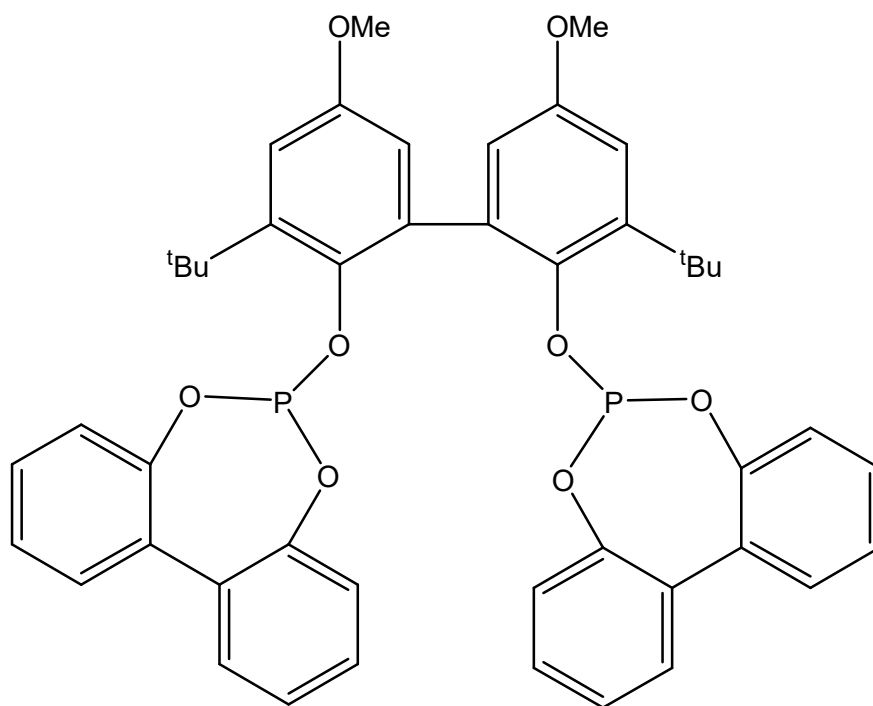


Pt-biphenyl-iodine complex and Pt-biphenyl-bromine complex

The present invention relates to a Pt-biphenyl-iodine complex and Pt-biphenyl-bromine complex, and the use thereof for catalysis of a hydroformylation reaction.

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EP 2663573 B1 describes a process for the preparation of (1).



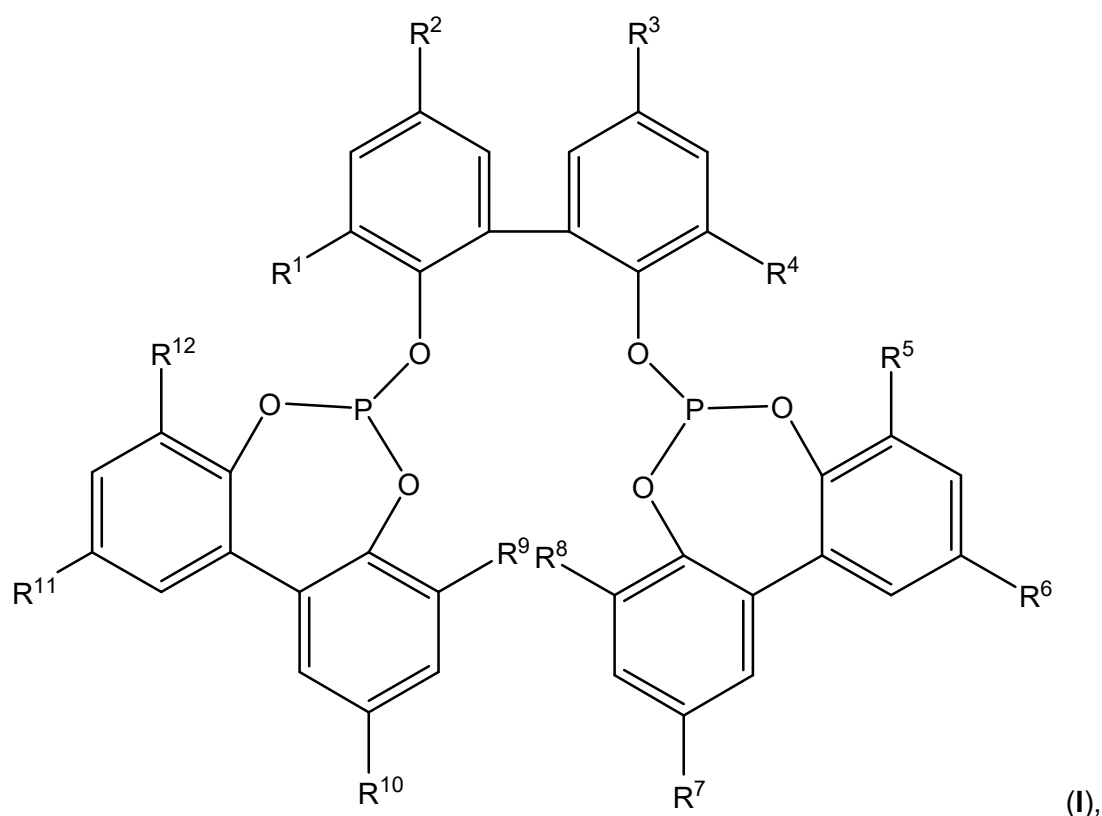
(1) (BiPhePhos)

- 10 It was an object of the present invention to provide a novel complex. In the case of catalysis of hydroformylation reactions, the complex should afford an increased yield.

This object is achieved by a complex according to Claim 1.

- 15 Complex comprising:

- a) Pt;
- b) a ligand corresponding to formula (I):



where $R^1, R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}$ are selected from: -H, $-(C_1-C_{12})$ -alkyl, $-O-(C_1-C_{12})$ -alkyl, $-(C_6-C_{20})$ -aryl;

c) an iodine ligand or a bromine ligand.

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The expression (C_1-C_{12}) -alkyl encompasses straight-chain and branched alkyl groups having 1 to 12 carbon atoms. These are preferably (C_1-C_8) -alkyl groups, more preferably (C_1-C_6) -alkyl, most preferably (C_1-C_4) -alkyl.

- 10 Suitable (C_1-C_{12}) -alkyl groups are especially methyl, ethyl, propyl, isopropyl, *n*-butyl, *isobutyl*, *sec*-butyl, *tert*-butyl, *n*-pentyl, 2-pentyl, 2-methylbutyl, 3-methylbutyl, 1,2-dimethylpropyl, 1,1-dimethylpropyl, 2,2-dimethylpropyl, 1-ethylpropyl, *n*-hexyl, 2-hexyl, 2-methylpentyl, 3-methylpentyl, 4-methylpentyl, 1,1-dimethylbutyl, 1,2-dimethylbutyl, 2,2-dimethylbutyl, 1,3-dimethylbutyl, 2,3-dimethylbutyl, 3,3-dimethylbutyl, 1,1,2-trimethylpropyl, 1,2,2-
- 15 trimethylpropyl, 1-ethylbutyl, 1-ethyl-2-methylpropyl, *n*-heptyl, 2-heptyl, 3-heptyl, 2-ethylpentyl, 1-propylbutyl, *n*-octyl, 2-ethylhexyl, 2-propylheptyl, nonyl, decyl.

The definition of (C_1-C_{12}) -alkyl also applies analogously to the (C_1-C_{12}) -alkyl in $-O-(C_1-C_{12})$ -alkyl.

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The expression (C₆-C₂₀)-aryl encompasses mono- or polycyclic aromatic hydrocarbon radicals having 6 to 20 carbon atoms. These are preferably (C₆-C₁₄)-aryl, more preferably (C₆-C₁₀)-aryl.

5 Suitable (C₆-C₂₀)-aryl groups are especially phenyl, naphthyl, indenyl, fluorenyl, anthracenyl, phenanthrenyl, naphthacenyl, chrysenyl, pyrenyl, coronenyl. Preferred (C₆-C₂₀)-aryl groups are phenyl, naphthyl and anthracenyl.

In one embodiment, R¹, R², R³, R⁴ are selected from: -(C₁-C₁₂)-alkyl, -O-(C₁-C₁₂)-alkyl.

10 In one embodiment, R¹ and R⁴ are -(C₁-C₁₂)-alkyl.

In one embodiment, R¹ and R⁴ are -^tBu.

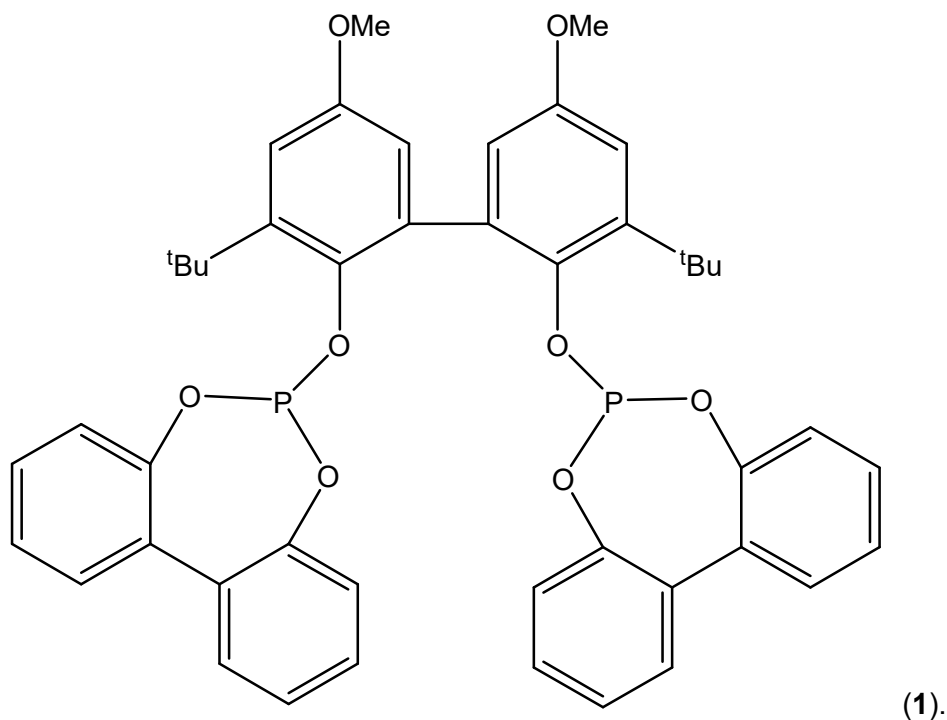
In one embodiment, R² and R³ are -O-(C₁-C₁₂)-alkyl.

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In one embodiment, R² and R³ are -OMe.

In one embodiment, R⁵, R⁶, R⁷, R⁸, R⁹, R¹⁰, R¹¹, R¹² are -H.

20 In one embodiment, the compound of formula (I) has the structure (1):



In one embodiment, the complex has exactly one ligand corresponding to formula (I).

In one embodiment, the complex has at least two iodine ligands.

In one embodiment, the complex has exactly two iodine ligands.

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In one embodiment, the complex has at least two bromine ligands.

In one embodiment, the complex has exactly two bromine ligands.

- 10 As well as the complex per se, the use thereof for catalysis of a hydroformylation reaction is also claimed.

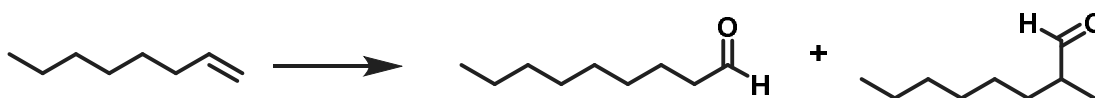
Use of a complex as described above for catalysis of a hydroformylation reaction.

- 15 The invention shall be elucidated in more detail hereinbelow with reference to working examples.

Experimental description

- 20 A vial was charged with PtX_2 (X = halogen), ligand, and an oven-dried stirrer bar. The vial is then sealed with a septum (PTFE-coated styrene-butadiene rubber) and phenolic resin cap. The vial is evacuated and refilled with argon three times. Toluene and 1-octene were added to the vial using a syringe. The vial was placed in an alloy plate, which was transferred to an autoclave of the 4560 series from Parr Instruments under an argon atmosphere. After purging
- 25 the autoclave three times with CO/H_2 , the synthesis gas pressure was increased to 40 bar at room temperature. The reaction was conducted at 120°C for 20 h. On termination of the reaction, the autoclave was cooled to room temperature and cautiously decompressed. Yield and selectivity were determined by GC analysis.

- 30 Variation of the halogen

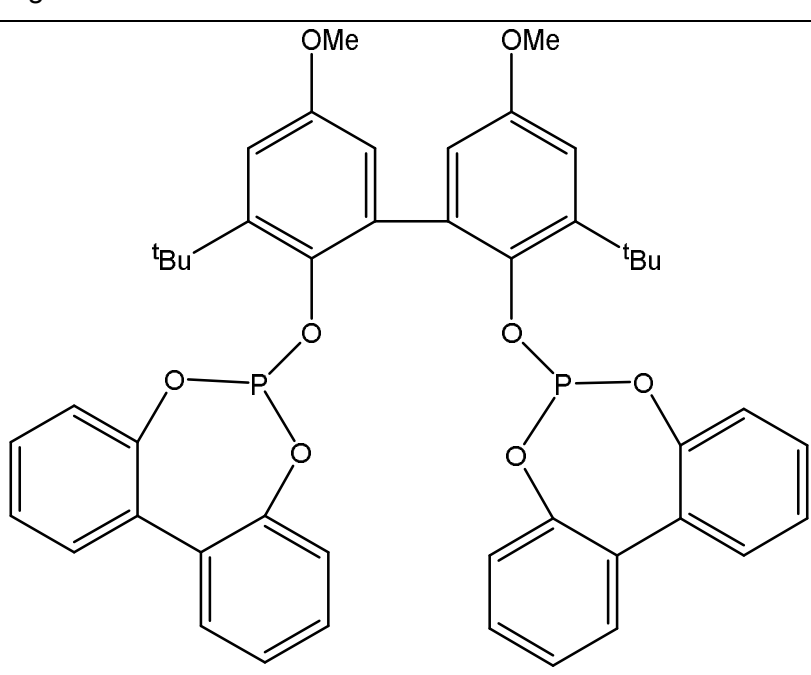


Reaction conditions:

1.0 mmol of 1-octene, 1.0 mol% PtX_2 , 2.2 equivalents of ligand **(1)**, solvent: toluene, $p(\text{CO}/\text{H}_2)$: 40 bar, T: 120°C, t: 20 h.

Yields:

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Ligand	Halogen	Yield [%]
 (1)	I / Br	69 / 27

As the experimental results show, the object is achieved by the complex according to the invention.

1. Complex comprising:

a) Pt;

b) a ligand corresponding to formula (I):



where R¹, R², R³, R⁴, R⁵, R⁶, R⁷, R⁸, R⁹, R¹⁰, R¹¹, R¹² are selected from: -H, -(C₁-C₁₂)-alkyl, -O-(C₁-C₁₂)-alkyl, -(C₆-C₂₀)-aryl;

c) an iodine ligand or a bromine ligand.

2. Complex according to Claim 1,

where R¹, R², R³, R⁴ are selected from: -(C₁-C₁₂)-alkyl, -O-(C₁-C₁₂)-alkyl.

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3. Complex according to either of Claims 1 and 2,

where R¹ and R⁴ are -(C₁-C₁₂)-alkyl.

4. Complex according to any of Claims 1 to 3,

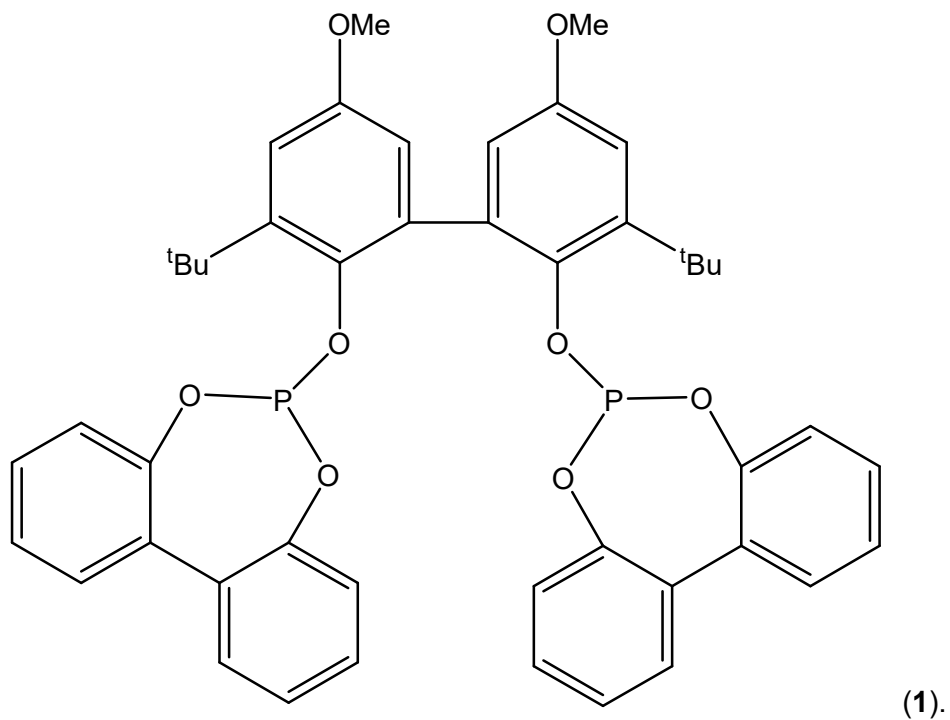
where R² and R³ are -O-(C₁-C₁₂)-alkyl.

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5. Complex according to any of Claims 1 to 4,

where $R^5, R^6, R^7, R^8, R^9, R^{10}, R^{11}, R^{12}$ are -H.

6. Complex according to any of Claims 1 to 5,
wherein the compound of formula (I) has the structure (1):



7. Complex according to any of Claims 1 to 6,
wherein the complex has exactly one ligand corresponding to formula (I).

10 8. Complex according to any of Claims 1 to 7,
wherein the complex has two iodine ligands.

9. Complex according to Claim 8,
wherein the complex has exactly two iodine ligands.

15 10. Complex according to any of Claims 1 to 7,
wherein the complex has at least two bromine ligands.

11. Complex according to Claim 10,
20 wherein the complex has exactly two bromine ligands.

12. Use of a complex according to any of Claims 1 to 11 for catalysis of a hydroformylation reaction.