

Supporting Information

Americium(III) and Europium(III) Complex Formation with Lactate at Elevated Temperatures Studied by Spectroscopy and Quantum Chemical Calculations

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monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

Figure S2. Fit of decay curve of 5 μM Am^{3+} , 0.1 M lactate (pH = 6.0, 25 °C)
monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

Figure S3. Fit of decay curve of 10 μM Eu^{3+} , 5 mM lactate (pH = 6.0, 25 °C)
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Figure S7. Eu(III) lactate 1:1 complex modeled with DFT with atomic distances referred to
Eu. Green: Eu; red: O; blue: C; grey: H.

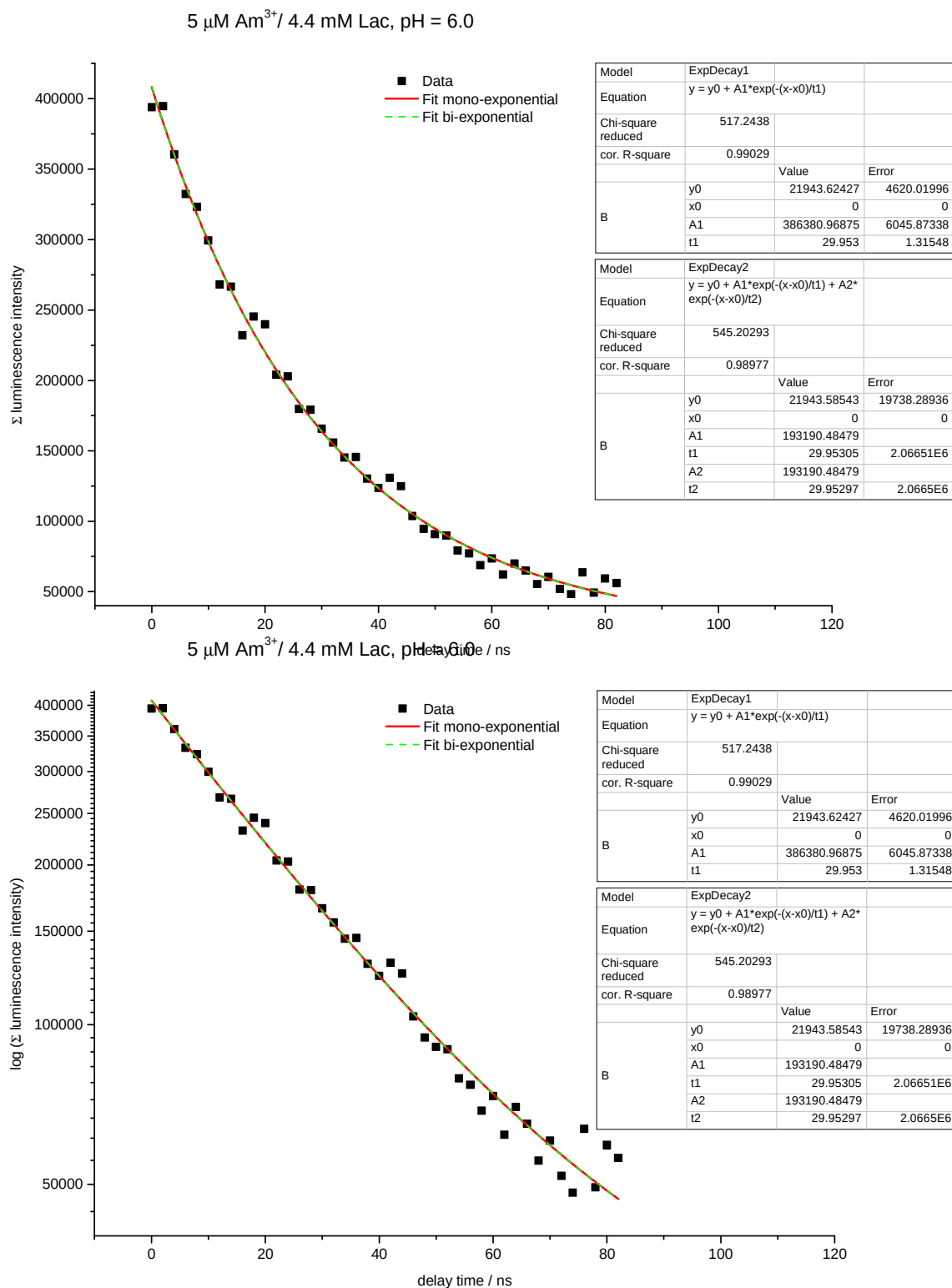


Figure S1. Fit of decay curve of 5 μM Am^{3+} , 4.4 mM lactate (pH = 6.0, 25 °C) monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

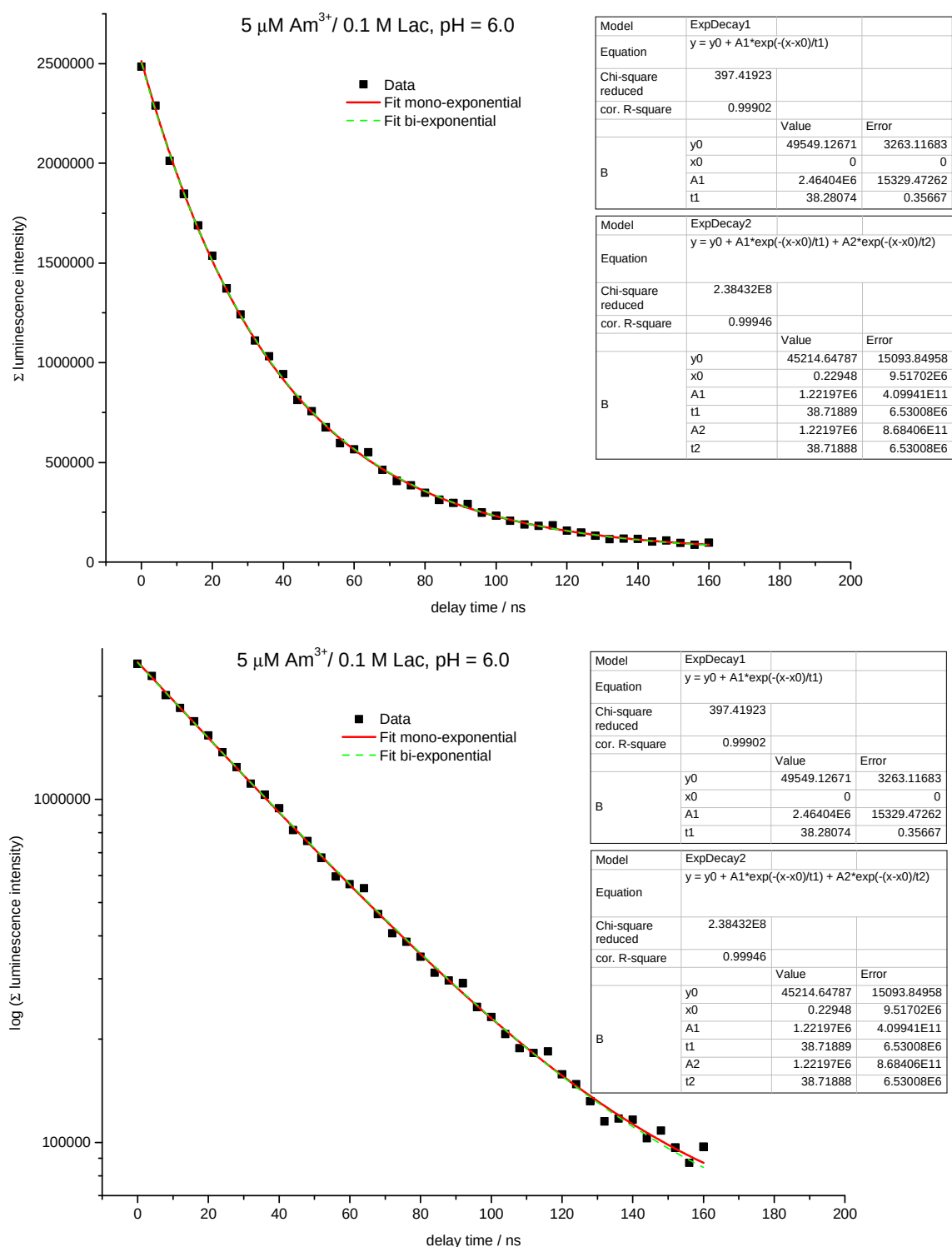


Figure S2. Fit of decay curve of 5 μM Am^{3+} , 0.1 M lactate (pH = 6.0, 25 °C) monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

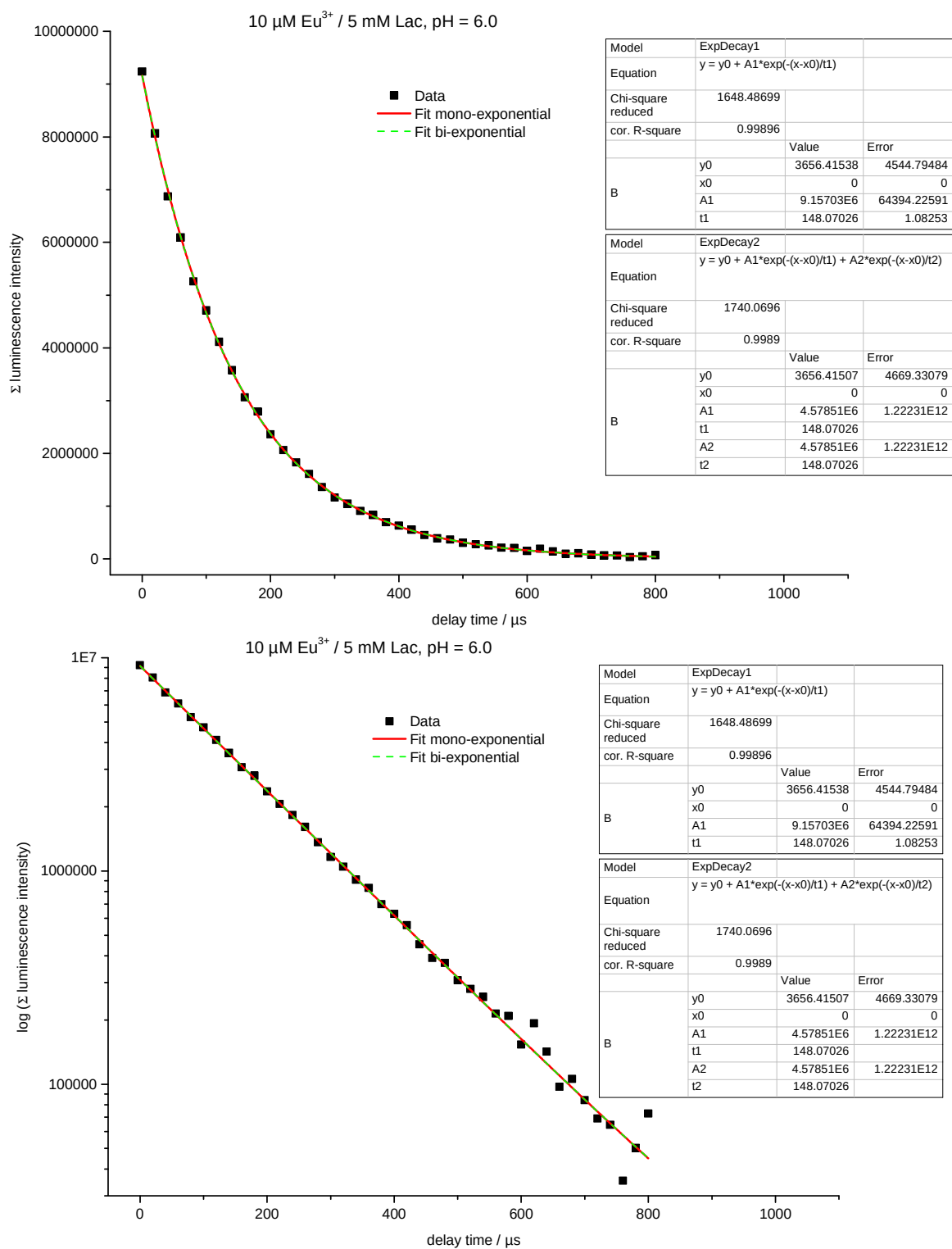


Figure S3. Fit of decay curve of 10 μM Eu^{3+} , 5 mM lactate (pH = 6.0, 25 $^{\circ}\text{C}$) monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

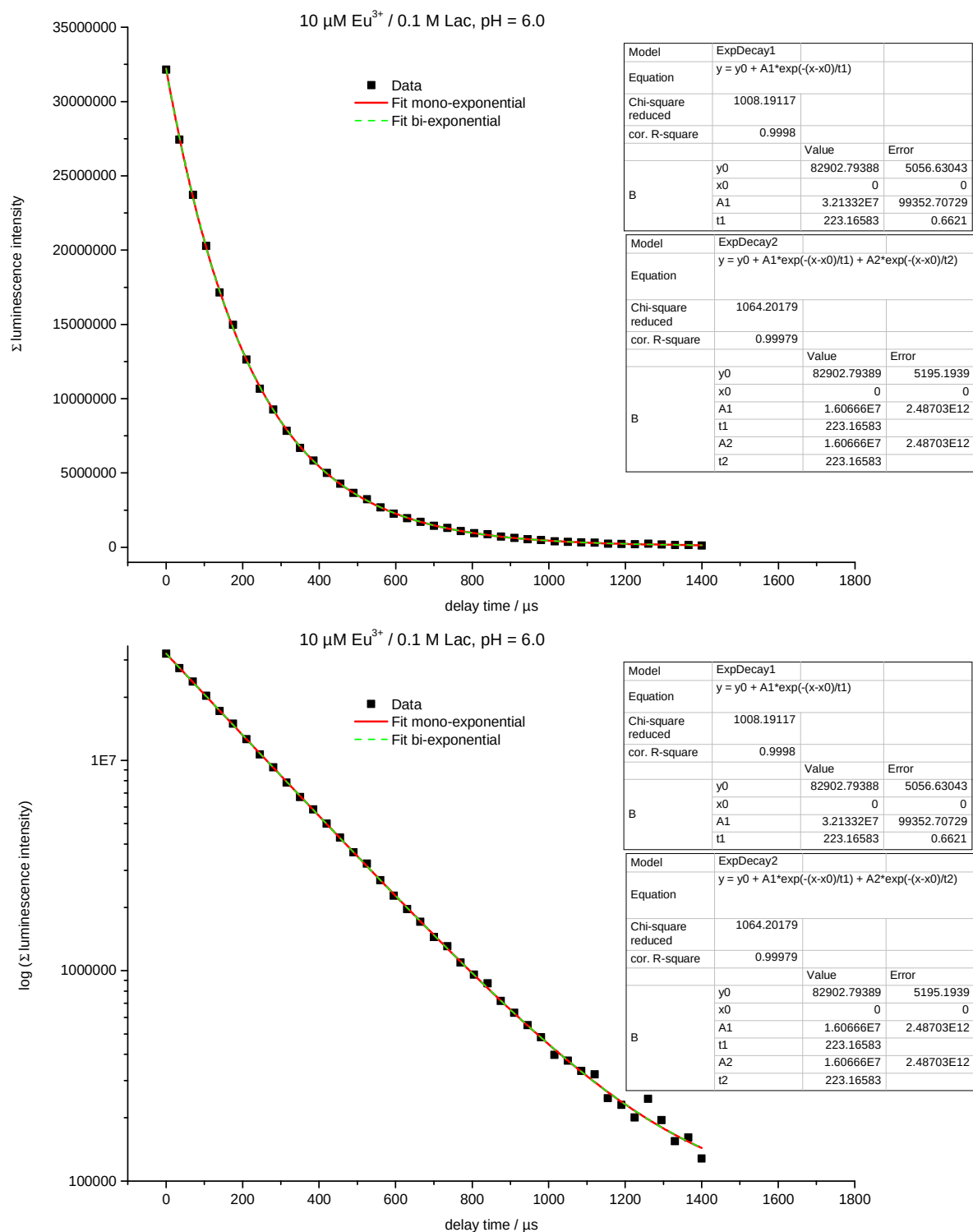


Figure S4. Fit of decay curve of 10 μM Eu^{3+} , 0.1 M lactate (pH = 6.0, 25 $^{\circ}\text{C}$) monoexponential vs. biexponential (top: linear y-axis, bottom: logarithmic y-axis).

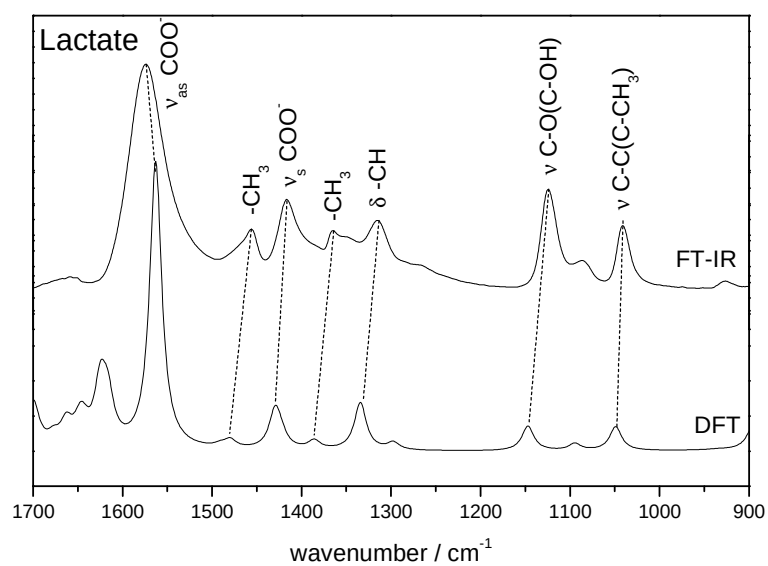


Figure S5. Experimental (FT-IR) and calculated (DFT) vibrational spectra of lactate at pH 5.

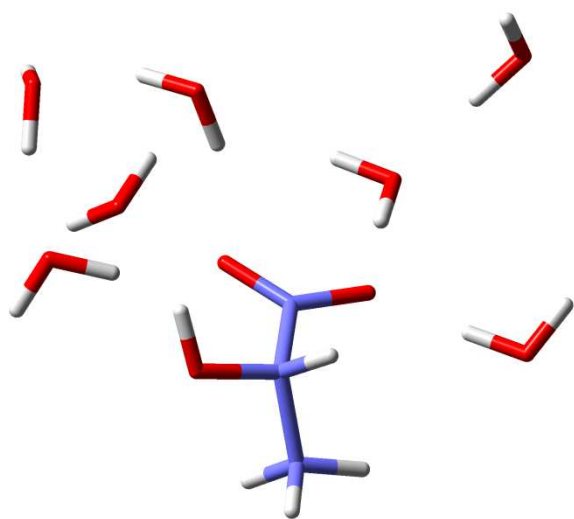
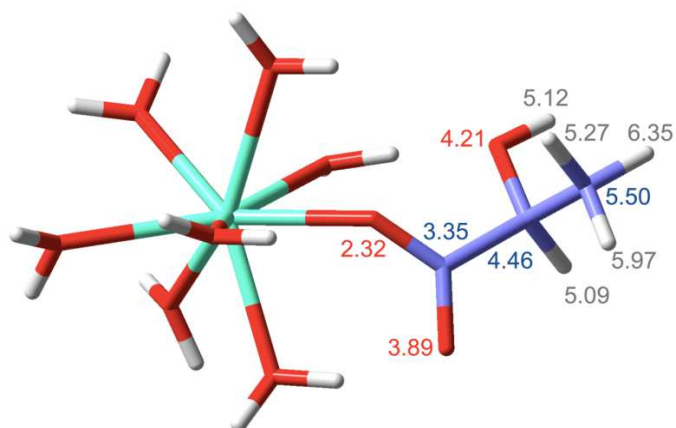
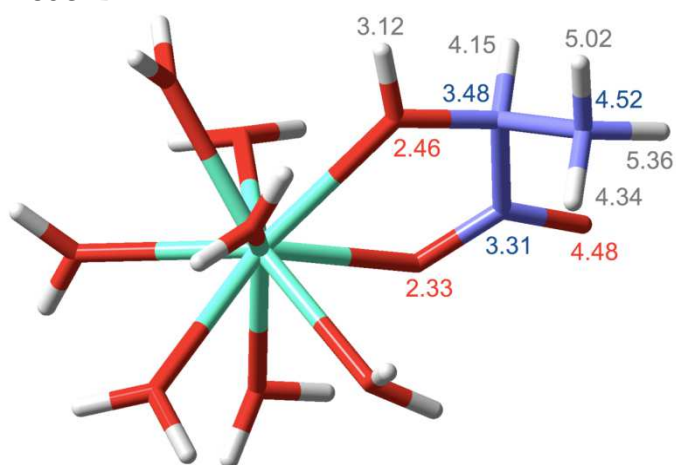


Figure S6. Lactate model for DFT calculation of IR spectrum with deprotonated carboxylate group, protonated hydroxyl group and 7 water molecules. Red: O; blue: C; grey: H.

Model A



Model B



Model C

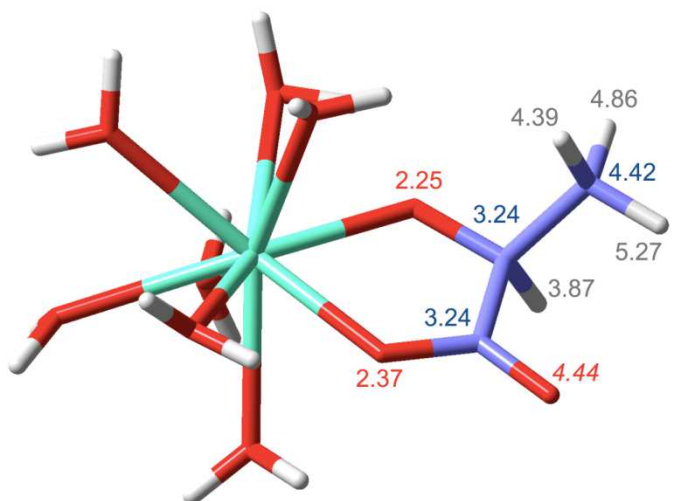


Figure S7. Eu(III) lactate 1:1 complex modeled with DFT with atomic distances referred to Eu. Green: Eu; red: O; blue: C; grey: H.