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Supplementary Information

Zwitterionic Surfactant Stabilized Palladium Nanoparticles as Catalysts in Aromatic Nitro Compound Reductions

Franciane D. Souza,* Haidi Fiedler and Faruk Nome*

Departamento de Química, Universidade Federal de Santa Catarina, 88040-900 Florianópolis-SC, Brazil

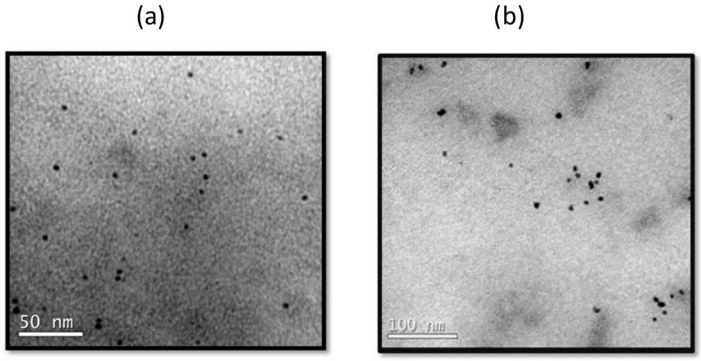

Figure S1. TEM microscopy and the average diameter (of approximately 300 particles) of palladium nanoparticles synthesized in: (a) w_0 4.6 (value taken from reference 1) and (b) w_0 14.7 (value taken from reference 2).

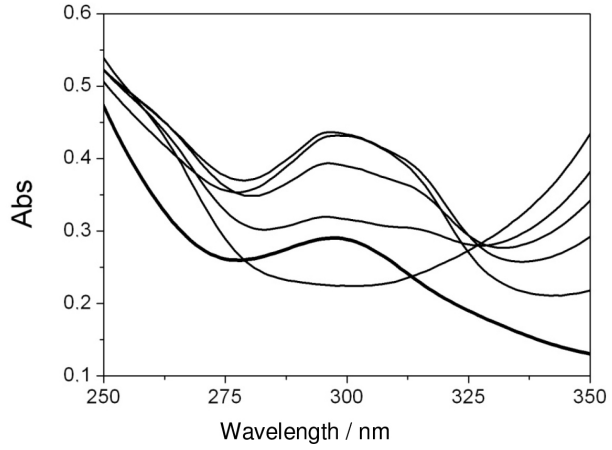

Figure S2. Variation of UV-Vis absorption spectra of reduction of 4-nitrophenol (0.066 mmol L^{-1}) with $NaBH_4$ (9.71 mmol L^{-1}) catalyzed by palladium nanoparticles (Pd NPs 1-0.0167 mmol L^{-1}) ([NaCl] = 0.033 mmol L^{-1}). The thicker line refers to the end of the reaction.

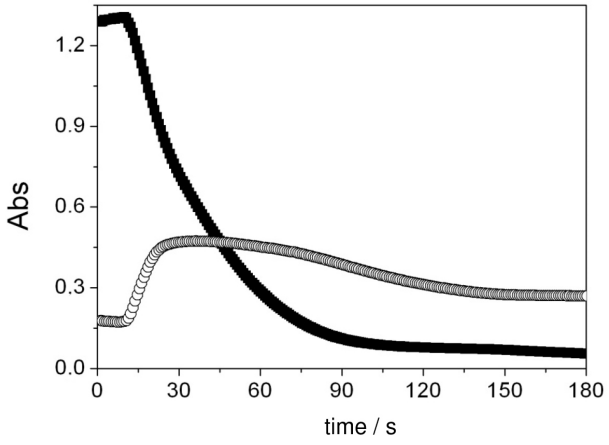

Figure S3. Time-dependence of the absorption of 4-nitrophenolate ions at (■) 400 nm and (○) 296 nm ([4-nitrophenol] = 0.066 mmol L^{-1}; [$NaBH_4$] = 9.71 mmol L^{-1}; [Pd NPs 1] = 0.0167 mmol L^{-1}, [NaCl] = 0.033 mmol L^{-1}). The reactions were carried out at 25 °C.

*e-mail: franciane_dutra@hotmail.com, faruk.nome@ufsc.br

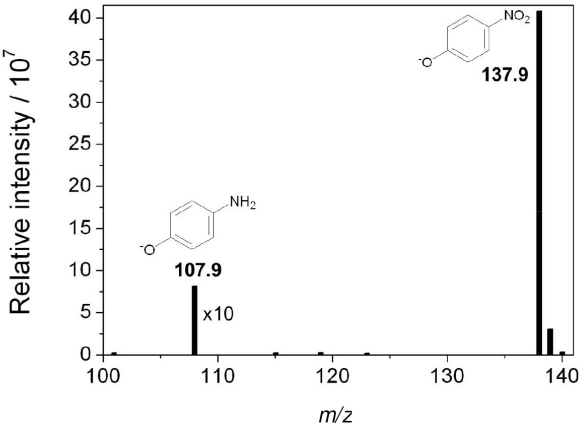

Figure S4. ESI-MS spectrum in negative mode of an aliquot taken after approximately 5 min of the mixing of reactants in the presence of Pd NPs. The initial conditions were [Nip] = 0.093 mmol L^{-1}; [$NaBH_4$] = 9.71 mmol L^{-1}; [NaCl] = 0.033 mmol L^{-1}; [Pd] = 0.0019 mmol L^{-1}. After addition of $NaBH_4$ solution, the solution was diluted ten times and injected into the mass spectrometer.

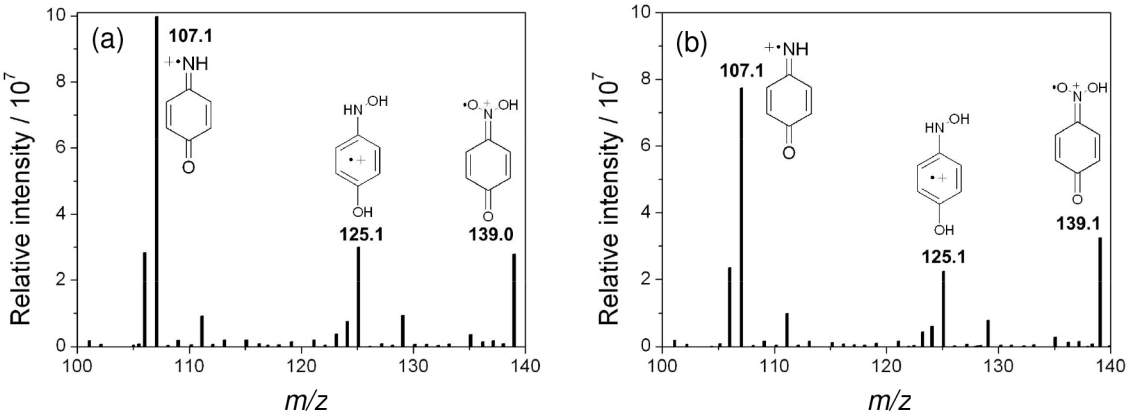

Figure S5. ESI-MS spectrum in positive mode of an aliquot taken after approximately 5 min of the mixing of reactants in the presence of Pd NPs. The initial conditions were [Nip] = 0.093 mmol L^{-1}; [$NaBH_4$] = 9.71 mmol L^{-1}; [NaCl] = 0.033 mmol L^{-1}; [Pd] = 0.0019 mmol L^{-1}. After addition of $NaBH_4$ solution, the solution was diluted ten times and injected into the mass spectrometer.

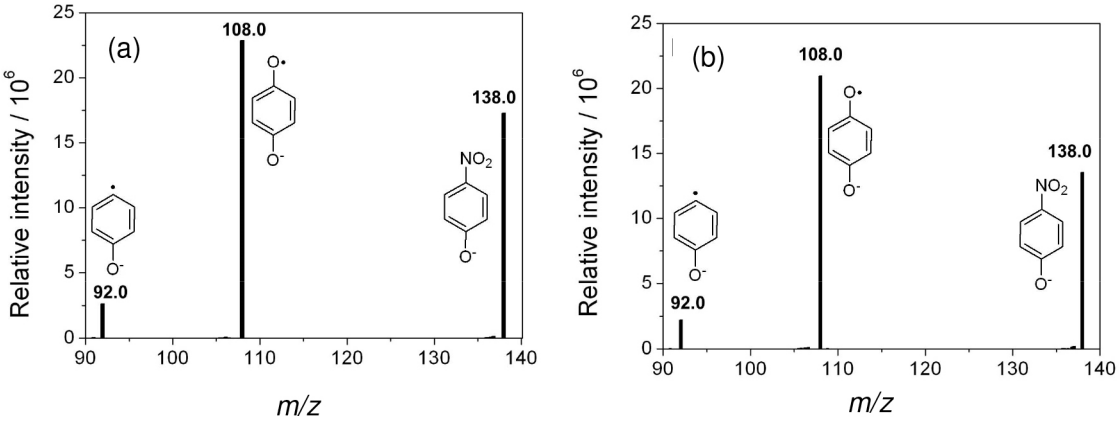

Figure S6. ESI-MS/MS of the intermediate anion of *m/z* 138 in negative mode: (a) Pd NPs 2; (b) Pd NPs 2.

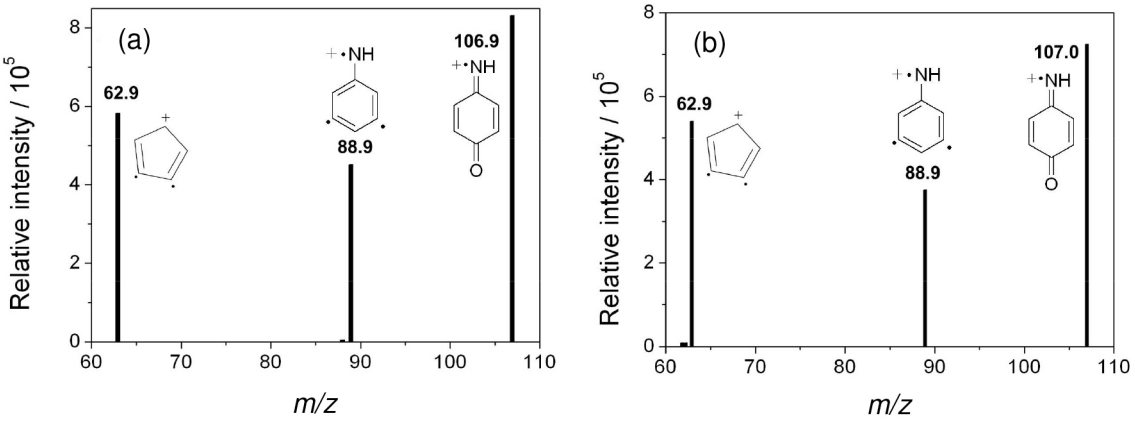

Figure S7. ESI-MS/MS of the intermediate anion of *m/z* 125 in positive mode: (a) Pd NPs 2; (b) Pd NPs 2.

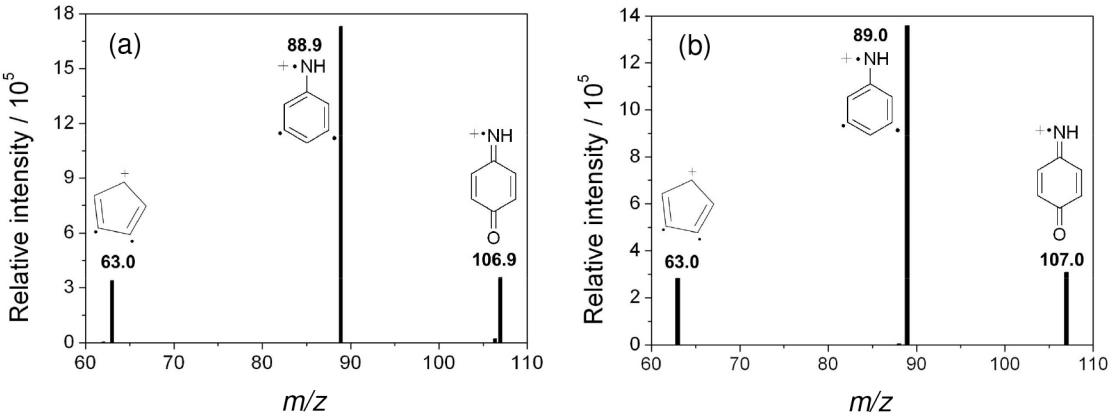

Figure S8. ESI-MS/MS of the intermediate anion of *m/z* 107 in positive mode: (a) Pd NPs 2; (b) Pd NPs 2.

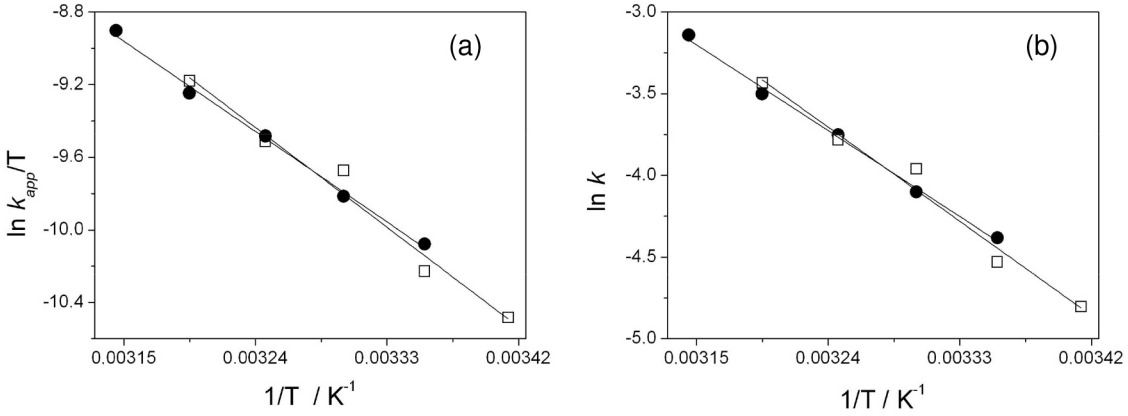

Figure S9. (a) Eyring and (b) Arrhenius plots for determination of activation parameters for reaction systems at [4-nitrophenol] = 0.093 mmol L^{-1}; [BH_4^-] = 9.71 mmol L^{-1}; [NaCl] = 0.033 mmol L^{-1}, [Pd] = 0.0167 mmol L^{-1}. (●) Pd NPs 1; (□) Pd NPs 2.

References

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2. Souza, F. D.; Souza, B. S.; Tondo, D. W.; Leopoldino, E. C.; Fiedler, H. D.; Nome, F.; *Langmuir* 2015, ***31***, 3587.