# ELECTRONIC SUPPLEMENTARY INFORMATION

# Synthetic Transformations of a Pendant Nitrile Moiety in Group 4 Metallocene Complexes

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## 1. Solid-state structure of compound 7

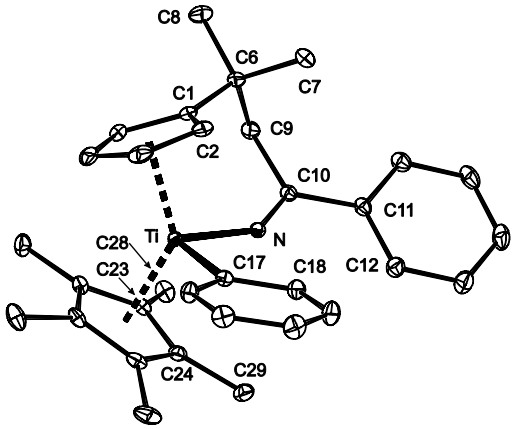


**Fig. S1.** A view of the molecular structure of compound **7** with thermal displacement ellipsoids at 30% probability level and hydrogen atoms omitted for clarity. Selected distances (Å) and angles (°): Ti–N 1.9227(10), Ti–C17 2.2004(13), Ti–centroid1 ($C_5Me_5$) 2.1036(6), Ti–centroid2 ($C_5H_4$) 2.0864(6), C1–C6 1.514(2), C6–C9 1.555(2), C9–C10 1.516(2), C10–N 1.271(2), centroid1–Ti–centroid2 135.20(3), N–Ti–C17 98.26(5), Ti–N–C10 145.07(9), C1–C6–C9 110.13(10), C6–C9–C10 107.89(11), C9–C10–N 117.82(11), C11–C10–N 121.69(11), C2–C1–C6–C9 118.39(14), C1–C6–C9–C10 – 63.81(13).

## 2. VT NMR analysis of the dynamic behaviour of imines 14 and 15

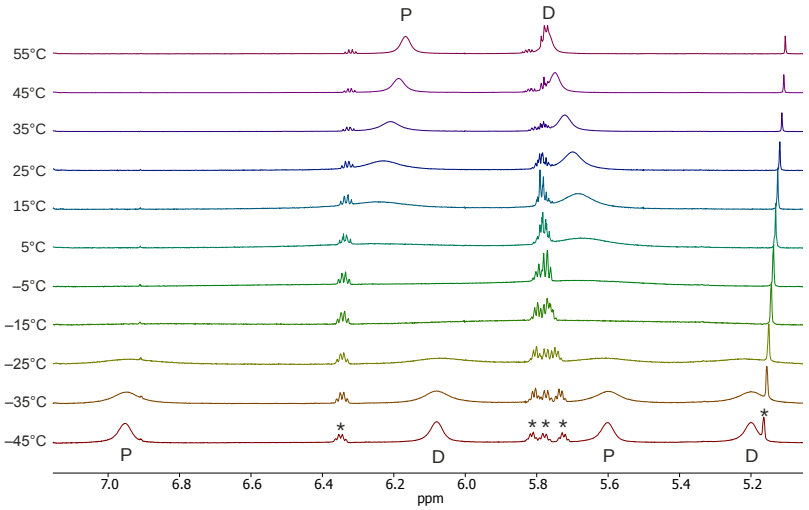


**Fig. S2.** $^1$H VT NMR spectra of compound **14** (only the $C_5H_4$ region is shown) measured in $CDCl_3$. P and D denotes the proximal and distal protons of the $C_5H_4$ ring with respect to the pendant substituent; asterisk denotes signals for the tentative enamine tautomer (see experimental part).

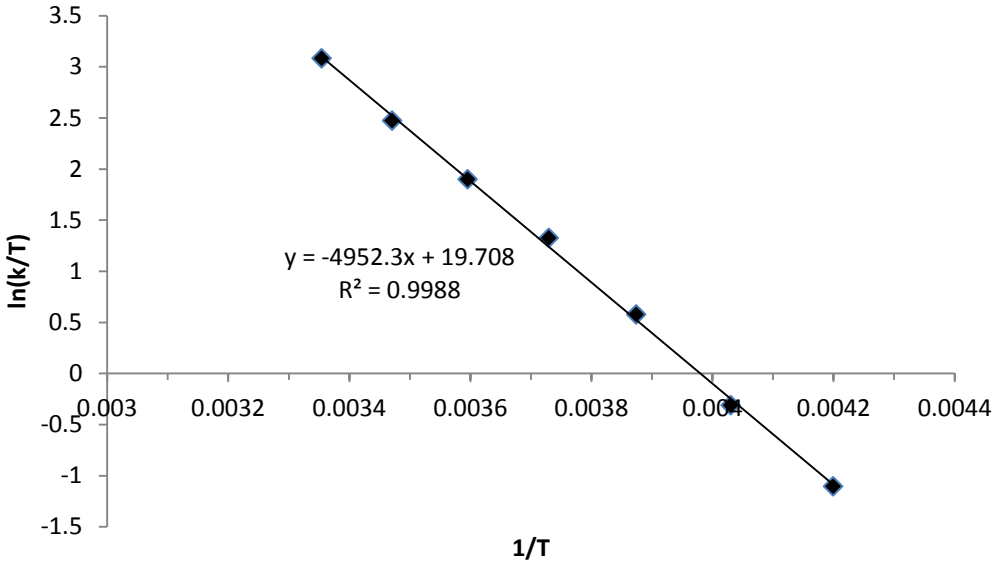


**Fig. S3.** Eyring plot for compound **14**.

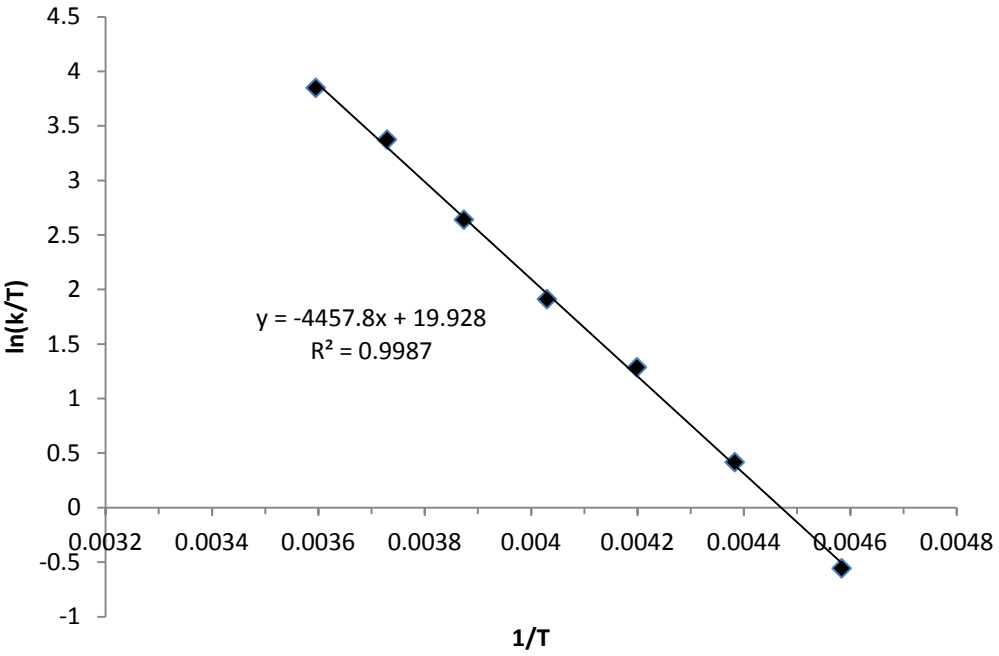


**Fig. S4.** Eyring plot for compound **15**.

**Table S1.** Thermodynamic parameters for the fluxional processes observed for compounds **14** and **15**.

| | $\Delta H^{\ddagger}$ [kJ mol$^{-1}$] | $\Delta S^{\ddagger}$ [J K$^{-1}$ mol$^{-1}$] | $\Delta G^{\ddagger}_{298}$ [kJ mol$^{-1}$] |
|---|---|---|---|
| **14** | 41.4 ± 0.7 | –32.8 ± 2.6 | 51.2 |
| **15** | 37.1 ± 0.6 | –31.9 ± 2.5 | 46.6 |