

Supporting Information

Electrocatalytic Water Oxidation by a Ni(II) Salophen-type Complex

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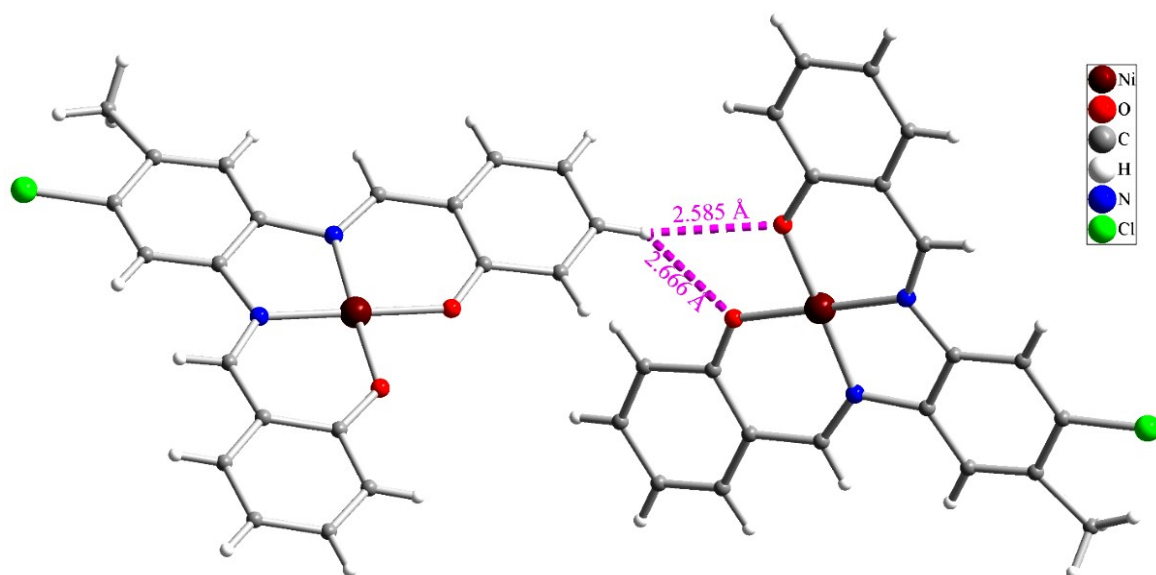


Fig. S1: Intermolecular C–H···O interactions in the crystal structure of complex **1**

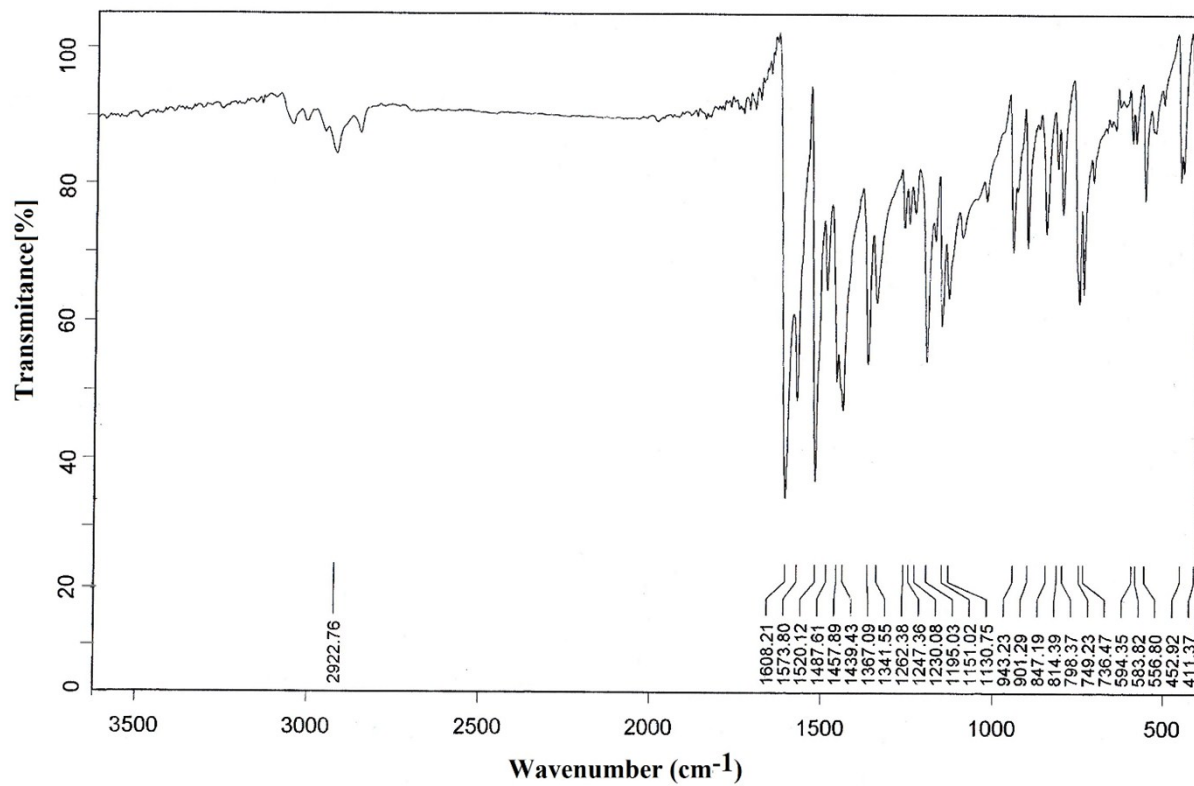


Fig. S2: The FT-IR spectrum of NiL (1)

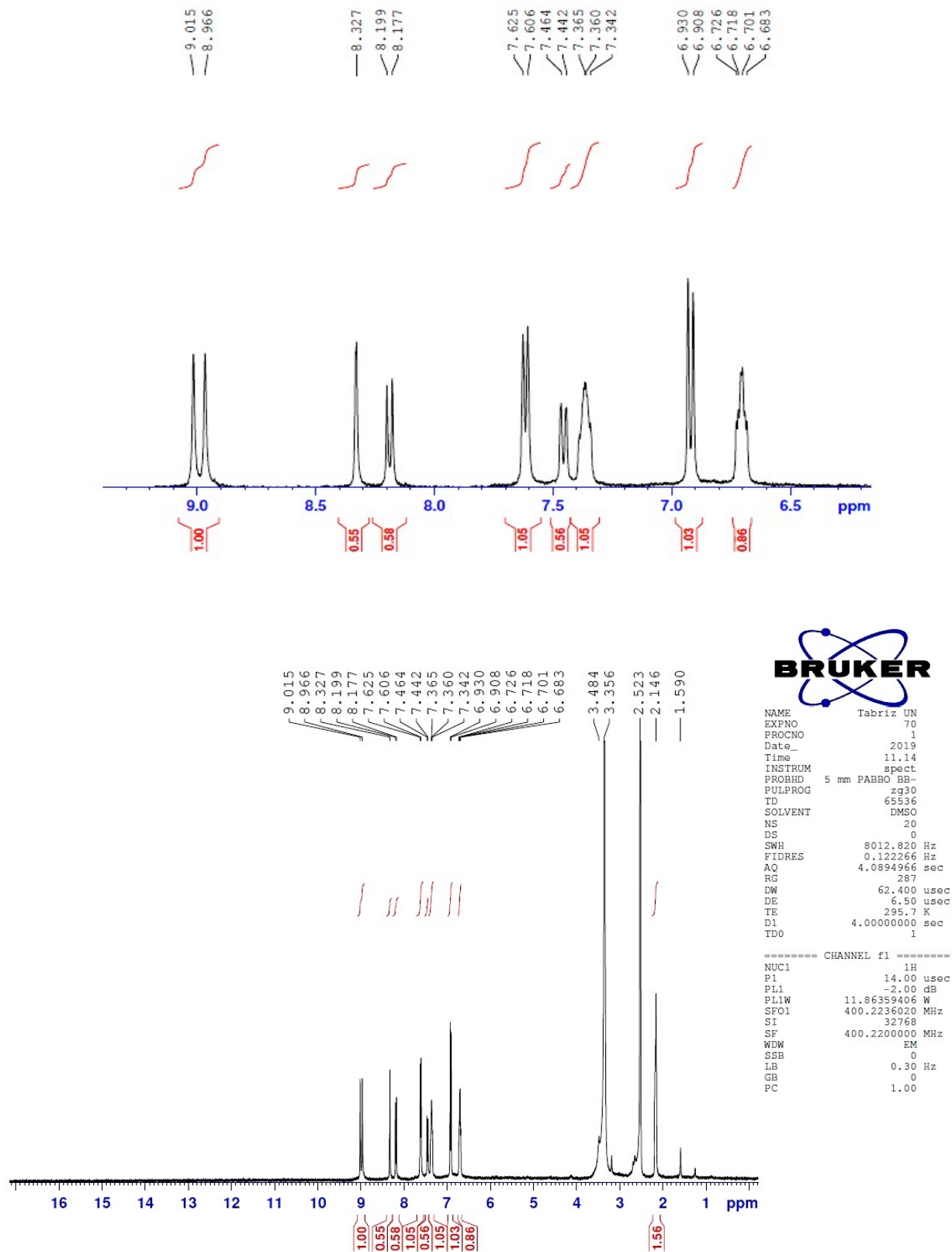


Fig. S3: The ^1H NMR spectrum of NiL (1)

Thermogravimetric analysis

The TGA plot of Ni(II) complex **1** shows that the complex is stable up to 400 °C with a $DTG_{max}=410$ °C. Decomposition for **1** involves four steps (see Fig. S3). The weight loss in the first stage is probably related to the omission of some small molecules such as CO₂ and N₂ molecules from the main body of the complex with a mass loss of 16.42% (calc. 17.09%). The second weight loss occurs in the range of 450-520 °C, which can be assigned to the release of –CH₃ group of complex **1** with a mass loss of 5.27% (Calc. 4.86 %). The third weight loss takes place in the 520-590 °C which corresponds to the decomposition of some parts of aromatic ring containing chloro substitute with a mass loss of 13.29% (Calc. 14.29 %). Finally, the highest weight loss occurs in the range of 590-800 °C which corresponds to the decomposition of the residue aromatic groups and the formation of metal oxide lattice.

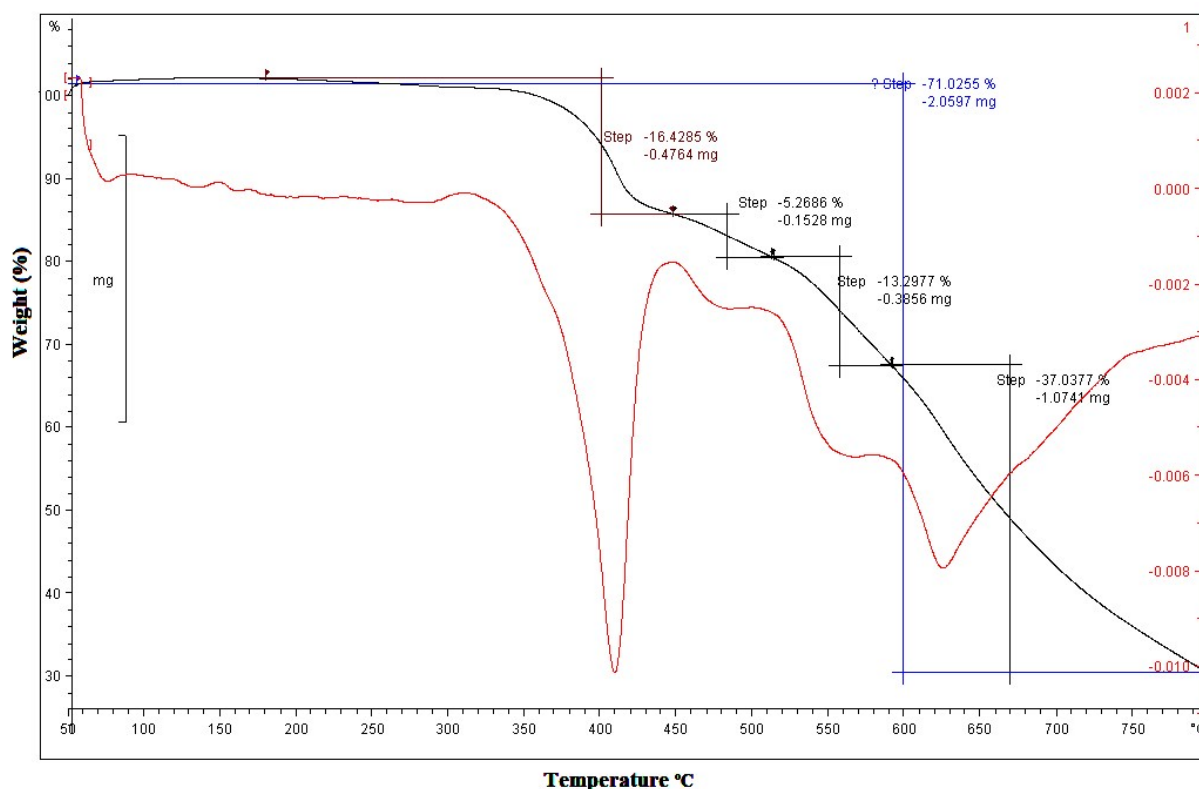


Fig. S4: The thermogravimetric plot of NiL (**1**)

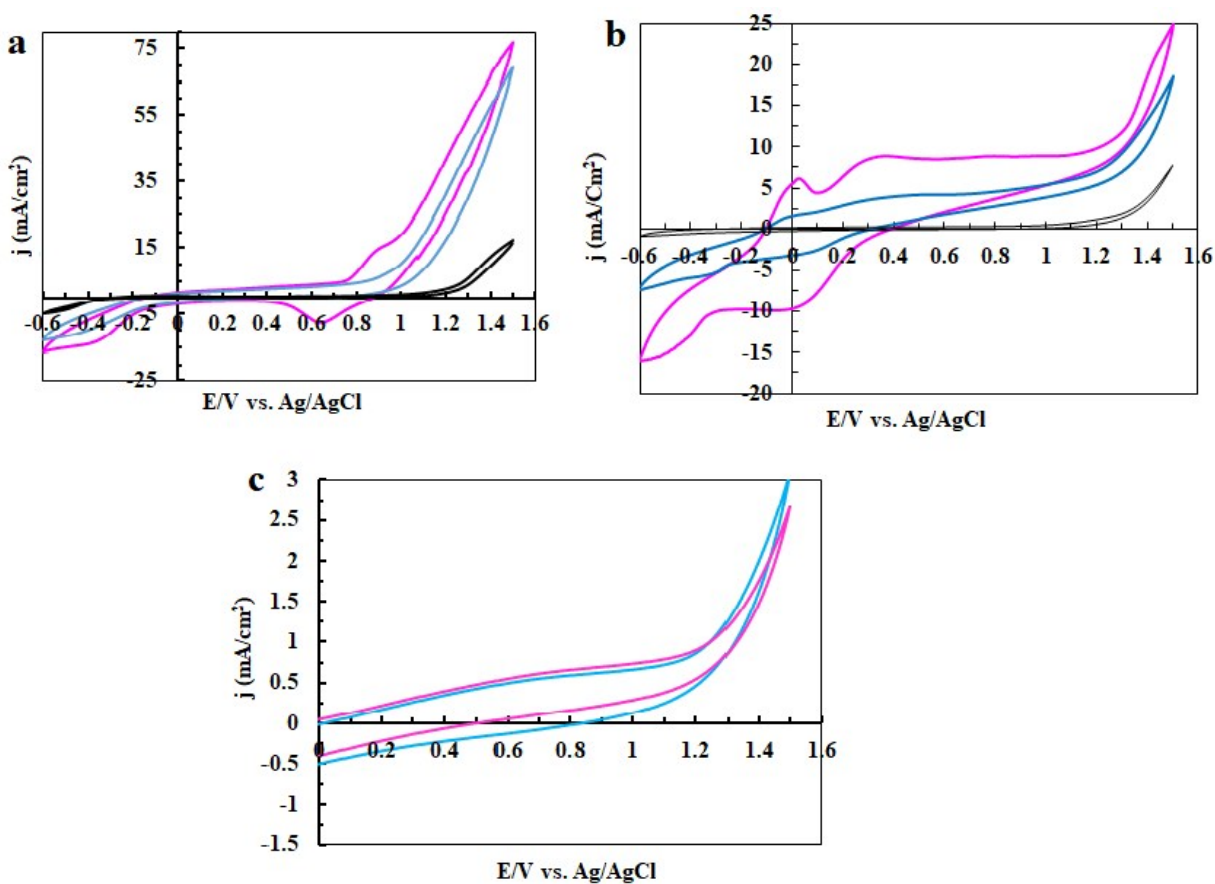


Fig. S5: CV for a fresh CPE (black), CPE-complex **1** (blue) and CPE-complex **1** after performing amperometry of 5 hours (pink) in the buffer solution (0.5 M) in the range of -0.6 to 1.6 V. vs Ag/AgCl at pH=11 (a), pH=7 (b) and in the range of 0-0.6 at pH=3 (c)

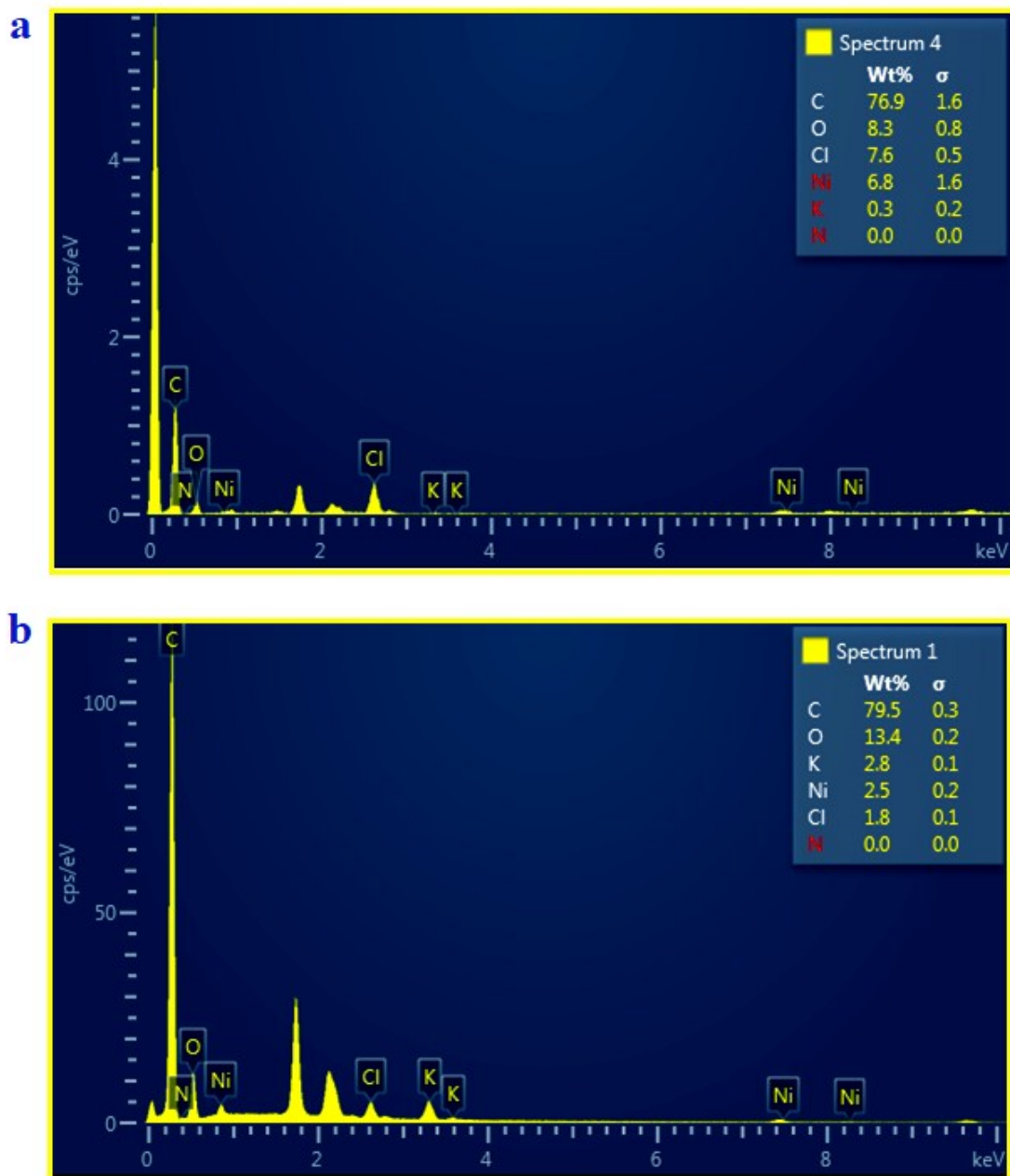


Fig. S6: EDX spectra of the surface of CPE modified with complex **1** after amperometry for 5h at pH=11 (a) and pH=7 (b)

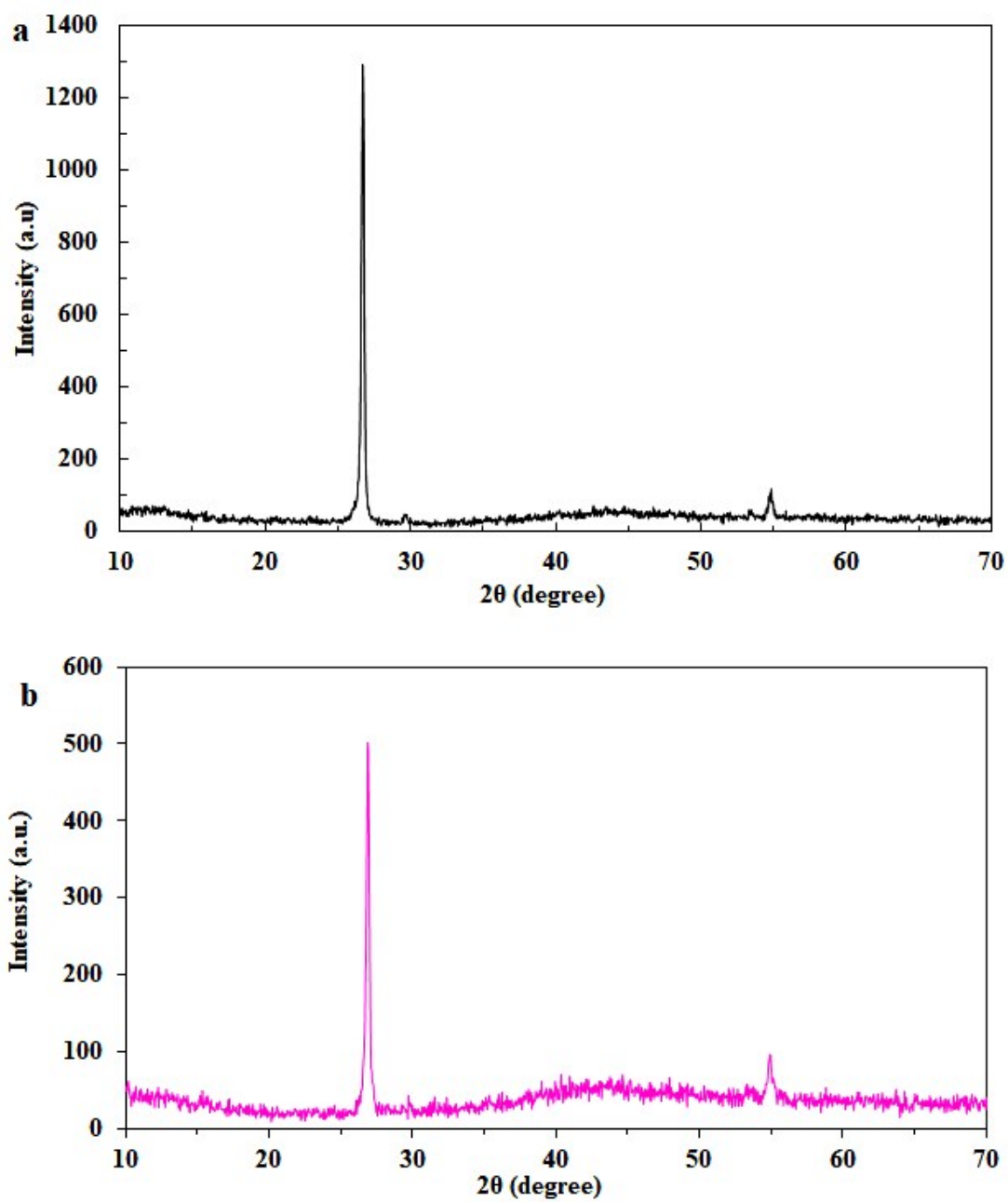


Fig. S7: The XRD pattern of the surface of bare CPE (a) and CPE-complex **1** after 5h amperometry at pH=11(b)

Table S1: Information of intermolecular hydrogen bond interactions in the crystal structure of complex **1**

D–H···A	d(D–H)	d(H···A)	<DHA	d(D···A)
C4–H4A...O24 ⁱ	0.930	2.585	163.28	3.487(18)
C4–H4A...O1 ⁱ	0.930	2.666	141.43	3.443(17)
C25–H25C...Cl1 ⁱⁱ	0.960	2.740	111.14	3.207(17)
Symmetry code: ⁱ <i>I</i> - <i>x</i> , <i>I</i> /2+ <i>y</i> , <i>I</i> /2- <i>z</i> ; ⁱⁱ 2- <i>x</i> , <i>I</i> /2+ <i>y</i> +2, 3/2- <i>z</i> ;				