Supplementary Information

Orthometallation of *N*-Substituents at the NHC Ligand of [Rh(Cl)(COD)(NHC)] Complexes: Its Role on the Catalytic Hydrosilylation of Ketones

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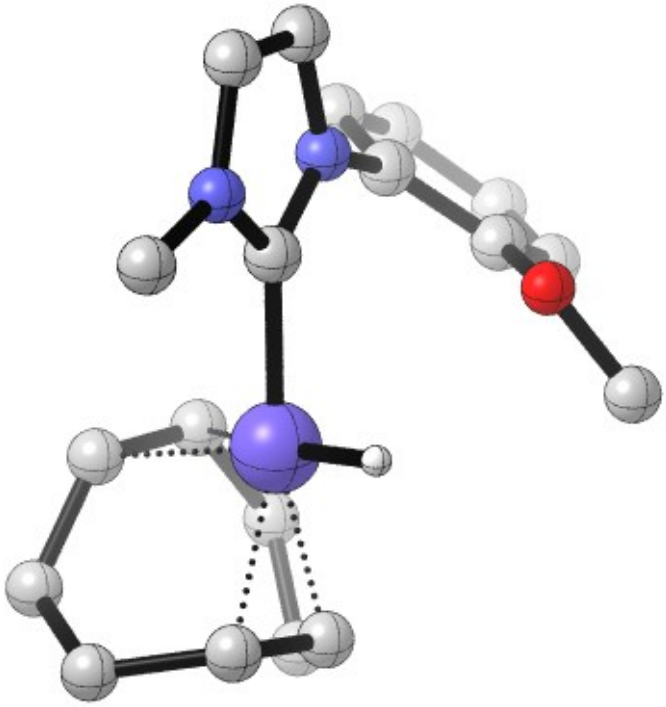
Reaction of C_6D_6 solutions of 3 and excess of $HSiMe(OSiMe_3)_2$ with PCy_3 at NMR scale. $HSiMe(OSiMe_3)_2$ (0.27 mL, 1.0 mmol), **2a** (33.4 mg, 0.05 mmol) and C_6D_6 (0.5 mL) were placed in a NMR tube. The reaction mixture was heated at 90ºC for 8 hours. After that, the solution was cooled at 25 °C and PCy_3 (0.05 mmol) was added to the reaction mixture. ^1H and $^{31}P\{^1H\}$ NMR spectra were recorded after 2 hours at 25 °C. Afterwards, the mixture was heated at 70ºC and monitored by ^1H and $^{31}P\{^1H\}$ NMR spectroscopy.

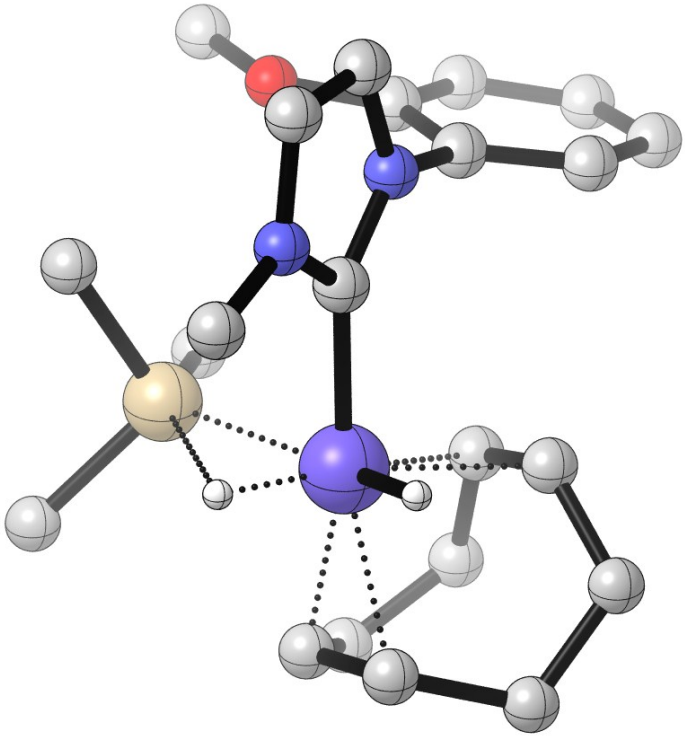
Table. B3LYP-D3/def2-SVP total energies in gas phase and Gibbs free energies (at 298 K and 1 atm) for all calculated structures.

	Eel/hartree	G/hartree	ΔG/kcal
A	-1033.80156	-1033.44936	0.0
TSA-B	-1443.51805	-1443.05376	18.8
B	-1443.53696	-1443.06827	9.6
TSB-C	-1443.52790	-1443.06181	13.7
C	-1443.55524	-1443.08736	-2.3
TSC-D	-1443.53806	-1443.07287	6.8
D	-1443.55984	-1443.09089	-4.5
TSD-E	-1443.52936	-1443.06389	12.4
E	-1443.55052	-1443.08780	-2.6
F	-2261.02064	-2260.45470	-25.2
G	-1323.51872	-1323.16874	17.2
Me2CO	-193.02324	-192.96882	
HSiMe3	-409.72219	-409.63429	
COE	-313.06728	-312.89654	

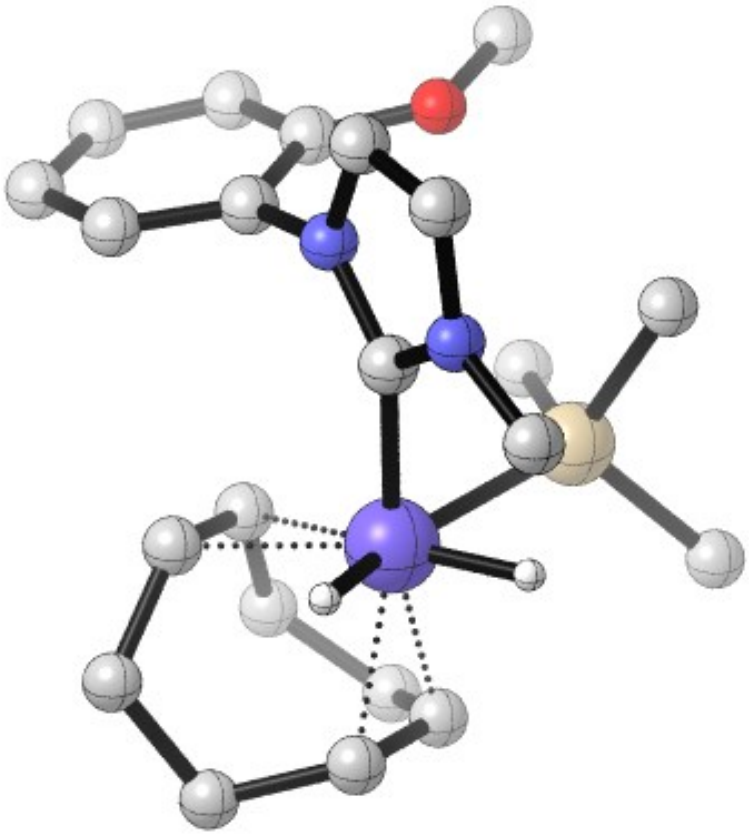
Geometrical representation of the B3LYP-D3/def2-SVP optimized structures



A



TSA-B



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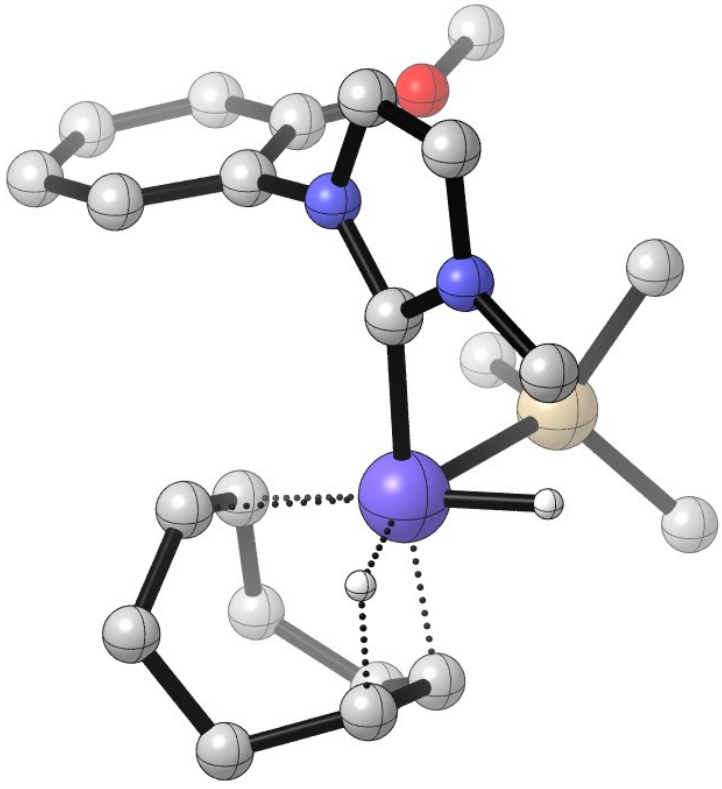
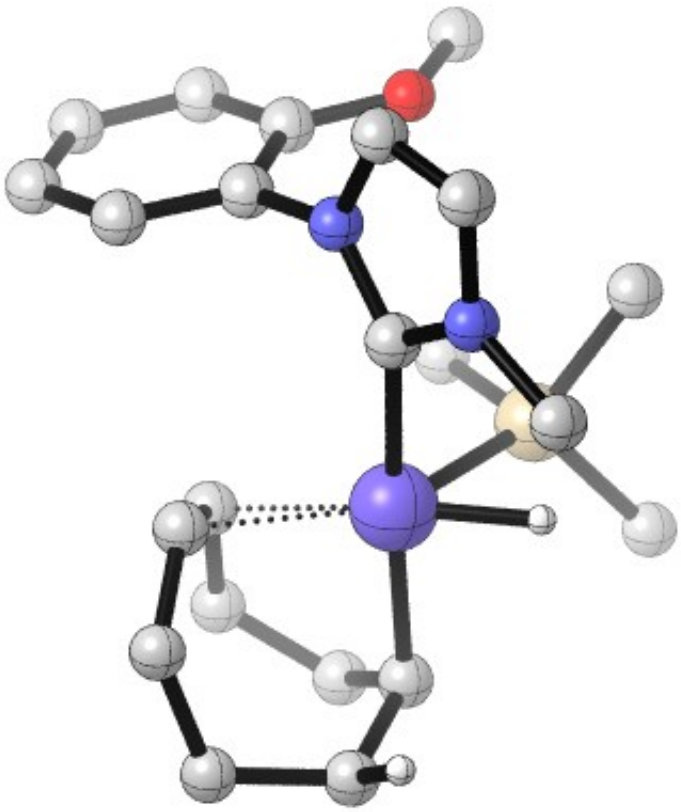


TSB-C



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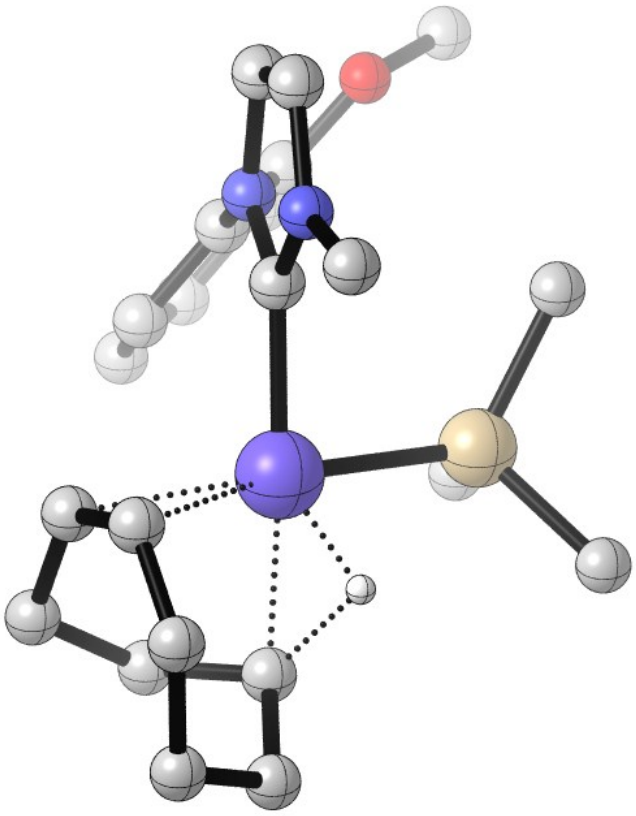

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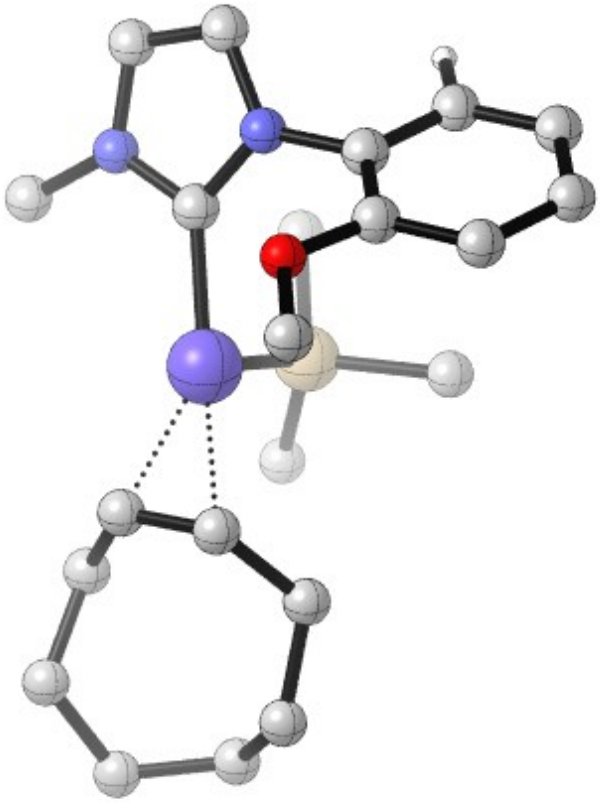

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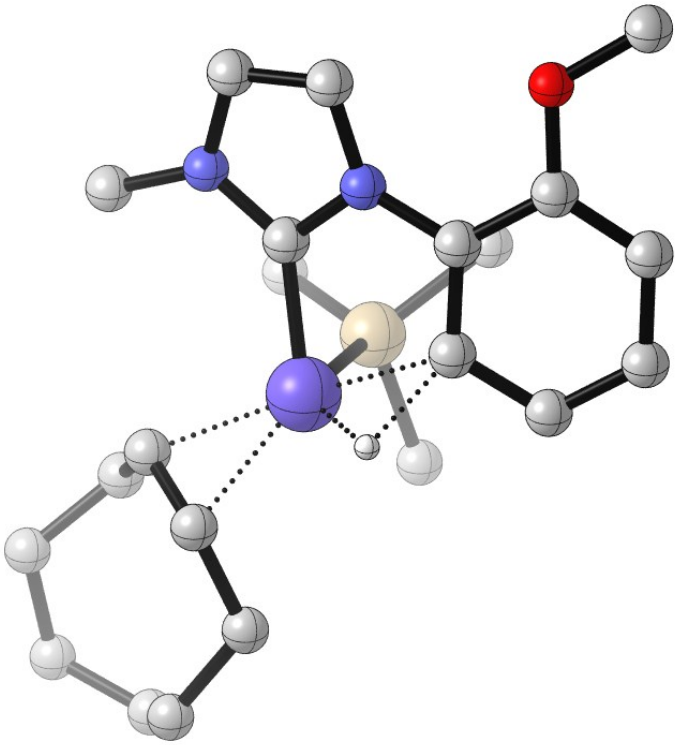
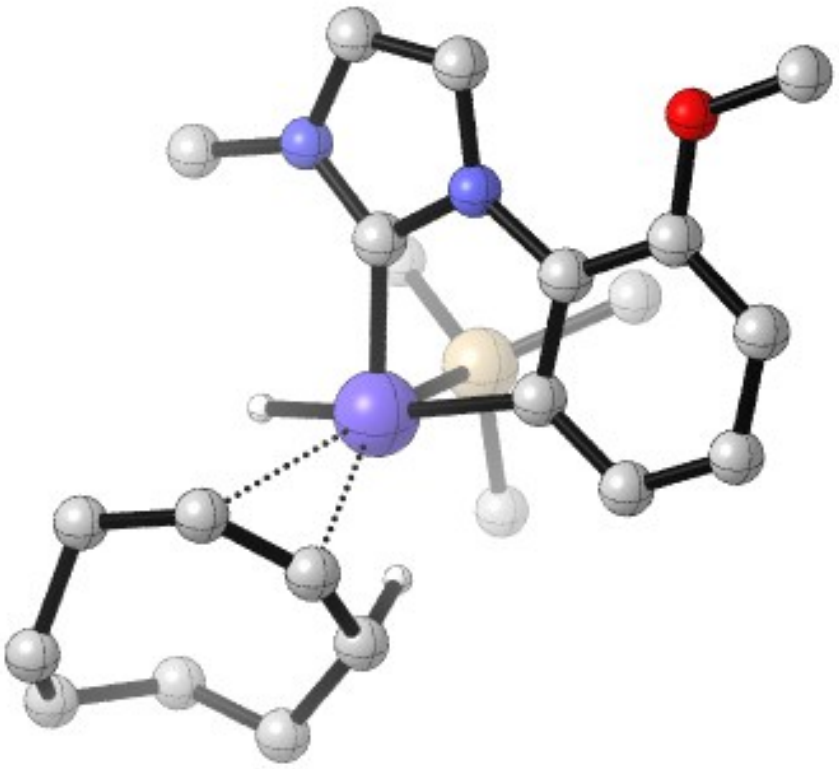
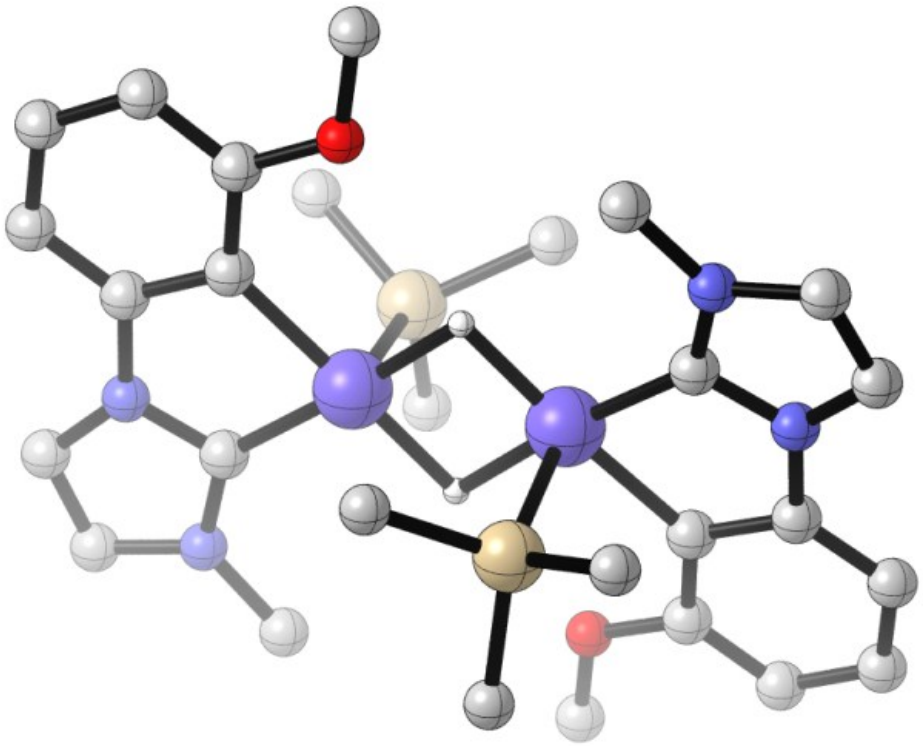


TSD-E



E



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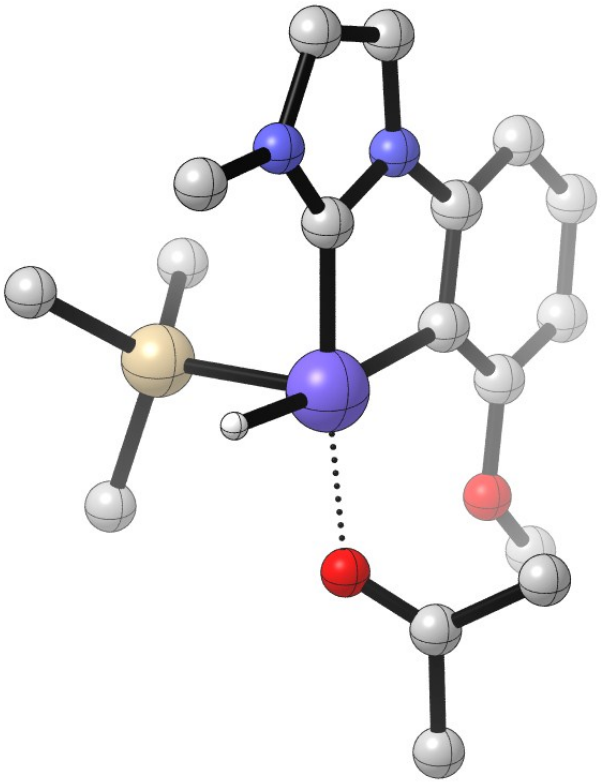

G

Cartesian coordinates (in Å) for all calculated structures using the B3LYP-D3/def2-SVP method

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6	-3.922532	-0.143834	-0.348846
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1	-4.210038	0.919672	-0.310046
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1	-3.363190	-1.476309	-1.985057
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6	-0.722602	-0.978586	-1.406917
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6	0.447900	1.607028	0.012649
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1	3.521252	2.595709	-0.713425
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6	2.359924	0.089558	-0.396648
6	2.351051	-0.780636	0.715971
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1 3.771255 -3.505868 -0.769777
8 1.879135 -0.283526 1.870157
6 -0.899480 3.678632 0.220888
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6 1.440576 -1.167408 2.880610
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TSA-B

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B

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TSB-C

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1 3.932710 0.559680 -1.243054

TSC-D

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