Supplementary Material for Chemical Communications

Electronic Supplementary Information

ad

Highly enantioselective iridium-catalysed allylic aminations with anionic N-nucleophiles

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Determination of enantiomeric excess of branched products 2 **(cf. Table 1 of publication) by HPLC:**
column: Daicel Chiralcel AD-H/OD-H, 4.6 x 250 mm with pre-column AD-H/OD-H, 10 x 4 mm; eluent: *n*-hexane/*iso*-propanol, flow 0.5 mL/min, UV detection λ = 210 nm, 254 nm)

R^1	Ar	R^2	*n*-hexane/ *iso*-propanol	Column	t_R (min) minor	t_R (min) major
Ph	*p*-Ts	CH_2Ph	90:10	AD-H	31.69	36.67
CH_2CH_2Ph	*p*-Ts	CH_2Ph	90:10	OD-H	20.66	17.31
Ph	*o*-Ns	CH_2Ph	90:10	AD-H	46.98	43.98
CH_2CH_2Ph	*o*-Ns	CH_2Ph	90:10	AD-H	39.02	31.10
Ph	*p*-Ns	CH_2Ph	90:10	AD-H	43.68	58.47
CH_2CH_2Ph	*p*-Ns	CH_2Ph	95:5	AD-H	90.16	96.56
CH=CHPh	*p*-Ns	CH_2Ph	75:25	AD-H	34.37	31.24
3-Pyridyl	*p*-Ns	CH_2Ph	70:30	AD-H	31.17	41.85
Ph	*p*-Ns	H	90:10	OD-H	53.71	60.68
Ph	*p*-Ns	H	90:10	AD-H	37.27	43.49
Ph	*p*-Ns	$CH_2CH=CH_2$	95:5	AD-H	33.86	34.79
3-Pyridyl	*p*-Ns	$CH_2CH=CH_2$	80:20	AD-H	39.16	58.72
Ph	*p*-Ns	$(CH_2)_2CH=CH_2$	95:5	AD-H	30.13	32.54
3-Pyridyl	*p*-Ns	$(CH_2)_2CH=CH_2$	80:20	AD-H	34.95	37.25

X-ray crystal structure analysis of compound 7t:

Supplier of crystal: A. Dahnz (AK Helmchen)
File name : ad1.*
Operator : Thomas Oeser
Instrument : Bruker Smart APEX

The data are available from the Cambridge Crystallographic Data Center: CCDC No 267826.

Bond lengths (Å) and angles (deg) for ad1.

S1-O2	1.4346(9)	C4-C7	1.4999(16)
S1-O1	1.4353(8)	C4-H4	0.953(15)
S1-N1	1.6052(10)	C5-C6	1.3198(17)
S1-C11	1.7751(11)	C5-H5	0.907(16)
O3-N2	1.2238(14)	C6-H6A	0.958(18)
O4-N2	1.2294(15)	C6-H6B	0.946(17)
N1-C1	1.4928(15)	C7-C8	1.3210(18)
N1-C4	1.4984(14)	C7-H7	0.940(19)
N2-C14	1.4780(14)	C8-H8A	0.93(2)
C1-C5	1.5021(15)	C8-H8B	0.937(17)
C1-C2	1.5351(16)	C11-C12	1.3937(15)
C1-H1	0.972(15)	C11-C16	1.3940(15)
C2-C3	1.5310(19)	C12-C13	1.3915(15)
C2-H2A	0.996(17)	C12-H12	0.952(16)
C2-H2B	0.974(16)	C13-C14	1.3868(16)
C3-C4	1.5365(17)	C13-H13	0.918(16)
C3-H3A	0.947(19)	C14-C15	1.3855(17)
C3-H3B	0.956(17)	C15-C16	1.3860(16)

C15-H15	0.969(15)	C7-C4-C3	112.52(10)
C16-H16	0.912(17)	N1-C4-H4	109.3(9)
O2-S1-O1	119.88(5)	C7-C4-H4	108.5(9)
O2-S1-N1	107.25(5)	C3-C4-H4	112.7(9)
O1-S1-N1	108.14(5)	C6-C5-C1	124.20(11)
O2-S1-C11	107.55(5)	C6-C5-H5	120.9(10)
O1-S1-C11	105.79(5)	C1-C5-H5	114.9(10)
N1-S1-C11	107.71(5)	C5-C6-H6A	119.9(11)
C1-N1-C4	113.65(9)	C5-C6-H6B	122.4(10)
C1-N1-S1	121.63(7)	H6A-C6-H6B	117.6(15)
C4-N1-S1	123.10(8)	C8-C7-C4	122.81(12)
O3-N2-O4	124.18(10)	C8-C7-H7	118.2(11)
O3-N2-C14	118.15(10)	C4-C7-H7	119.0(11)
O4-N2-C14	117.68(11)	C7-C8-H8A	119.6(12)
N1-C1-C5	111.50(9)	C7-C8-H8B	122.1(11)
N1-C1-C2	101.66(9)	H8A-C8-H8B	118.3(16)
C5-C1-C2	111.69(10)	C12-C11-C16	121.32(10)
N1-C1-H1	110.1(9)	C12-C11-S1	119.19(8)
C5-C1-H1	108.8(9)	C16-C11-S1	119.49(8)
C2-C1-H1	113.0(9)	C13-C12-C11	119.70(10)
C3-C2-C1	103.59(10)	C13-C12-H12	119.5(9)
C3-C2-H2A	110.8(10)	C11-C12-H12	120.7(9)
C1-C2-H2A	111.6(10)	C14-C13-C12	117.85(10)
C3-C2-H2B	115.1(9)	C14-C13-H13	121.4(10)
C1-C2-H2B	110.4(9)	C12-C13-H13	120.7(10)
H2A-C2-H2B	105.5(13)	C15-C14-C13	123.30(10)
C2-C3-C4	104.10(10)	C15-C14-N2	118.59(10)
C2-C3-H3A	112.9(12)	C13-C14-N2	118.11(10)
C4-C3-H3A	110.7(11)	C14-C15-C16	118.45(11)
C2-C3-H3B	111.3(10)	C14-C15-H15	120.1(9)
C4-C3-H3B	108.1(11)	C16-C15-H15	121.4(9)
H3A-C3-H3B	109.4(15)	C15-C16-C11	119.38(11)
N1-C4-C7	113.36(9)	C15-C16-H16	119.9(10)
N1-C4-C3	100.35(9)	C11-C16-H16	120.8(10)