Supplementary Material (ESI) for New Journal of Chemistry

A 1,1'-ferrocenyl phosphine-borane: synthesis, structure and evaluation in Rh-catalyzed hydroformylation

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ELECTRONIC SUPPLEMENTARY INFORMATION

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Selected crystal data. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–766316 (**2**). These data can be obtained free of charge via www.ccdc.cam.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

2: $C_{40}H_{40}BFeP$, M = 618.35, monoclinic, space group $P2(1)/c$, a = 8.2786(11), b = 42.999(5), c = 9.2730(12) Å, α = 90°, β = 93.458(3)°, γ = 90°, V = 3294.9(7) Å^3, Z = 4, crystal size 0.2 x 0.1 x 0.07 mm^3, 14541 reflections collected (4681 independent, R_{int} = 0.1484), 394 parameters, $R1$ [I>2σ(I)] = 0.0756, wR_2 [all data] = 0.1269, GOF = 1.018, largest diff. peak and hole: 0.435 and -0.302 eÅ^{-3}.

Data were collected at 173(2) K using an oil–coated shock–cooled crystal on a Bruker–AXS CCD 1000 diffractometer (λ = 0.71073 Å). Semi-empirical absorption corrections were employed.[1] The structure was solved by direct methods (SHELXS–97),[2] and refined using the least–squares method on F^2.[3]

[1] SADABS, Program for data correction, Bruker-AXS.
[2] G. M. Sheldrick, *Acta Crystallogr.*, 1990, **A46**, 467.
[3] SHELXL-97, Program for Crystal Structure Refinement, G. M. Sheldrick, University of Göttingen, 1997.

Catalytic Results

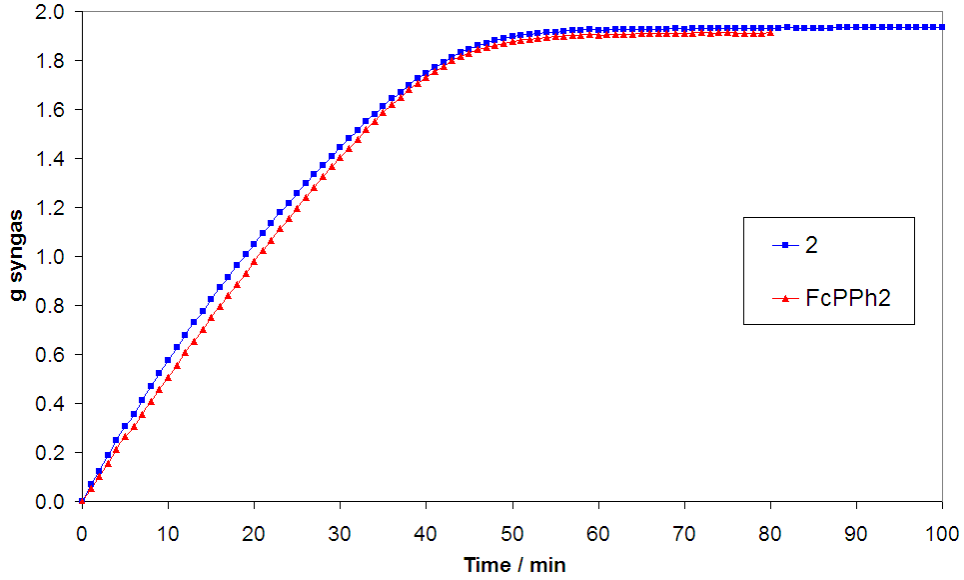

Fig. S1 Uptake of syngas observed with the 1,1'-ferrocenyl phosphine-borane ligand **2** and the boron-free ligand $FcPPh_2$.

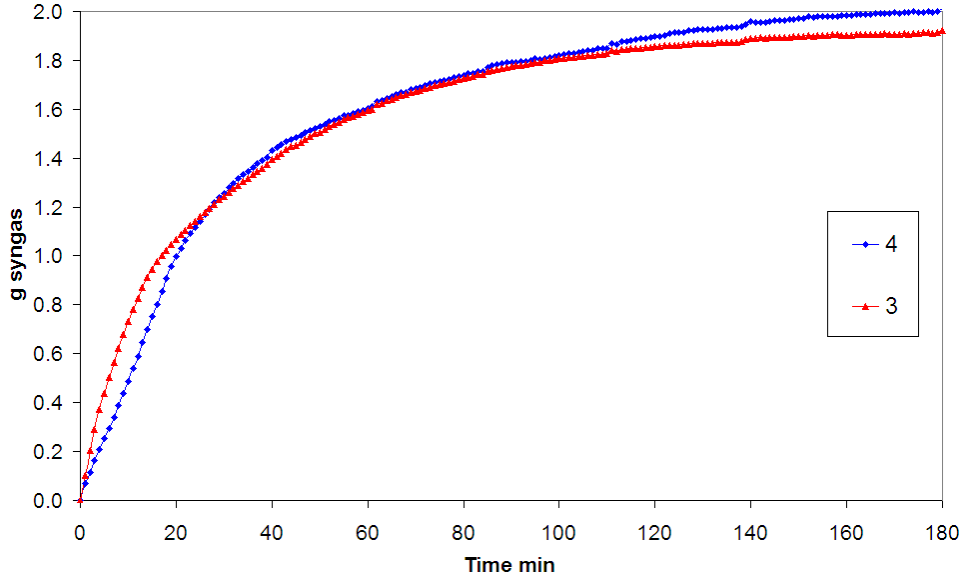

Fig. S2 Uptake of syngas observed with the *ortho*-phenylene phosphine-borane ligand **3** and the sterically encumbered biaryldiphosphine ligand **4**.