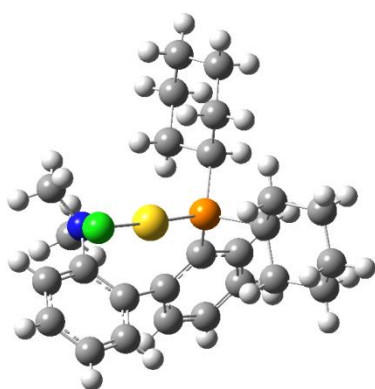


## Supporting Information

## Gold Catalysis: Biarylphosphine Ligands as Key for the Synthesis of Dihydroisocoumarines

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## Computational Results on Au-BiarylP



complex	Au-cl	Au-c2	Au-Cl	Au-P	P-Au-Cl
Mp2					
DFT (Lanl2dz) HF=-1224.0237256 1 Au -0.286143 2 Cl -0.274293 3 P 0.593996 4 C -0.147529	3.35	3.39	2.40	2.37	176
----- DFT (CEP-31g) HF=-335.2775321 S.point 1 Au -0.479815 2 Cl -0.314688 3 N 0.144588 4 P -0.333166	3.19	3.17	2.28	2.23	175.4
----- DFT Lanl2dz + 6-31g HF=-2004.2946953 1 Au -0.367124 2 Cl -0.309747 3 N -0.422166 4 P 0.646858	3.33	3.44	2.36	2.31	174.25
X-ray	3.12	3.20	2.28	2.22	176.4