Electrochemical coupling of a phenol to a naphthol

The invention which follows relates to an electrochemical process for coupling a phenol to a naphthol, these having different oxidation potentials. The invention further relates to compounds which can be prepared, for example, by electrochemical coupling.

The terms "phenols" and "naphthols" are used as generic terms in this application and hence also encompass substituted phenols and substituted naphthols.

To date, only an electrochemical coupling of phenol to a naphthol not having any OH group has been described: Kirste et al. Angew. Chem. 2010, 122, 983-987 and Kirste et al. J. Am. Chem. Soc. 2012, 134, 3571-3576.

A problem which occurs in the electrochemical coupling of different molecules is that they have different oxidation potentials E_{Ox}. The result of this is that the molecule having the higher oxidation potential has a lower propensity to release an electron (e^-) to the anode and an H^+ ion to the solvent, for example, than the molecule having the lower oxidation potential. The oxidation potential E_{Ox} can be calculated via the Nernst equation:

$$E_{Ox} = E^\circ + (0.059/n) * \lg([Ox]/[Red])$$

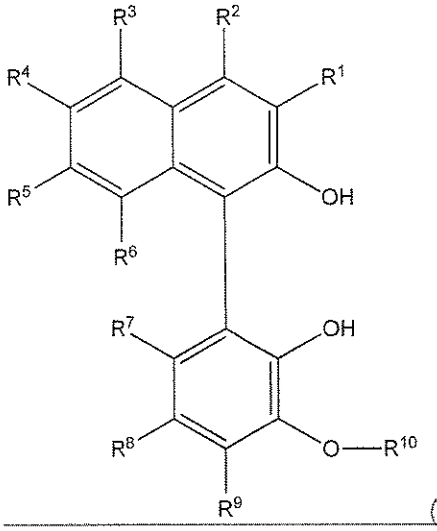
E_{Ox}: electrode potential for the oxidation reaction (= oxidation potential)
E°: standard electrode potential
n: number of electrons transferred
[Ox]: concentration of the oxidized form
[Red]: concentration of the reduced form

The problem addressed by the invention which follows was that of providing an electrochemical process in which a phenol is coupled to a naphthol, these two molecules having different oxidation potentials

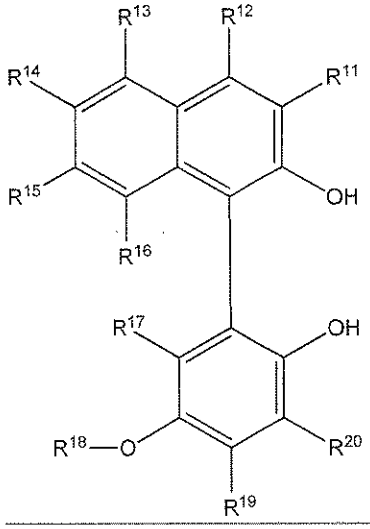
In addition, novel compounds were to be synthesized.

Summary

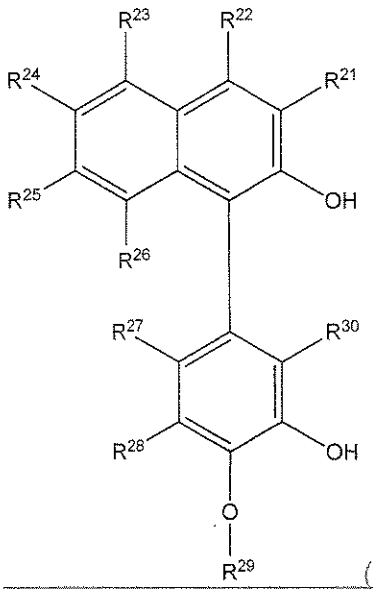
In a first aspect, there is provided a compound of one of the general formulae (I) to (III)



(I)



(II)



(III)

where R^1, R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^9, R^{11}, R^{12}, R^{13}, R^{14}, R^{15}, R^{16}, R^{17}, R^{19}, R^{20}, R^{21}, R^{22}, R^{23}, R^{24}, R^{25}, R^{26}, R^{27}, R^{28}, R^{30} are selected from: -H, -alkyl, -O-alkyl, -O-aryl, -S-alkyl, -S-aryl and

where R^{10}, R^{18}, R^{29} are -alkyl.

In a second aspect, there is provided an electrochemical process comprising the process steps of:

a) introducing a solvent or solvent mixture and a conductive salt into a reaction vessel,

b) adding a phenol having an oxidation potential $|E_{Ox}1|$ to the reaction vessel,

c) adding a naphthol having an oxidation potential $|E_{Ox}2|$ to the reaction vessel, the substance having the higher oxidation potential being added in excess,

and where: $|E_{Ox}1| - |E_{Ox}2| = |\Delta E|$

and the solvent or solvent mixture is selected such that $|\Delta E|$ is in the range from 10 to 450 mV,

d) introducing two electrodes into the reaction solution,

e) applying a voltage to the electrodes,

f) coupling the phenol to the naphthol to give a cross-coupled product.

Detailed Disclosure

Compound of one of the general formulae (**I**) to (**III**):