

Electronic Supplementary Information

Ligand effect on the oxidative addition of dioxygen on gold(I)–hydride complexes

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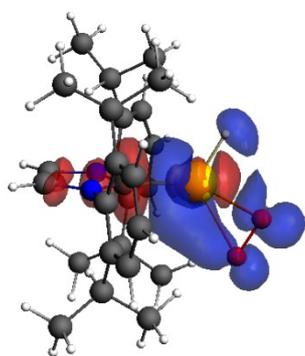
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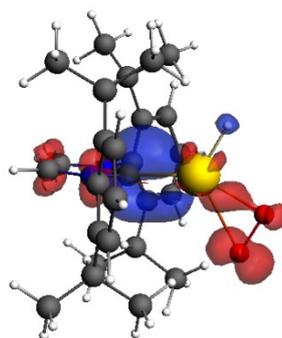
Figure S1: 3D isodensity plot of the electron density change upon formation of L-[AuH(O₂)] bond and of the first four NOCV components; L=IPr **S2**

Figure S2: 3D isodensity plot of the electron density change upon formation of L-[AuH(O₂)] bond and of the first four NOCV components; L=NAC.....**S3**

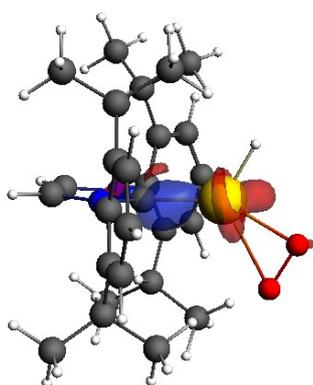
Table S1: CD-NOCV analysis of the L-AuH bond in the [LAuH] complexes and L-AuH(O₂) bond in the [LAuH(O₂)] transition states (L=NHC_H, IPr, NAC)..... **S4**



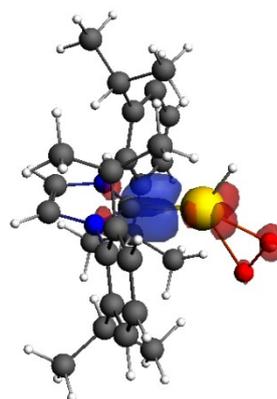
$\Delta\rho_1$



$\Delta\rho_2$

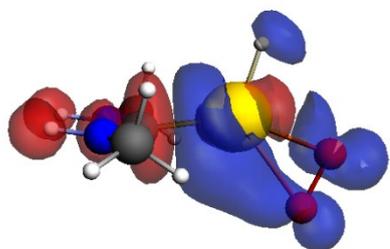


$\Delta\rho_3$

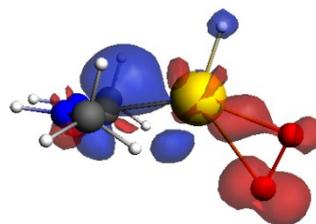


$\Delta\rho_4$

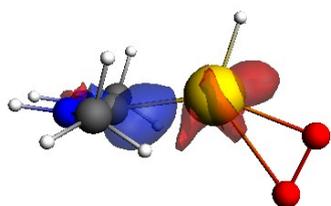
Figure S1: 3D isodensity plot of the electron density change upon formation of L-[AuH(O₂)] bond and of the first four NOCV components; L=IPr (isodensity value ± 0.001 e au⁻¹). Blue (red) isosurfaces identify regions in which the electron density increases (decreases).



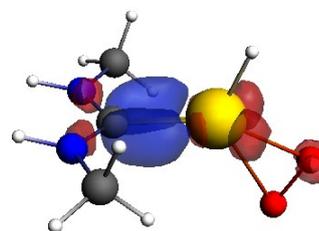
$\Delta\rho_1$



$\Delta\rho_2$



$\Delta\rho_3$



$\Delta\rho_4$

Figure S2: 3D isodensity plot of the electron density change upon formation of L-[AuH(O₂)] bond and of the first four NOCV components; L=NAC (isodensity value ± 0.001 e au⁻¹). Blue (red) isosurfaces identify regions in which the electron density increases (decreases).

	$\Delta\rho_1$ energy	$\Delta\rho_2$ energy	$\Delta\rho_1$ electrons	$\Delta\rho_2$ electrons
[L-AuH]				
NHC_H	-33.37 (0.47)	-8.21 (0.32)	-0.254	0.080
IPr	-34.11 (0.48)	-8.75 (0.31)	-0.258	0.078
NAC	-35.02 (0.51)	-8.02 (0.32)	-0.272	0.086
[L-AuH(O₂)]				
NHC_H	-47.86 (0.66)	-12.24 (0.41)	-0.336	0.095
IPr	-50.63 (0.69)	-12.36 (0.40)	-0.345	0.082
NAC	-50.58 (0.71)	-12.93 (0.42)	-0.371	0.111

Table S1: CD-NOCV analysis of the L-AuH bond in the [LAuH] complexes and L-AuH(O₂) bond in the [LAuH(O₂)] transition states (L=NHC_H, IPr, NAC). Decomposition energy contributions characterizing the donation ($\Delta\rho_1$ energy) and back-donation ($\Delta\rho_2$ energy) interactions (in kcal/mol) are given in the first and second column, respectively, with corresponding NOCV eigenvalues in parenthesis. Charge transfer values for the $\Delta\rho_1$ and $\Delta\rho_2$ components are reported in the third ($\Delta\rho_1$ electrons) and fourth ($\Delta\rho_2$ electrons) column, respectively.