Supplementary Materials: A Chiral Bis(salicylaldiminato)zinc(II) Complex with Second-Order Nonlinear Optical and Luminescent Properties in Solution

Paola Matozzo, Alessia Colombo, Claudia Dragonetti, Stefania Righetto, Dominique Roberto, Paolo Biagini, Simona Fantacci and Daniele Marinotto

Elemental Analysis of the Zinc Complex

Anal. calcd. for $C_{30}H_{28}N_2O_2Zn$: C 70.11, H 5.49, N 5.45; found: C, 70.35 H, 5.47; N,5.46.

[1] NMR and Elemental Analysis of the Zinc Complex

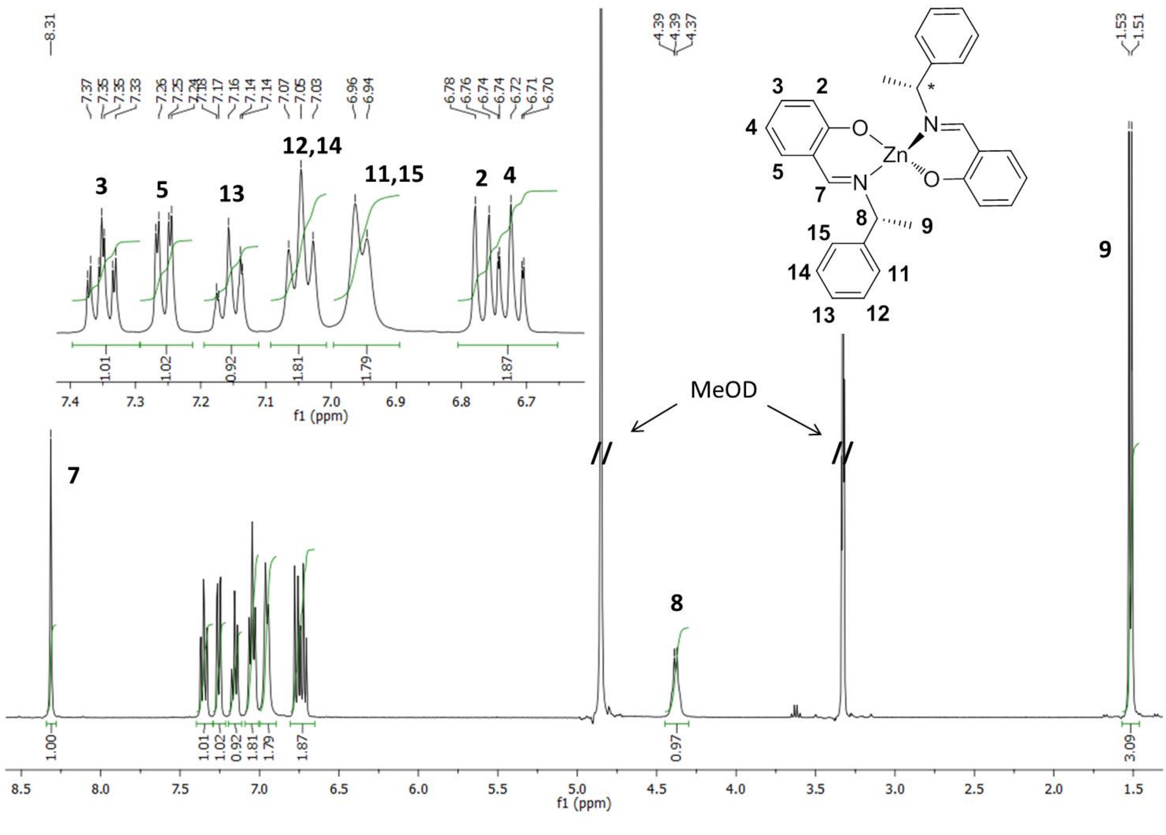

Figure S1. ^{1}H-NMR(400 MHz) spectrum in CD_3OD.

^{1}H NMR (400 MHz, CD_3OD δ): 8.31 (s, 1H, H_7), 7.40–7.29 (m, 1H, H_3), 7.26 (dd, J_1 = 7.9, Hz, J_2 = 6.7 Hz, 1H, H_5), 7.19–7.11 (m, 1H, H_{13}), 7.05 (t, J = 7.5 Hz, 2H, H_{12},H_{14}), 6.95 (d, J = 8.0 Hz, 2H, H_{11}, H_{15}), 6.77 (d, J_1 = 7.9 Hz, 1H, H_2), 6.72 (td, J_1 = 8.5 Hz, J_2 = 4.0 Hz, 1H, H_4), 4.39 (q, J = 6.91 Hz, 1H, H_8), 1.52 (d, J = 6.9 Hz, 3H, H_9).

EFISH Measurements

A $CHCl_3$ solution of the investigated compound was put in the EFISH cell, and a strong electric field (~30 KW/cm) was applied in order to align the molecules in the same direction. A laser beam at ω frequency was then pointed through the cell, which was shifted orthogonally to the beam. Because the EFISH cell has a wedge shape (Figure S2), when it is translated orthogonally to the laser beam, the latter has to cover an optical path that changes with time, leading to interferences which are represented by Maker fringes (Figure S3) [1–3]. The incident radiation ω was removed by suitable filters, so that only the 2ω, arising from the laser–sample interaction, was collected and sent to a photomultiplier. In order to remove the effect of the solvent, the measurements were done first with pure $CHCl_3$, then with the $CHCl_3$ solution of the investigated compound, and finally with pure $CHCl_3$. During the elaboration to obtain the value of μβ, the solution was compared with the solvent before and after. The Maker fringes periodicity and the amplitude are related to the solution macroscopic susceptibility and, therefore, to γ_{EFISH} and $\mu\beta_{EFISH}$ [1-3].

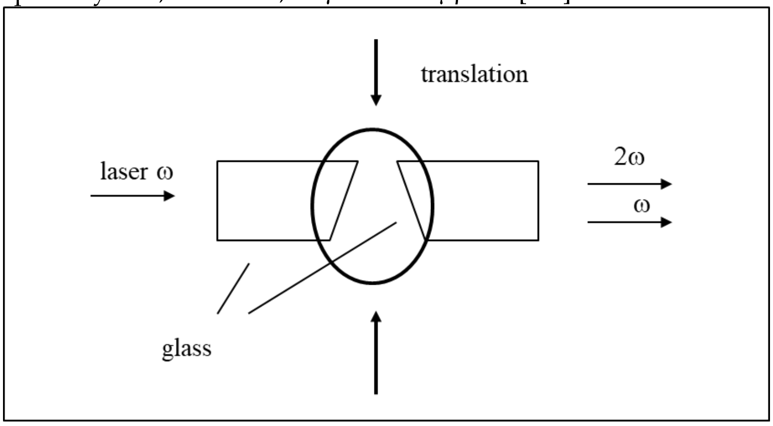

Figure S2. Top view of the EFISH cell.

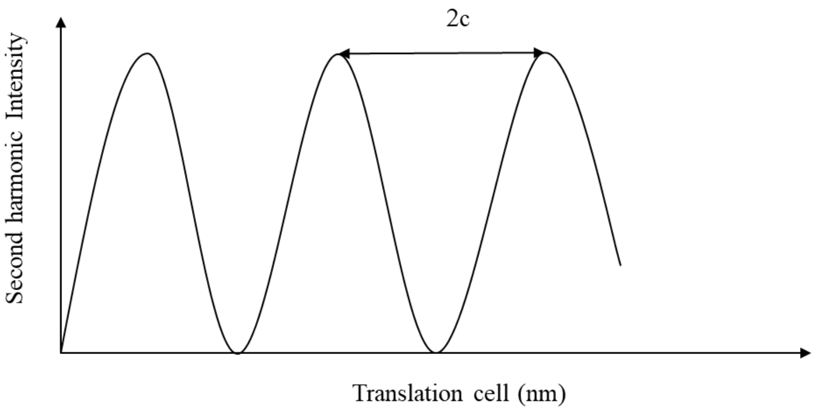

Figure S3. Maker fringes.

1. Ledoux, I.; Zyss, J. Influence of the molecular environment in solution measurements of the Second-order optical susceptibility for urea and derivatives. *J. Chem. Phys.* **1982**, *73*, 203–213.
2. Levine, B.F.; Bethea, C.G. Molecular hyperpolarizabilities determined from conjugated and nonconjugated organic liquids. *Appl. Phys. Lett.* **1974**, *24*, 445–447.
3. Levine, B.F.; Bethea, C.G. Second and third order hyperpolarizabilities of organic molecules. *J. Chem. Phys.*, **1975**, *63*, 2666–2682.