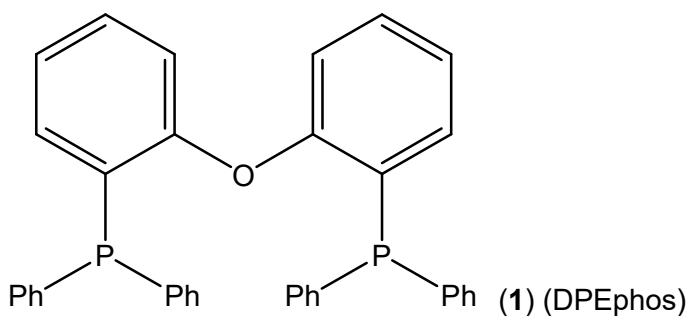


Pt-DPEphos-iodine complex and Pt-DPEphos-bromine complex

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

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P. Meessen et al., Journal of Organometallic Chemistry, 551, (1998), 165-170 describes the use of DPEphosPtCl₂ for the hydroformylation of methyl 3-pentenoate.



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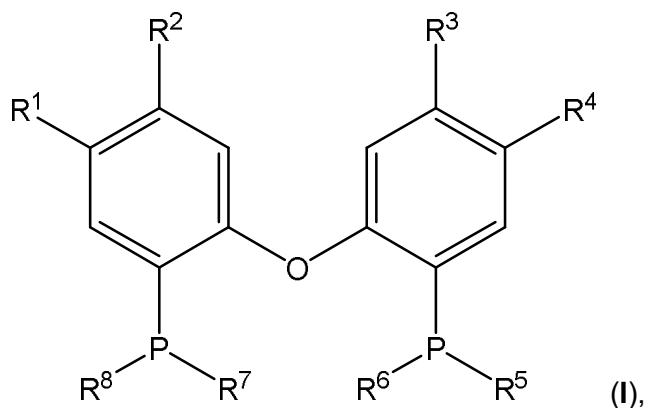
The present invention has the object of providing a novel complex. The complex here is to afford an enhanced yield in the catalysis of hydroformylation reactions compared to the complex described in the prior art.

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

Complex comprising:

a) Pt;

b) a ligand conforming to the formula (I):



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where R¹, R², R³, R⁴, R⁵, R⁶, R⁷, R⁸ are selected from: -H, -(C₁-C₁₂)-alkyl, -(C₆-C₂₀)-aryl, and at least two of the R⁵, R⁶, R⁷, R⁸ radicals are -(C₆-C₂₀)-aryl;

c) an iodine ligand or bromine ligand.

The expression (C₁-C₁₂)-alkyl encompasses straight-chain and branched alkyl groups having 1 to 12 carbon atoms. These are preferably (C₁-C₈)-alkyl groups, more preferably (C₁-C₆)-alkyl, most preferably (C₁-C₄)-alkyl.

5

Suitable (C₁-C₁₂)-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-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 expression (C₆-C₂₀)-aryl encompasses mono- or polycyclic aromatic hydrocarbyl radicals having 6 to 20 carbon atoms. These are preferably (C₆-C₁₄)-aryl, more preferably (C₆-C₁₀)-aryl.

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.

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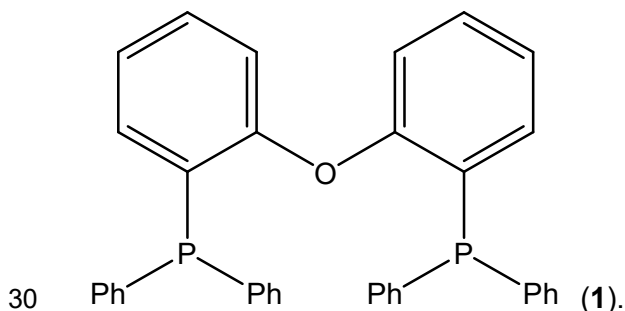
In one embodiment, R⁵, R⁶, R⁷, R⁸ are -(C₆-C₂₀)-aryl.

In one embodiment, R⁵, R⁶, R⁷, R⁸ are -Ph.

25 In one embodiment, R¹ and R⁴ are each -H.

In one embodiment, R² and R³ are each -H.

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.

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

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.

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

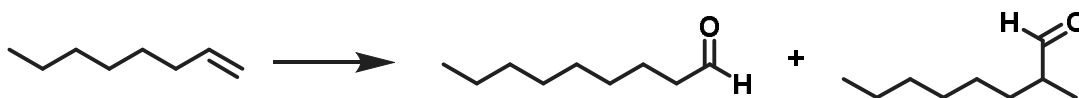
Experimental description

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A vial was charged with PtX_2 ($X = \text{halogen}$), ligand, and an oven-dried stirrer bar. The vial is then sealed with a septum (PTFE-coated styrene-butadiene rubber) and phenolic 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 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 $120^\circ C$ 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.

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Hydroformylation of 1-octene

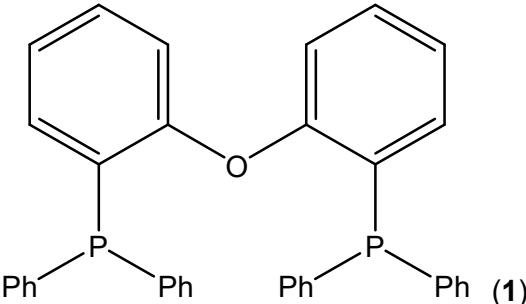


Reaction conditions:

10.0 mmol of 1-octene, 0.1 mol% PtX_2 , 2.2 equivalents of ligand, solvent: toluene, $p(\text{CO}/\text{H}_2)$: 40 bar, T: 120°C, t: 20 h.

Yields:

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Ligand	Halogen	Yield [%]
	I / Br / Cl	76 / 45 / 14

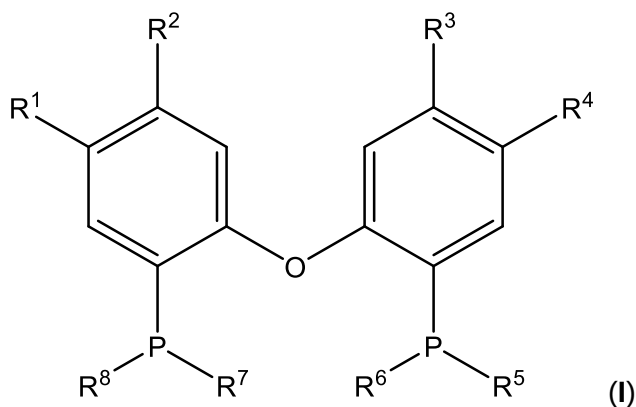
As the experimental results show, the object is achieved by the complex according to the invention.

Claims

1. A complex comprising:

5 a) Pt;

b) a ligand conforming to the formula (I):



where R^1 , R^2 , R^3 , R^4 , R^5 , R^6 , R^7 , R^8 are selected from: -H, -(C₁-C₁₂)-alkyl, -(C₆-C₂₀)-aryl, and at least two of the R^5 , R^6 , R^7 , R^8 radicals are -(C₆-C₂₀)-aryl;

10 c) at least two bromine ligands.

2. The complex according to Claim 1,

where R^5 , R^6 , R^7 , R^8 are -(C₆-C₂₀)-aryl.

15 3. The complex according to either of Claims 1 or 2,

where R^5 , R^6 , R^7 , R^8 are -Ph.

4. The complex according to any of Claims 1 to 3,

where R^1 and R^4 are each -H.

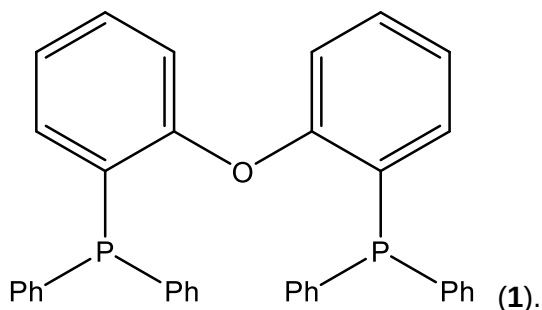
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5. The complex according to any of Claims 1 to 4,

where R^2 and R^3 are each -H.

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



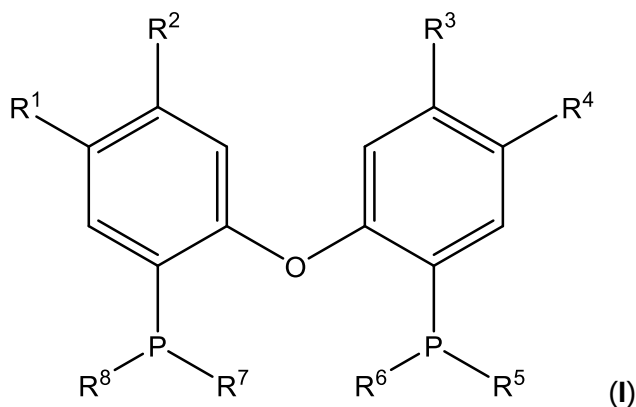
7. The complex according to any of Claims 1 to 6,
wherein the complex has exactly one ligand conforming to the formula (I).

8. The complex according to any of Claims 1 to 7,
wherein the complex has exactly two bromine ligands.

9. Use of a complex comprising:

a) Pt;

b) a ligand conforming to the formula (I):



where R^1 , R^2 , R^3 , R^4 , R^5 , R^6 , R^7 , R^8 are selected from: -H, $-(C_1-C_{12})$ -alkyl, $-(C_6-C_{20})$ -aryl,
and at least two of the R^5 , R^6 , R^7 , R^8 radicals are $-(C_6-C_{20})$ -aryl;

c) an iodine ligand or bromine ligand

for catalysis of a hydroformylation reaction.

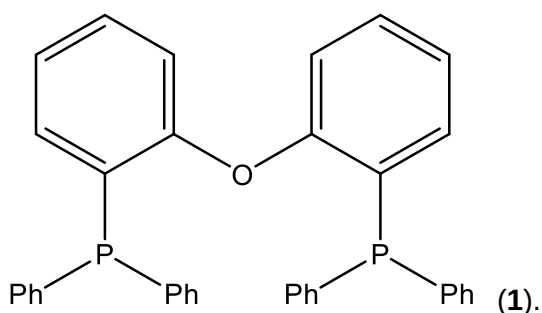
10. The use according to Claim 9,
where R^5 , R^6 , R^7 , R^8 are $-(C_6-C_{20})$ -aryl.

11. The use according to either of Claims 9 or 10,
where R^5 , R^6 , R^7 , R^8 are -Ph.

12. The use according to any of Claims 9 to 11,
5 where R^1 and R^4 are each -H.

13. The use according to any of Claims 9 to 12,
where R^2 and R^3 are each -H.

10 14. The use according to any of Claims 9 to 13,
wherein the compound of formula (I) has the structure (1):



15 15. The use according to any of Claims 9 to 14,
wherein the complex has exactly one ligand conforming to the formula (I).

16. The use according to any of Claims 9 to 15,
wherein the complex has two iodine ligands.

20 17. The use according to Claim 16,
wherein the complex has exactly two iodine ligands.

18. The use according to any of Claims 9 to 15,
wherein the complex has at least two bromine ligands.

25 19. The use according to Claim 18,
wherein the complex has exactly two bromine ligands.