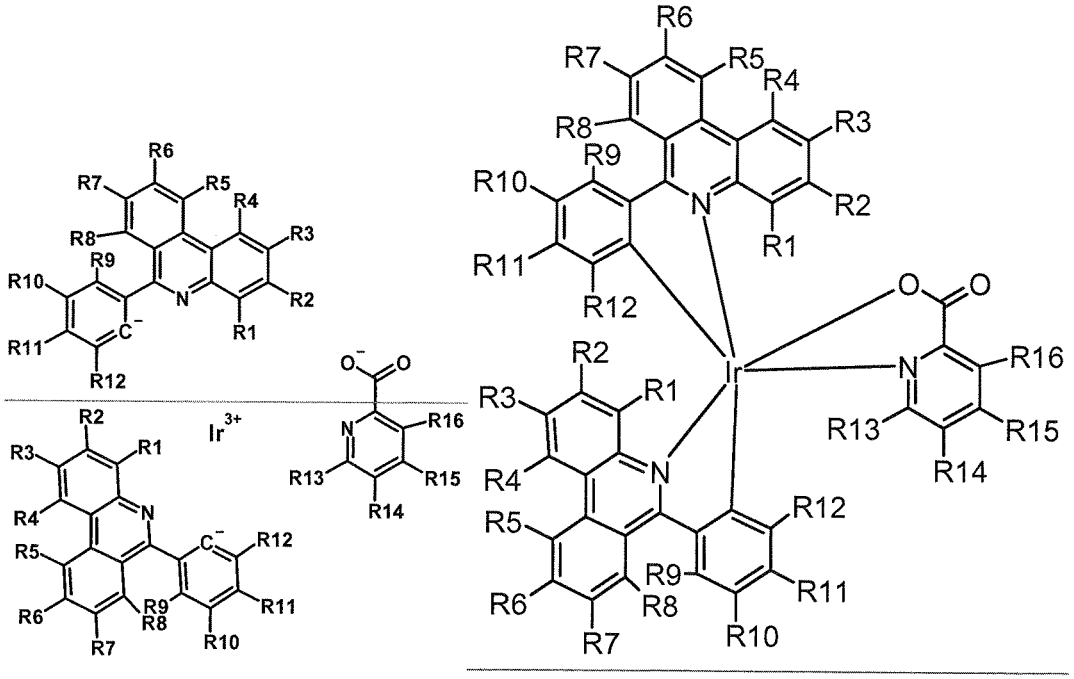
Summary of the Invention

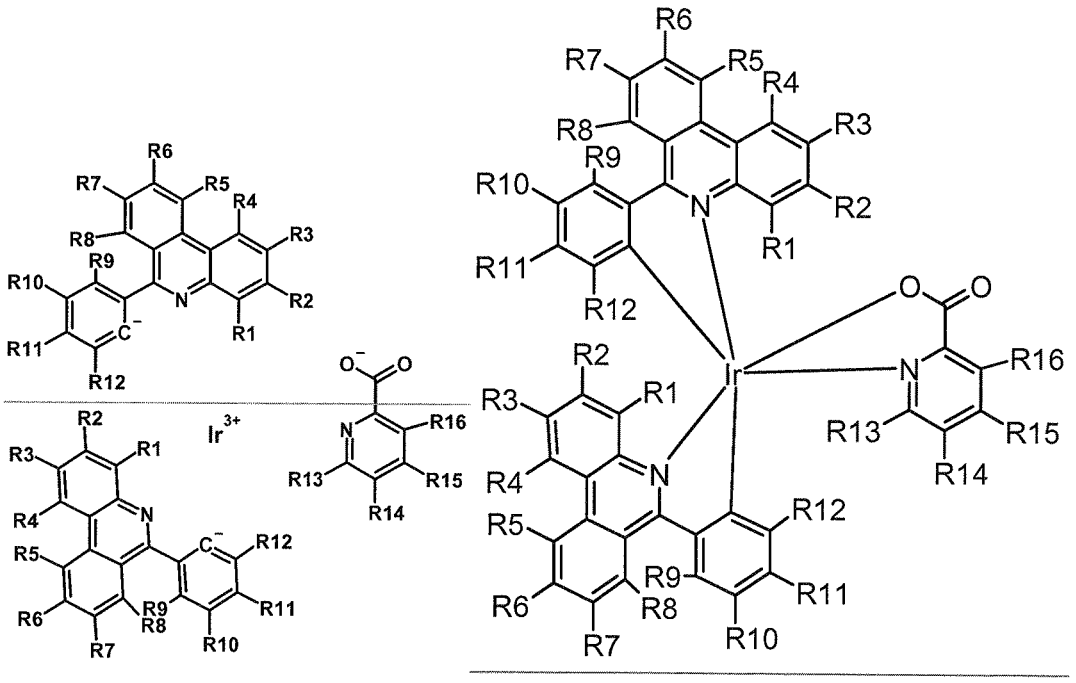
The present invention discloses an iridium-based chemiluminescent compound of Formula I



wherein R1-R16 is hydrogen, halide, cyano- or nitro-group, amino, alkylamino, substituted alkylamino, arylamino, substituted arylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituated or unsubstituated alkyloxy, substituted or unsubstituted aryloxy, sulfanyl, alkylsulfonyl, arylsulfonyl, sulfo, sulfino, sulfeno, sulfonamide, sulfoxide, sulfodioxide, phosphonate, phosphinate or R17, wherein R17 is aryl, substituted aryl, alkyl, substituted alkyl branched alkyl, substituted branched alkyl, arylalkyl, substituted arylalkyl, alkylaryl, substituted alkylaryl, alkenyl, substituted alkenyl, alkynyl, substituted alkynyl, wherein the substituent is selected from hydrogen, halide, cyano- or nitro-group, a hydrophilic group, like amino, alkylamino, substituted alkylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituted or unsubstituated alkyloxy,

Detailed Description of the Invention

The present invention relates to an iridium-based chemiluminescent compound of Formula I

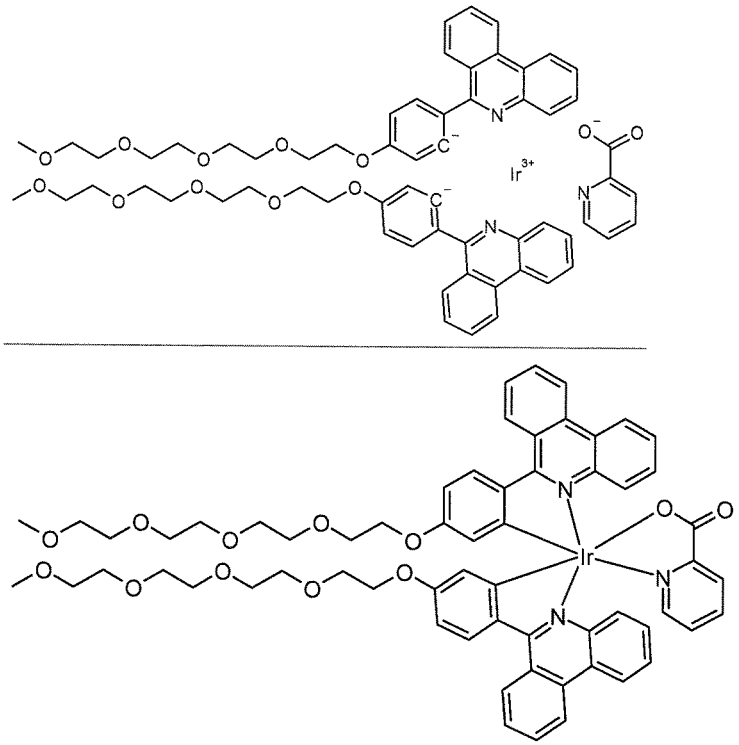


wherein R1-R16 is hydrogen, halide, cyano- or nitro-group, amino, alkylamino, substituted alkylamino, arylamino, substituted arylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituated or unsubstituated alkyloxy, substituted or unsubstituted aryloxy, sulfanyl, alkylsulfonyl, arylsulfonyl, sulfo, sulfino, sulfeno, sulfonamide, sulfoxide, sulfodioxide, phosphonate, phosphinate or R17, wherein R17 is aryl, substituted aryl, alkyl, substituted alkyl branched alkyl, substituted branched alkyl, arylalkyl, substituted arylalkyl, alkylaryl, substituted alkylaryl, alkenyl, substituted alkenyl, alkynyl, substituted alkynyl, wherein the substituent is selected from hydrogen, halide, cyano- or nitro-group, a hydrophilic group, like amino, alkylamino, substituted alkylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituted or unsubstituated alkyloxy, substituted or unsubstituted aryloxy, sulfanyl, alkylsulfonyl, arylsulfonyl, sulfo,

^{1}H-NMR (400 MHz, DMSO-d_6) δ 9.24 (m, 1H), 9.15 (d, J = 8.0 Hz, 1H), 8.97 (d, J = 8.4 Hz, 1H), 8.88 (d, J = 8.1 Hz, 1H), 8.73 (d, J = 7.6 Hz, 1H), 8.68 (d, J = 7.4 Hz, 1H), 8.50 (d, J = 7.8 Hz, 1H), 8.45 (d, J = 7.9 Hz, 1H), 8.34 (d, J = 2.0 Hz, 1H), 8.28 (d, J = 7.9 Hz, 1H), 8.13-8.00 (m, 4H), 7.92 (dd, J = 8.1, 2.1 Hz, 1H), 7.63 (t, J = 15.2, 7.0 Hz, 2H), 7.54-7.42 (m, 3H), 7.35 (d, J = 8.2 Hz, 2H), 7.17 (t, J = 15.2, 7.0 Hz, 1H), 7.10-7.06 (m, 3H), 7.02 (t, J = 15.7, 7.3 Hz, 1H), 6.89 (d, J = 6.7 Hz, 1H), 6.77 (t, J = 14.0, 7.1 Hz, 1H), 6.71 (t, J = 14.8, 7.0 Hz, 1H), 6.45 (d, J = 6.7 Hz, 1H), 2.86 (t, J = 15.2, 7.5 Hz, 2H), 2.55 (t, J = 15.4, 7.7 Hz, 2H).

MS: $[M+H]^+$ 972.3

Synthesis of JM 360:



JM 360

A suspension of Ir-dimer (150 mg, 0,065 mmol), picolinic acid (17 mg, 0.137 mmol) and Na_2CO_3 (70 mg, 0.65 mmol) in 20 mL dichloromethane/ethanol (4:1) was refluxed overnight. After cooling down, the mixture was concentrated to dryness. The residue was purified by flash cromatography in dichloromethane/MeOH (gradient from 100:0 to 10:1). The compound was recrystallized in dichloromethane/Et_2O.

Yield: 30%.

NMR:

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.06 (d, J = 8.2 Hz, 1H), 8.98 (d, J = 8.1 Hz, 1H), 8.61 (m, 3H), 8.46 – 8.21 (m, 4H), 8.13 (d, J = 8.9 Hz, 1H), 7.83 (m, 4H), 7.61 (m, 2H), 7.57 – 7.41 (m, 3H), 7.30 (d, J = 7.2 Hz, 1H), 7.24 – 7.12 (m, 1H), 6.89 (t, J =

7.2 Hz, 1H), 6.76 (dd, J = 8.9, 2.5 Hz, 1H), 6.61 (dd, J = 8.8, 2.6 Hz, 1H), 6.54 (d, J = 2.5 Hz, 1H), 5.99 (d, J = 2.6 Hz, 1H), 3.85 – 3.41 (m, 32H), 3.34 (s, 3H), 3.33 (s, 3H).

MS: $[2M+2Na]^{2+}$ calc. 1258.4012, found 1258.4030. $[M+H]^{+}$ calc. 1236.4197, found 1236.4227

Example 5

ECL with a novel Iridium complex

The electrochemiluminescence signal of several metal complexes was assessed in an ELECSYS® analyzer (Roche Diagnostics GmbH). Measurements were carried out homogeneously in the absence of streptavidin-coated paramagnetic microparticles. Stock solutions of each metal complex at 0.1 mg/ml DMSO were diluted with PBS buffer resulting in 10 nM solutions. The 10 nM solutions were handled as samples on the ELECSYS® analyzer. 20 µl sample was incubated together with 90 µl Reagent 1 (ProCell) and 90 µl Reagent 2 (ProCell) for 9 min at 37°C and subsequently the electrochemiluminescence signal was quantified.

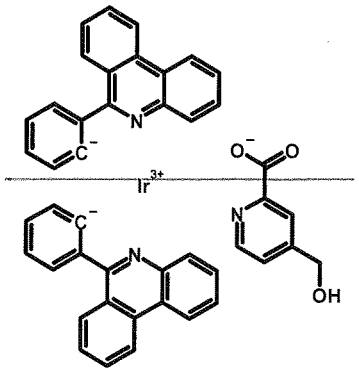
ECL results:

Reference Ru(bpy)3 = 10000 counts in 10 nmolar concentration

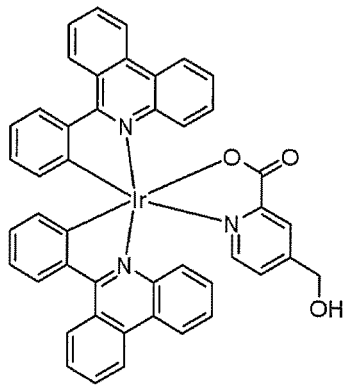
- JM 360 = 31258 counts 10 nmolar concentration

- RC 72 = 45512 count in 10 nmolar concentration

RC 72

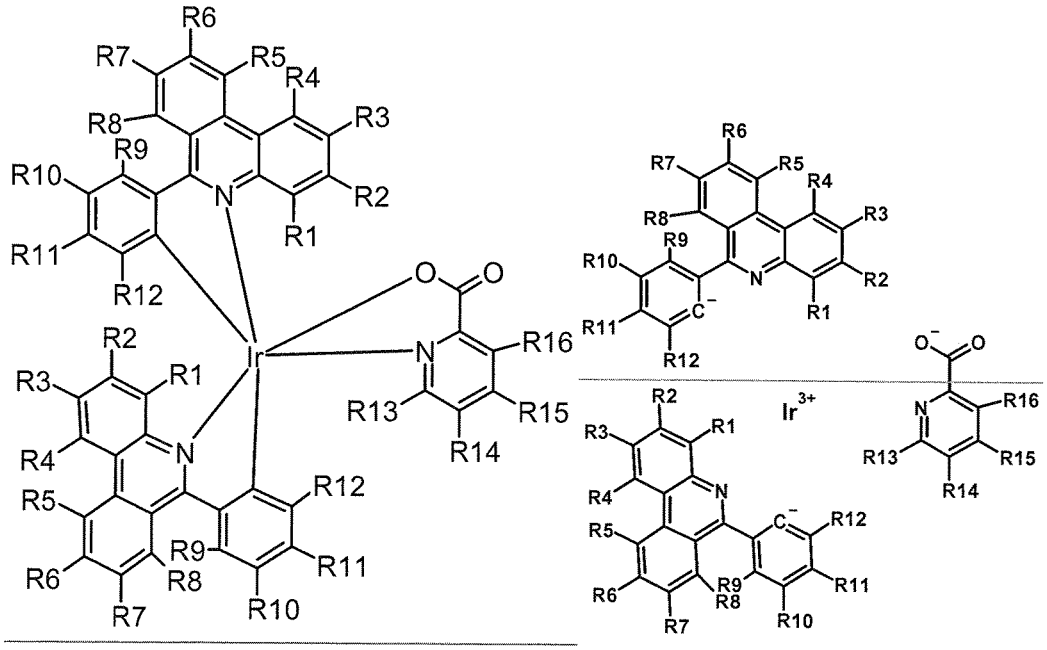


RC 72



Patent Claims

1. An iridium-based chemiluminescent compound of Formula I



wherein R1-R16 is hydrogen, halide, cyano- or nitro-group, amino, alkylamino, substituted alkylamino, arylamino, substituted arylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituated or unsubstituated alkyloxy, substituted or unsubstituted aryloxy, sulfanyl, alkylsulfonyl, arylsulfonyl, sulfo, sulfino, sulfeno, sulfonamide, sulfoxide, sulfodioxide, phosphonate, phosphinate or R17, wherein R17 is aryl, substituted aryl, alkyl, substituted alkyl branched alkyl, substituted branched alkyl, arylalkyl, substituted arylalkyl, alkylaryl, substituted alkylaryl, alkenyl, substituted alkenyl, alkynyl, substituted alkynyl, wherein the substituent is selected from hydrogen, halide, cyano- or nitro-group, a hydrophilic group, like amino, alkylamino, substituted alkylamino, alkylammonium, substituted alkylammonium, carboxy, carboxylic acid ester, carbamoyl, hydroxy, substituted or unsubstituated alkyloxy, substituted or unsubstituted aryloxy, sulfanyl, alkylsulfonyl,