

Multiparameter molecular sensor based on a compound containing tetrathiafulvalenium, thiophene and pyridine fragments

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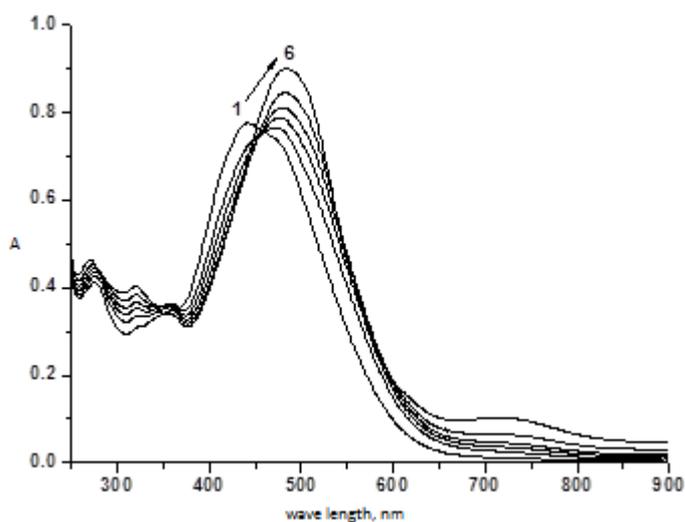


Figure S1 Electronic absorption spectra of dye **1** solution at different iron perchlorate concentration (spectrophotometric titration). Initial dye concentration $C_1 = 2.2 \cdot 10^{-5}$ M, iron perchlorate concentration changes in the range of 0 – 0.1 M. Solvent – acetonitrile, $T = 294$ K.

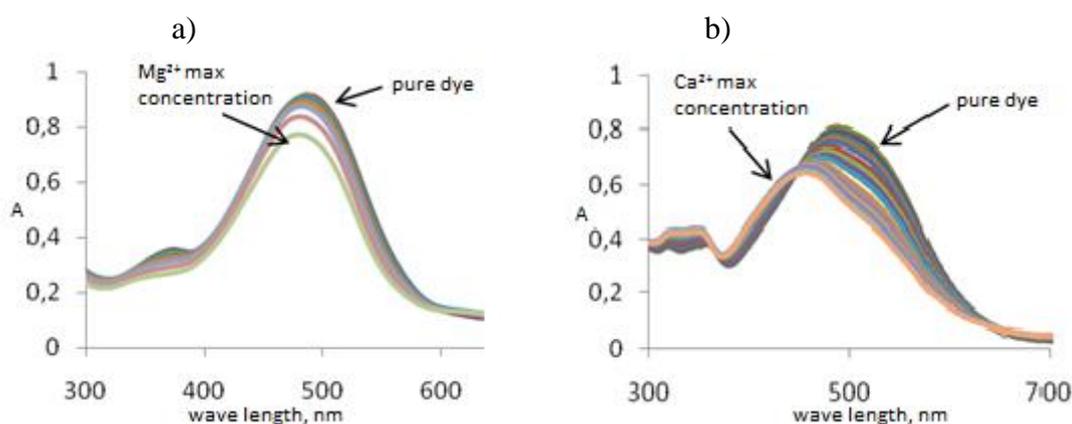
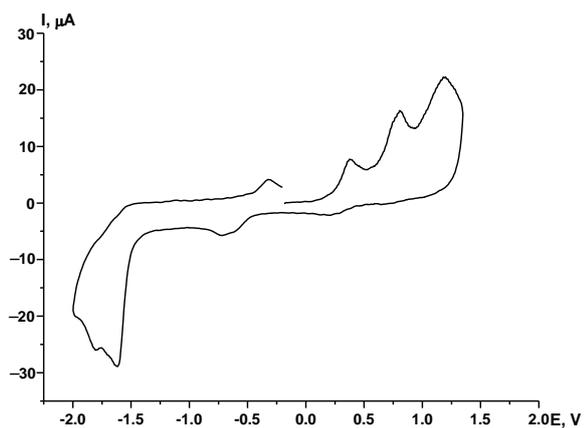
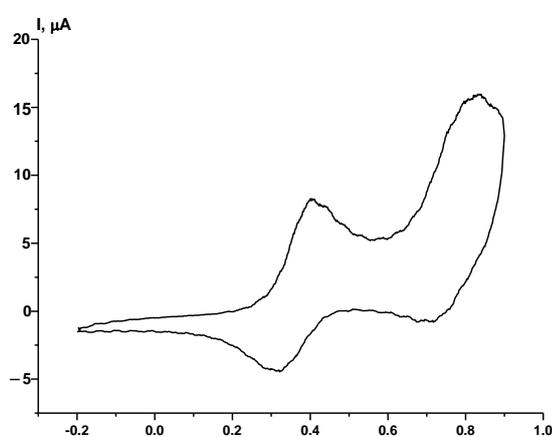


Figure S2 a) electronic absorption spectra of dye $1 \cdot H^+$ solution at different magnesium perchlorate concentration (spectrophotometric titration). Initial dye concentration $C_{1 \cdot H^+} = 2.5 \cdot 10^{-5}$ M, magnesium perchlorate concentration changes in the range of 0 – 0.5 M. Solvent – acetonitrile, $T = 294$ K; b) Electronic absorption spectra of dye $1 \cdot H^+$ solution at different calcium perchlorate concentration (spectrophotometric titration). Initial dye concentration $C_{1 \cdot H^+} = 2.2 \cdot 10^{-5}$ M, calcium perchlorate concentration changes in the range of 0 – 0.5 M. Solvent – acetonitrile, $T = 294$ K.



a)



b)

Figure S3 CVA of the ligand **1** $C_1 = 10^{-3}\text{M}$ in the range of potentials from -2 V to 1.5 V (a) (Pt, $\text{CH}_3\text{CN} - \text{CH}_2\text{Cl}_2$ 3:1, 200 mV/s, Ag/AgCl/KCl aq, Bu_4NBF_4) and from -0.2 V to 0.9 V (b).

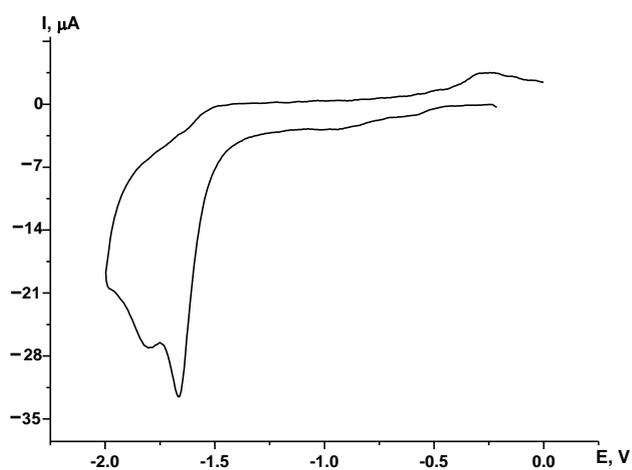


Figure S4 CVA of the ligand **1** $C_1 = 10^{-3}\text{M}$ in the range of potentials from 0 V to -2.0 V (Pt, $\text{CH}_3\text{CN} - \text{CH}_2\text{Cl}_2$ 3:1, 200 mV/s, Ag/AgCl/KCl aq, Bu_4NBF_4).

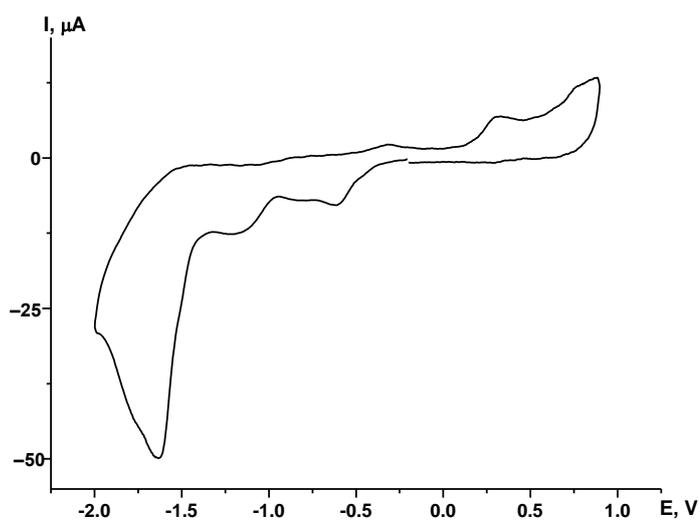


Figure S5 CVA of the ligand **1** $C_1 = 10^{-3}$ M after addition of 2 equivalents of $\text{Cd}(\text{ClO}_4)_2$ in the range of potentials from -2 V to 1.5 V (Pt, $\text{CH}_3\text{CN} - \text{CH}_2\text{Cl}_2$ 3:1, 200 mV/s, Ag/AgCl/KCl aq, Bu_4NBF_4).

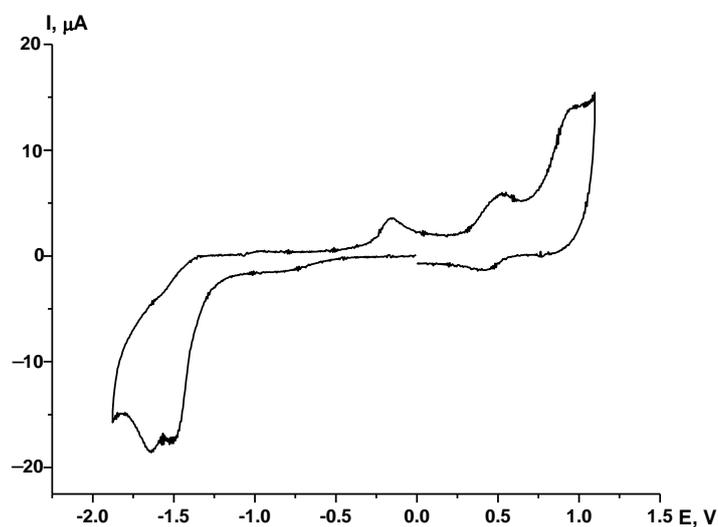


Figure S6 CVA of the ligand **1** $C_1 = 10^{-3}$ M after addition of 1 equivalent of $\text{Fe}(\text{ClO}_4)_2$ in the range of potentials from -2 V to 1.5 V $+\text{Fe}(\text{ClO}_4)_2$ (Pt, $\text{CH}_3\text{CN} - \text{CH}_2\text{Cl}_2$ 3:1, 200 mV/s, Ag/AgCl/KCl aq, Bu_4NBF_4).

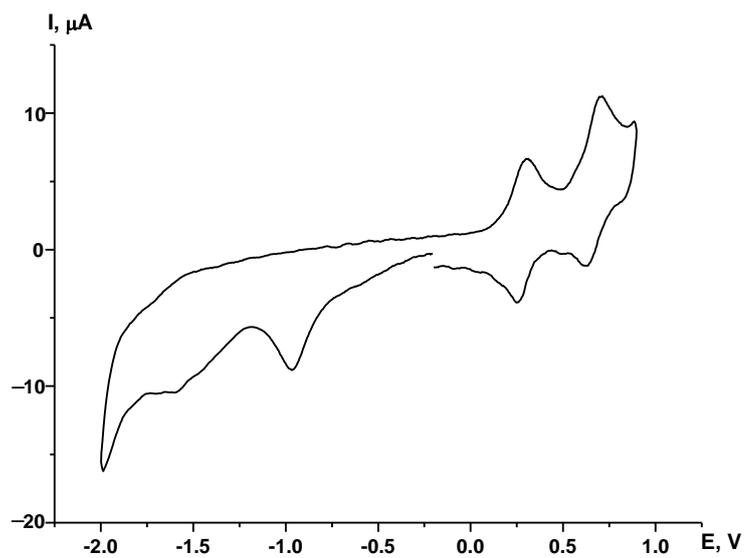


Figure S7 CVA of the ligand **1** $C_1 = 10^{-3}$ M after addition of 2 equivalents of $\text{Ca}(\text{ClO}_4)_2$ in the range of potentials from -2 V to 1.5 V (Pt, $\text{CH}_3\text{CN} - \text{CH}_2\text{Cl}_2$ 3:1, 200 mV/s, Ag/AgCl/KCl aq, Bu_4NBF_4).