Chem. Eur. J. **2004**

Supporting Information

for

Chemistry: A European Journal

New Chiral Ruthenium(II) Catalysts Containing 2,6-Bis(4'-(*R*)-phenyloxazolin-2'-yl)pyridine (Ph-pybox) Ligands for Highly Enantioselective Transfer Hydrogenation of Ketones

By

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Table S1. Transfer Hydrogenation of 2-Br-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	60	18	59
2	**2a**	60	21	60
3[a]	**3a**	15(60)	23(28)	73(74)
4	**6a**	5(60)	4(7)	43(27)
5	**6b**	1(60)	32(65)	86(80)
6	**7a**	45	>99.5	2

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S2. Transfer Hydrogenation of 3-Br-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	60	36	45
2	**2a**	60	55	16
3[a]	**3a**	60	>99.5	77
4	**6a**	5	>99	93
5	**6b**	3	>99	93
6	**7a**	30	>99.5	2

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S3. Transfer Hydrogenation of 4-Br-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	30	23	44
2	**2a**	60	17	7
3[a]	**3a**	120	97	70
4	**6a**	120	68	45
5	**6b**	60	69	54
6	**7a**	30	99	1

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S4. Transfer Hydrogenation of 2-MeO-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	180	92	64
2	**2a**	60	38	40
3[a]	**3a**	60	44	62
4	**6a**	120	61	23
5	**6b**	120	94	47
6	**7a**	15	99	76

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S5. Transfer Hydrogenation of 3-MeO-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	30	92	82
2	**2a**	60	98	77
3[a]	**3a**	15	97	91
4	**6a**	10	94	87
5	**6b**	5	97	82
6	**7a**	15	97	43

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S6. Transfer Hydrogenation of 4-MeO-Acetophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	15(60)	40(68)	69(61)
2	**2a**	15	82	59
3[a]	**3a**	30	82	86
4	**6a**	30	83	80
5	**6b**	5	83	89
6	**7a**	10	86	62

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S7. Transfer Hydrogenation of Propiophenone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	15	95	91
2	**2a**	60	96	85
3[a]	**3a**	30	97	92
4	**6a**	60	94	83
5	**6b**	5	97	92
6	**7a**	30	98	58

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S8. Transfer Hydrogenation of 2'-Acetonaphtone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee* (*S*)
1	**1b**	60	96	81
2	**2a**	90	94	77
3[a]	**3a**	15	96	91
4	**6a**	10	96	82
5	**6b**	5	96	86
6	**7a**	30	98	37

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S9. Transfer Hydrogenation of 2-Butanone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee*
1	**1b**	60	93	13 (*R*)
2	**2a**	30	>99.5	7 (*R*)
3[a]	**3a**	30	97	10 (*R*)
4	**6a**	60	98	11 (*R*)
5	**6b**	10	>99	11 (*R*)
6	**7a**	10	>99	11 (*S*)

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.

Table S10. Transfer Hydrogenation of Methyl Isopropyl Ketone Catalyzed by Ph-pybox Complexes under Optimized Conditions.

entry	cat.	time (min)	%conv	%*ee*
1	**1b**	60	70	20 (*R*)
2	**2a**	120	85	6 (*R*)
3[a]	**3a**	60	86	16 (*R*)
4	**6a**	90	95	12 (*R*)
5	**6b**	60	97	10 (*R*)
6	**7a**	10	99	31 (*S*)

Reactions were carried out at 82 ºC with a 0.1 M acetophenone solution in 50 mL of 2-propanol (ketone:cat:NaOH = 500:1:24). [a] Base was added 10 min before ketone.