W **(C)** YddV-heme-CO adducts at pD 8 subsequent to CO photolysis.

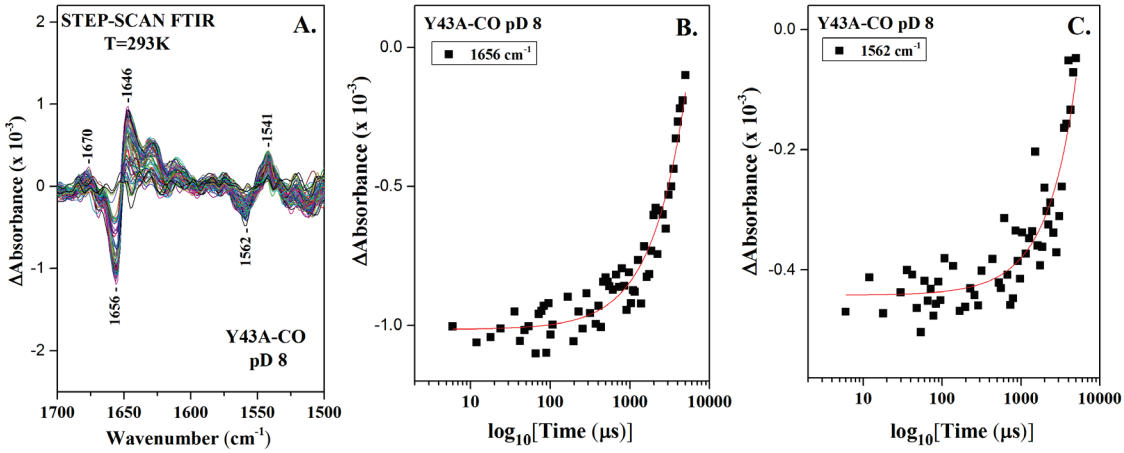

Fig. S4. Time-resolved step-scan FTIR difference spectra of the Y43A YddV-heme-CO adduct **(A)**. Plot of the ΔA of the 1656 cm^{-1} **(B)** and 1562 cm^{-1} modes **(C)** versus time on a logarithmic scale subsequent to CO photolysis.

The calculated rate constants for different modes in the TRS^2-FTIR spectra of the Y43A mutant are shown in Table S1:

Table S1

	t_1 (μs)	k (s^{-1})
1962 cm^{-1}	2424 ± 92	285
1656 cm^{-1}	2330 ± 443	297
1562 cm^{-1}	2183 ± 512	318