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Functionalized cyclopentadienyl rhodium(III) bipyridine complexes: Synthesis, characterization, and catalytic Application in hydrogenation of ketones

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Electronic Supporting Information

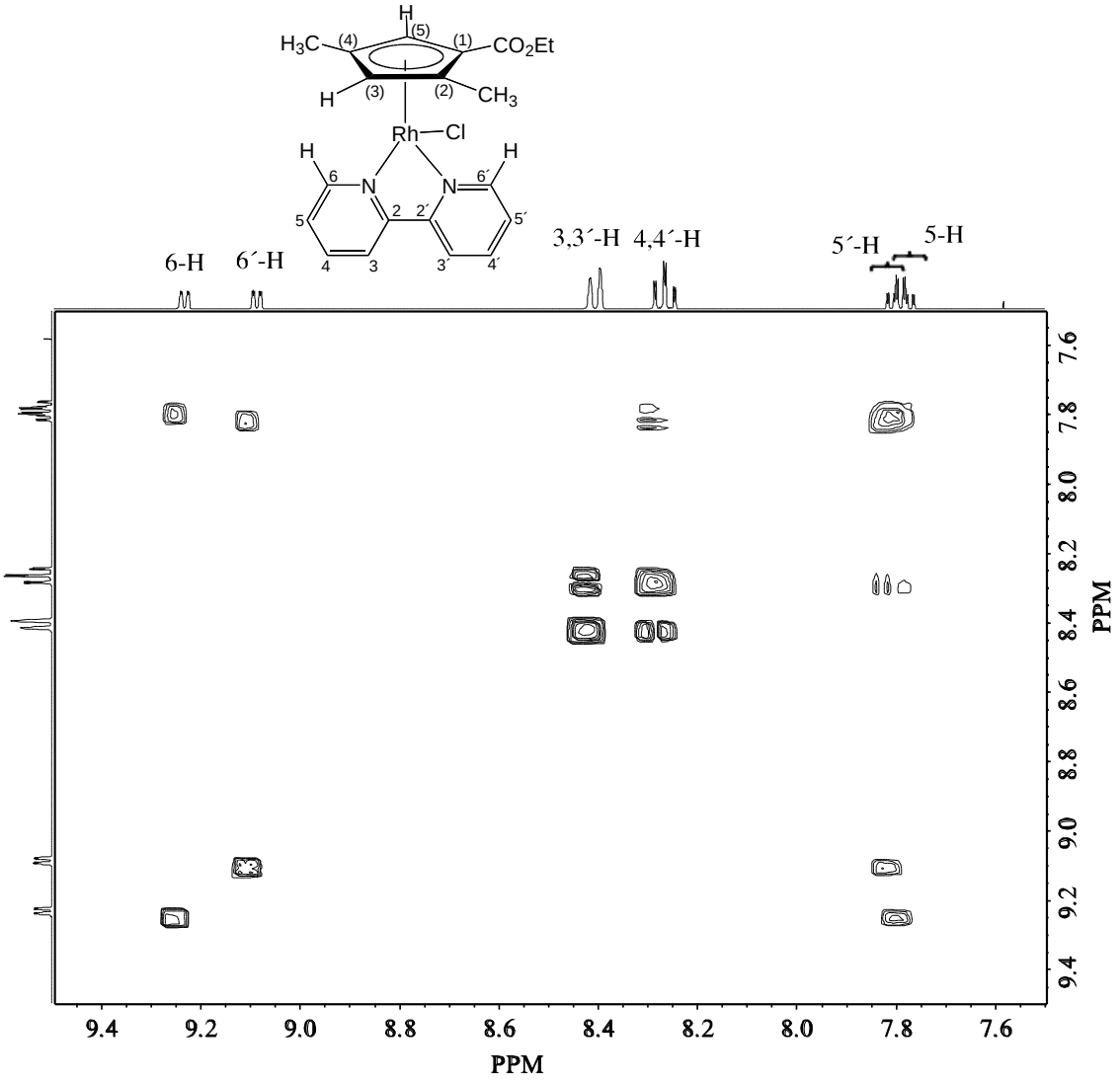

Figure S1. H-H COSY spectrum of **3** in CD_3CN.

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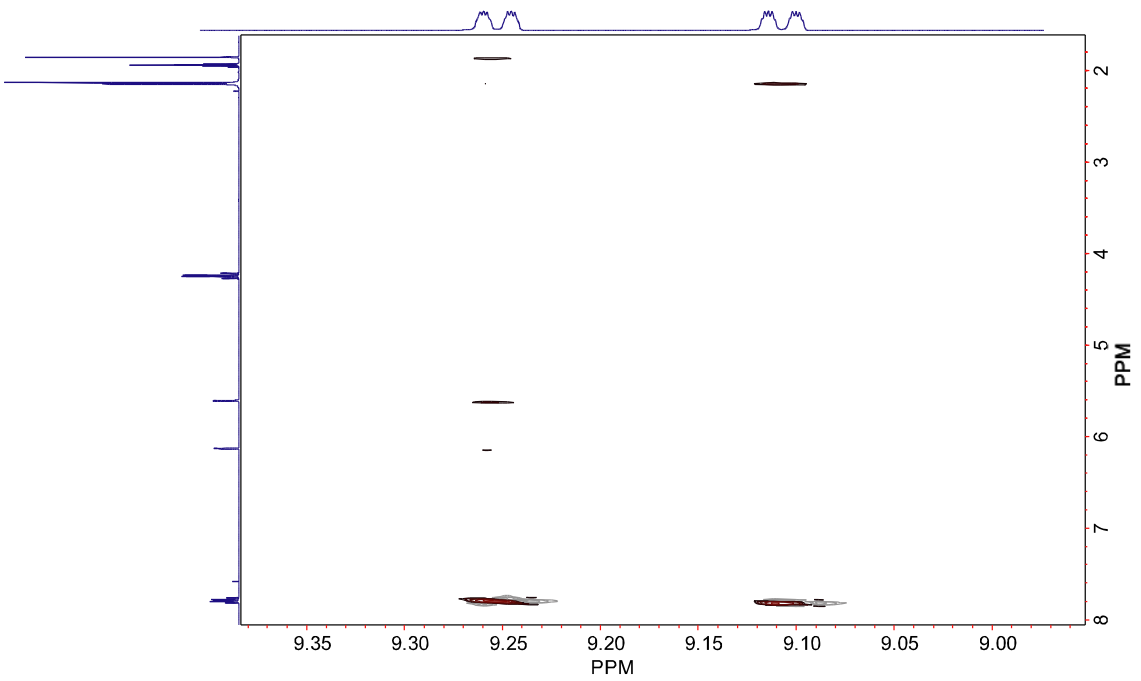

Figure S2. NOESY spectrum of **3** in CD_3CN.

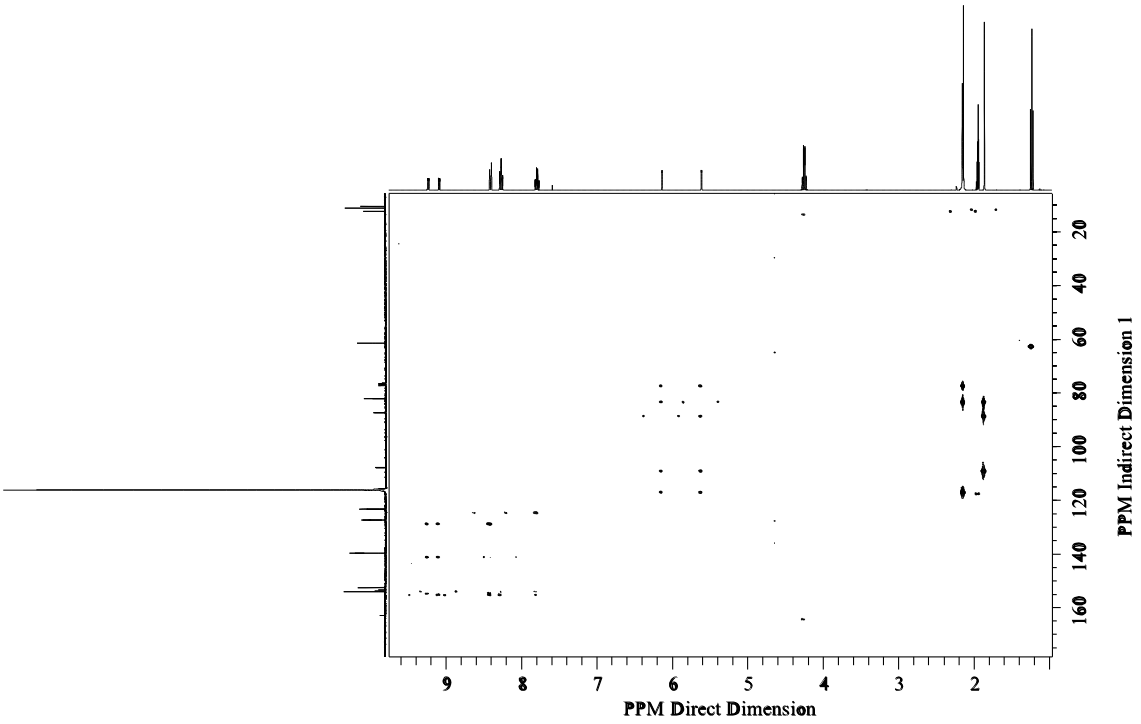

Figure S3. HMBC spectrum of **3** in CD_3CN.

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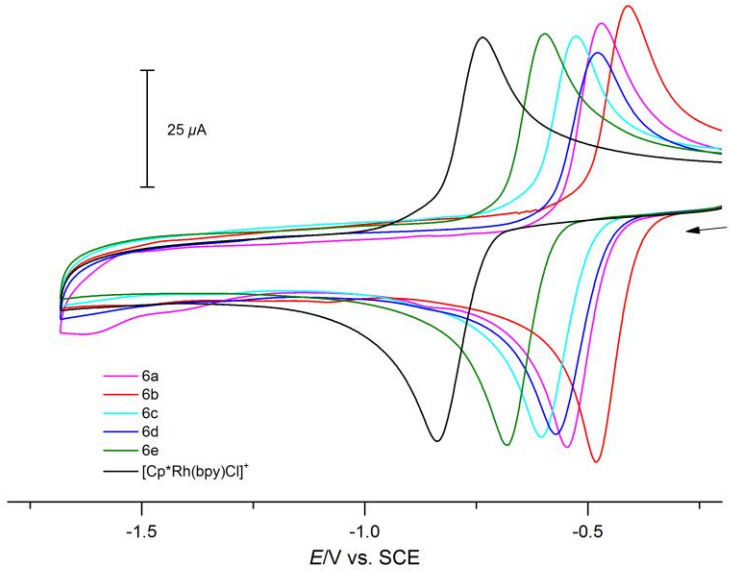

Figure S4. Cyclic voltammograms of $[Cp^*Rh(bpy)Cl]^+$ and **6a–e** obtained in CH_3CN containing 0.1 M $TBAPF_6$ with a scan rate of 100 mV s^{-1}. Ferrocene was employed as an internal standard, and its $Fe^{(II/III)}$ half-wave potential ($E_{1/2}$) was taken to be +0.40 V *vs* SCE.

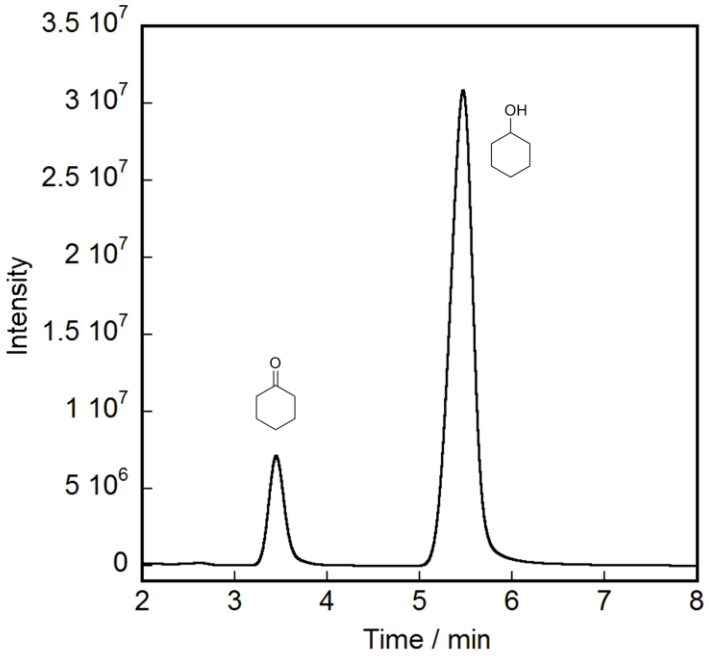

Figure S4. GC analysis of the hydrogenation of cyclohexanone with complex **6d**.

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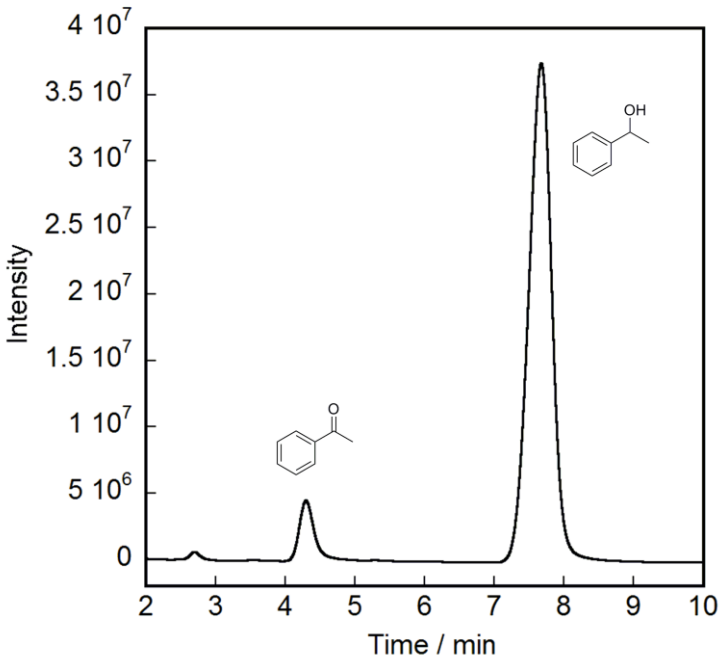

Figure S5. GC analysis of the hydrogenation of acetophenone with complex **6e**.

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X-ray crystallographic experiment: X-ray data were obtained with a Brucker SMART-CCD diffractometer. Structural determination and refinement were performed by using Crystals.[1] Molecular graphics is drawn with Mercury.[2]

Table S1. Crystal data and structure refinement details for complex **6e**.

Formula	C24 H27 Br1 Cl1 N2 O7 Rh1
Formula Weight	673.75
Crystal System	Monoclinic
Space group	P21/c
a, [Å]	14.9471(8)
b, [Å]	10.5506(6)
c, [Å]	16.8312(10)
α, [°]	90
β, [°]	95.793(1)
γ, [°]	90
V, [Å^3]	2640.7(3)
Z	4
D(calc), [g cm^{-3}]	1.695
Temperature, (K)	293
Crystal Size, [mm]	0.21 x 0.25 x 0.55
μ (Mo-Ka), [mm^{-1}]	2.307
F(000)	1352
Reflections collected / Unique	16362 / 6050
R(int)	0.025
Used reflections	3763
Parameters	326
R	0.0369
wR2	0.0583
S	1.09

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References:

[1] a) Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487. b) Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435. c) Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112-122.

[2] Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453-457.