

Flexible Coordination of Bulky Amidinates and Guanidines Towards Rhodium(I):

Conversion of Kinetic to Thermodynamic Isomers

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Supplementary Material

Crystal data for $[\{\text{Rh}(\eta^4\text{-COD})\}_4(\kappa^4\text{-O}_2\text{SiMe}_2)_2]$: $\text{C}_{36}\text{H}_{60}\text{O}_4\text{Rh}_4\text{Si}_2$, $a = 11.7331(2) \text{ \AA}$, $b = 18.5200(3) \text{ \AA}$, $c = 19.0441(3) \text{ \AA}$, $\alpha = 111.723(1)^\circ$, $\beta = 97.088(1)^\circ$, $\gamma = 97.293(1)^\circ$, triclinic, $P-1$, $Z = 4$, $V = 3747.49(11) \text{ \AA}^3$, $FW = 1024.66$, $D_c = 1.816 \text{ g cm}^{-3}$, $F(000) = 2064$, $\mu(\text{Mo-K}\alpha) = 1.832 \text{ mm}^{-1}$, 123(2) K, 16908 unique reflections [$R(\text{int})$ 0.0315], R (on F) 0.0414, wR (on F^2) 0.0749 ($I > 2\sigma I$). Two crystallographically independent molecules reside in the asymmetric unit of the crystal structure. As there are no significant geometric differences between them, the ORTEP diagram and metrical parameters for only one are given below.

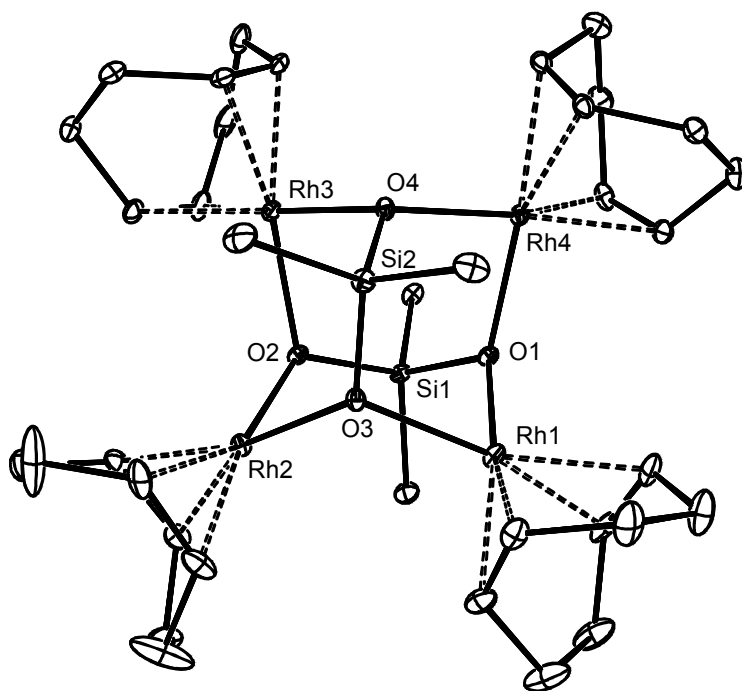


Figure S1. Molecular structure of $[\{\text{Rh}(\eta^4\text{-COD})\}_4(\kappa^4\text{-O}_2\text{SiMe}_2)_2]$ (25% thermal ellipsoids are shown). Selected bond lengths (Å) and angles (°): Rh(1)-O(3) 2.126(3), Rh(1)-O(1) 2.130(3), Rh(2)-O(3) 2.088(3), Rh(2)-O(2) 2.091(3), Rh(3)-O(2) 2.122(3), Rh(3)-O(4) 2.127(3), Rh(4)-O(1) 2.092(3), Rh(4)-O(4) 2.094(3), Si(1)-O(2) 1.636(3), Si(1)-O(1) 1.639(3), Si(2)-O(3) 1.633(3), Si(2)-O(4) 1.639(3), O(3)-Rh(1)-O(1) 91.24(10), O(3)-Rh(2)-O(2) 88.70(11), O(2)-Rh(3)-O(4) 91.46(10), O(1)-Rh(4)-O(4) 88.60(11), O(2)-Si(1)-O(1) 112.20(14), O(3)-Si(2)-O(4) 111.57(15).

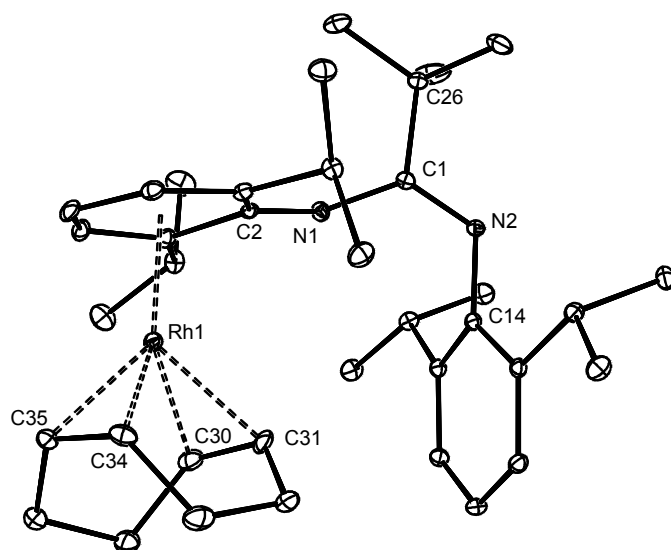


Figure S2. Molecular structure of $[\text{Rh}\{(\eta^5\text{-ArN})(\text{ArN})\text{CtBu}\}(\text{COD})]$ **1** (25% thermal ellipsoids are shown).

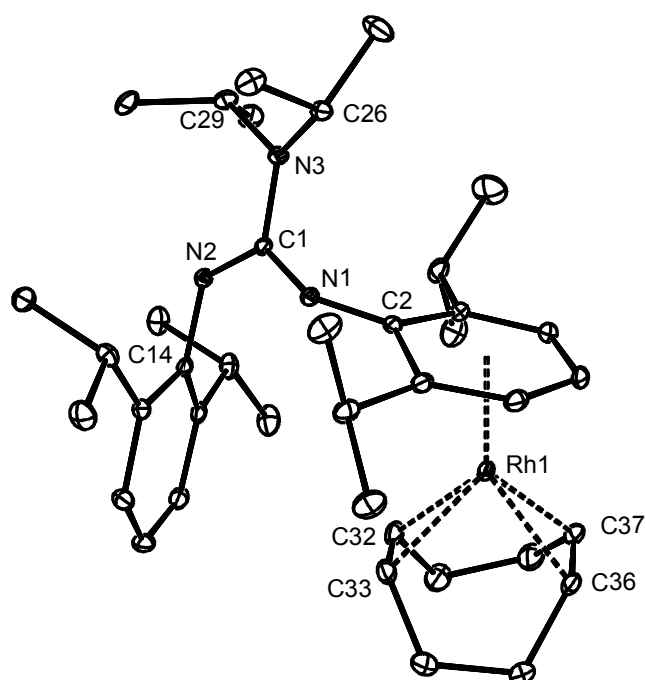


Figure S3. Molecular structure of $[\text{Rh}\{(\eta^5\text{-ArN})(\text{ArN})\text{CNPr}_2\}(\text{COD})]$ **2** (25% thermal ellipsoids are shown).

Figure S5. Molecular structure of $[\text{Rh}\{\kappa^2\text{-N,N'-(ArN)}_2\text{CNPr}_2^i\}(\text{COD})]$ **7** (25% thermal ellipsoids are shown).