Sulfonated Schiff base dinuclear and polymeric copper(II) complexes: crystal structures, magnetic properties and catalytic application in Henry reaction

Susanta Hazra,* Anirban Karmakar,* Maria de Fátima C. Guedes da Silva,* Lubor Dlhán, Roman Boča and Armando J. L. Pombeiro* 

*Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisbon, Portugal. E-mail: hazra_susanta1@yahoo.co.in, fatima.guedes@tecnico.ulisboa.pt and pombeiro@tecnico.ulisboa.pt

b Institute of Inorganic Chemistry, FCHPT, Slovak University of Technology, SK-812 37, Bratislava, Slovakia

c Department of Chemistry, FPV, University of SS Cyril and Methodius, SK-917 01, Trnava, Slovakia
Fig. S1. UV-vis spectra (200–900 nm) of 1–3 and [CuLCl]_2 in aqueous solution at room temperature. Red and black lines indicate the spectra obtained at the beginning and after 8 h of the solution preparation, respectively. Graphs A, B, C and D are for 1, 2, 3 and [CuLCl]_2, respectively. Inset graphs concern the visible spectral range.
**Fig. S2.** Experimental (circles) and calculated (lines) magnetic susceptibility data converted to the effective magnetic moment for 1, 2 and 3.

**Fig. S3.** Plot of β-nitroalkanol yield vs. time for the Henry reaction of benzaldehyde and nitroethane with 3 (points 1–6 concern the corresponding entries in Table 2).
Fig. S4. ESI-MS spectrum of complex 1 in aqueous solution.
Fig. S5. ESI-MS spectrum of complex 2 in aqueous solution.
Fig. S6. ESI-MS spectrum of complex 3 in aqueous solution.
Fig. S7. ESI-MS spectrum of complex 1 in catalytic reaction solution.
Fig. S8. ESI-MS spectrum of complex 2 in catalytic reaction solution.
**Fig. S9.** ESI-MS spectrum of complex 3 in catalytic reaction solution.