Supporting Information

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Chelating NHC Ruthenium(II) Complexes as Robust Homogeneous Hydrogenation Catalysts

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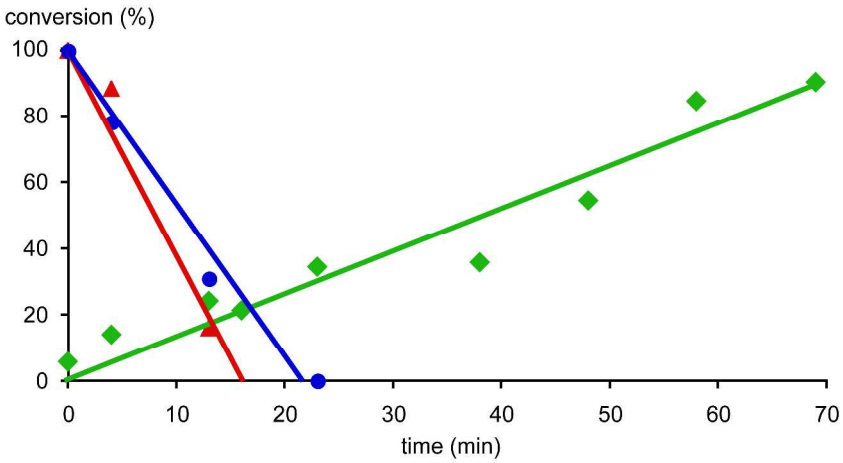

Figure S1. Time-dependent decoordination of the olefin (▲), and cymene (●) from complex **8**, and formation of imidazolium salt (◆) monitored by high pressure ^{1}H NMR spectroscopy in absence of styrene.

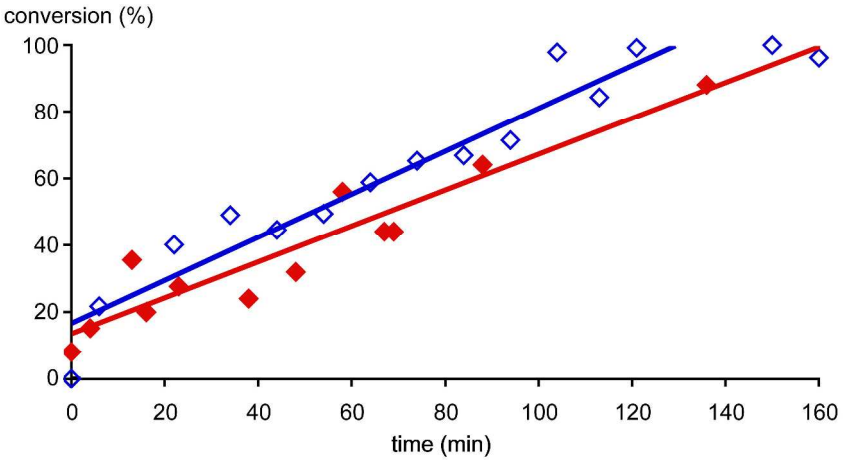

Figure S2. Time-dependent formation of imidazolium salt from complex **8** in the presence (◆) and in the absence (◇) of styrene monitored by high pressure ^{1}H NMR spectroscopy

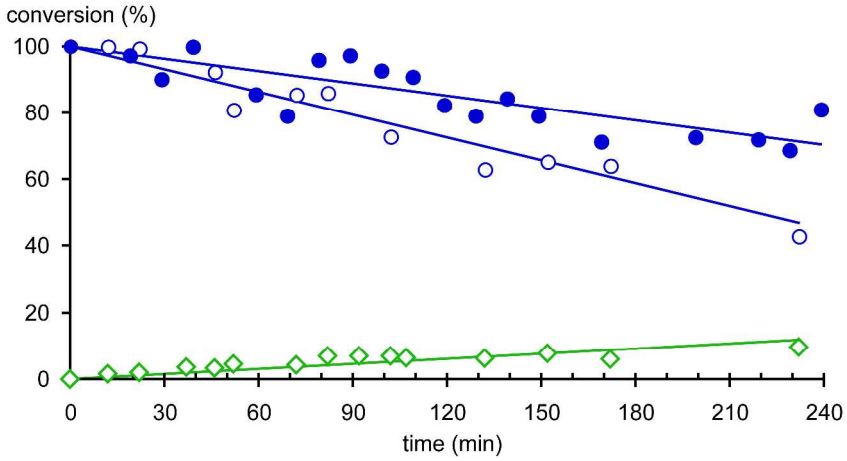

Figure S3. Comparison of the stability of complex **10** in the presence (●) and absence (○) of styrene monitored by high pressure ^{1}H NMR spectroscopy. Formation of imidazolium salt (◇) in the absence of styrene occurs at similar rates as complex decomposition.

Table S1. Crystallographic Data for Complexes **5a**, **6**, **10** and **12**

	5a	**6**	**10**	**12**
color, shape	yellow, needle	yellow, needle	orange, needle	yellow, block
crystal size/mm	0.45 × 0.15 × 0.10	0.45 × 0.15 × 0.10	0.40 × 0.25 × 0.15	0.45 × 0.40 × 0.35
empirical formula	$C_{30}H_{30}ClN_2PRu$ × CH_2Cl_2 × 2 H_2O	$C_{30}H_{32}BF_4N_2PRu$ S × CH_2Cl_2	$C_{24}H_{29}ClN_2O_2Ru$ × C_3H_6O	$C_{23}H_{34}ClF_6N_4PRu$
Fw	707.01	756.41	572.09	648.03
T/K	173(2)	173(2)	173(2)	173(2)
crystal system	orthorhombic	Monoclinic	monoclinic	tetragonal
space group	*P*bca (No. 61)	*C* 2/c (No. 15)	*P* 2_1/n (No. 14)	*P* 4_2/n (No. 86)
unit cell				
a/Å	33.7082(10)	36.288(3)	8.0931(7)	23.6976(18)
b/Å	10.0040(3)	10.6994(6)	10.5933(11)	23.6976(18)
c/Å	37.0802(17)	17.6923(13)	30.176(3)	9.7412(10)
α/deg	90	90	90	90
β/deg	90	110.377(6)	93.321(8)	90
γ/deg	90	90	90	90
V/Å^3	12504.1(8)	6439.4(8)	2582.8(4)	5470.4(8)
Z	16	8	4	8
D_{calc}/g cm^{-3}	1.502	1.560	1.471	1.574
μ/mm^{-1} (Mo K_α)	0.840	0.816	0.741	0.790
no. of total, unique reflns	106561, 11147	20694, 5732	17550, 4597	18300, 4843
R_{int}	0.0948	0.0607	0.1047	0.0401
transmission range	0.499–0.841	0.709–0.864	0.770–0.968	0.741–0.817
no. parameters, restraints	748, 7	361, 8	318, 0	332, 0
R, *Rw* [a]	0.0724, 0.1845	0.0887, 0.2310	0.0944, 0.2041	0.0363, 0.0847
GOF	1.074	1.083	1.185	0.903
min,max resid density/e Å^{-3}	–1.383, 0.958	–1.194, 1.155	–1.205, 1.064	–0.746, 0.465

[a] $R_1 = \Sigma||F_O|-|F_C||/\Sigma|F_O|$ and $wR_2 = [\Sigma w(F_O^2-F_C^2)^2/\Sigma(w(F_O^4)]^{1/2}$ for all $I > 2\sigma(I)$