

On the nature and feasibility of unsupported Au···Pd metallophilic interactions: a correlated computational study

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Computational details

All models were fully optimized at the gas-phase using the Gaussian 16 Revision C.01 suite of programs.¹ Geometries were constructed from scratch without any constraints and optimized at the RHF,² MP2,^{3,4} and density functional theory (DFT),^{5,6} employing the PBE0-D3BJ,^{7,8} M06-L,⁹ and M06-2X¹⁰ functionals. The Karlsruhe def2-TZVP basis set¹¹ was used for all atoms, 2f-type polarization functions together with def2 effective core potentials (ECPs) replacing 60 core electrons for gold and 28 core electrons for palladium. Harmonic frequency analyses at the same level of theory were performed to confirm that the optimized structures correspond to true minimum, as no imaginary frequencies were detected. Solvent effects were evaluated by re-optimizing selected models in tetrahydrofuran (THF) using the SMD implicit solvation model for geometry optimizations and single-point energy calculations. All structures were visualized and rendered using GaussView 6.1¹³ and UCSF ChimeraX 1.3.¹⁴

Additionally, the MP2 structures were re-optimized at the Spin-Component Scaled (SCS)-MP2 level of theory¹⁵ using either the Zero Order Regular Approximation (ZORA)¹⁶ or def2-ECPs, to evaluate the suitability of the MP2 geometries. For the ZORA calculations, all electron SARC-ZORA-TZVP basis sets were used for the metal atoms, and ZORA-TZVP basis sets were applied to the remaining atoms.¹⁷ For the ECP-based calculations, def2-TZVP basis sets were used for all atoms. Numerical frequency calculations at the same level of theory confirmed that the optimized geometries represent genuine minima on the potential energy surface, with no imaginary frequencies detected. All calculations were performed using the ORCA program (version 6.1.0),¹⁸ employing the RIJCOSX approximation¹⁹ to accelerate the evaluation of Coulomb and exact exchange integrals along with the corresponding default auxiliary basis sets: def2-TZVP/C and def2/J for def2-ECP-based calculations, and def2-TZVP/C and SARC/J for ZORA calculations.

The Potential Energy Curves (PECs) were obtained from interaction energies values (ΔE_{int}) calculated at the RHF and MP2 levels of theory with the def2-TZVP basis sets using **equation S1**. Therefore, counterpoise correction (cp) to the basis set superposition error (BSSE) on interaction energies was performed,²⁰

$$\Delta E_{int} = E_{AB}^{(AB)} - E_A^{(AB)} - E_B^{(AB)} \quad \text{S1}$$

where ΔE_{int} represents the interaction energy, $E_{AB}^{(AB)}$ is the energy of the dimer and $E_A^{(AB)}$, $E_B^{(AB)}$ are monomer's energies calculated using the basis sets of the dimer.

The calculated points were fitted using a four-parameter function (**equation S2**), which had been previously used to derive the Herschbach-Laurie relation,²¹

$$\Delta E_{int}(R) = Ae^{-BR} - C \cdot R^D \quad \text{S2}$$

where R is the corresponding interatomic distance and A, B, C, D are fitting parameters. The internal coordinate corresponding to the interatomic distance was manually adjusted to the target values, while all remaining internal coordinates were constrained to their optimized values. To assess the impact of relativistic effects on the interactions, additional potential energy curves (PECs) were computed using both non-relativistic (MHF)²² and fully relativistic (MDF)^{23,24} effective core potentials for metal atoms.

The electron correlation contribution to the total interaction energy at the minima of the PECs was calculated by subtracting the interaction energy at the MP2 level of theory at the MP2 minimum distance ($\Delta E_{min MP2}^{MP2}$) from the interaction energy at the RHF level of theory at the MP2 minimum distance ($\Delta E_{min MP2}^{RHF}$) and dividing it by the first term, as shown in **equation S3**.

$$electron\ correlation\ contribution = \frac{\Delta E_{min MP2}^{MP2} - \Delta E_{min MP2}^{RHF}}{\Delta E_{min MP2}^{MP2}} \cdot 100 \quad \text{S3}$$

Additionally, single-point counterpoise-corrected interaction energy calculations were carried out at the minimum of all PECs using both levels of theory to refine the interaction energies. Additional single-point counterpoise-corrected interaction energy calculations were also performed at the SCS-MP2 and DLPNO-CCSD(T) levels of theory with the def2-TZVP basis sets,²⁵ employing the ORCA 6 software package. The RIJCOSX approximation and the corresponding default auxiliary basis sets for def2-TZVP/C and def2/J were used to accelerate the calculations.

NBO analysis²⁶ and Wiberg Bond Order (WBO)²⁷ calculations were carried out in each computational model at the MP2/def2-TZVP level of theory using Gaussian 16 and NBO 7.0 programs.²⁸ Additionally, the Intrinsic Bond Strength Indices (IBSI)²⁹ and the Fuzzy Bond Orders (FBO)³⁰ were calculated at the MP2 and DLPNO-CCSD(T)/def2-TZVP levels of theory using the Multiwfn 3.8 software package.³¹

The interpenetration index (p_{AB}), recently introduced by Santiago Álvarez *et al.*,³² was calculated using **equation S4**,

$$p_{AB}(\%) = \frac{(v_A + v_B - d_{AB})}{(v_A + v_B - r_A - r_B)} \cdot 100 \quad \text{S4}$$

where v is the corresponding van der Waals radii, r the corresponding covalent radii and d the interatomic distance at the minimum of the MP2-PEC of each model. Defined as the ratio of the intersecting volume of the shells to the sum of their shell widths, p_{AB} offers a qualitative assessment of interaction strength: values near 0% indicate weak van der Waals contacts, while values above 100% suggest significant covalent or ionic character. Hence, the covalent and van der Waals radii proposed by the same authors were employed.^{33,34}

Energy Decomposition Analysis (EDA)³⁵ coupled with Natural Orbital for Chemical Valence (NOCV)³⁶ was carried out for all models using ORCA 6.1.0. program. EDA-NOCV calculations were performed at the DLPNO-MP2/def2-TZVP level of theory,³⁷ together with the complementary def2-TZVP/C basis sets and TightPNO settings. This approach allows the intrinsic total interaction energy (ΔE_{int}) between two fragments to be decomposed into individual energy terms, as shown in **equation S5**.

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{orb} + \Delta E_{pauli} + \Delta E_{disp} \quad \text{S5}$$

Here, the ΔE_{elstat} term corresponds to the electrostatic interaction between the unperturbed charge distributions of the prepared fragments. The ΔE_{orb} term accounts for orbital interactions, including orbital mixing, charge transfer, and polarization. The ΔE_{pauli} term represents the repulsive contribution arising from the antisymmetrization of the fragment wavefunctions, as required by the Pauli exclusion principle. Finally, the ΔE_{disp} term describes the attractive dispersion forces associated with instantaneous electron-density fluctuations before and after bond formation. This term can be further decomposed into two components, as shown in **equation S6**.

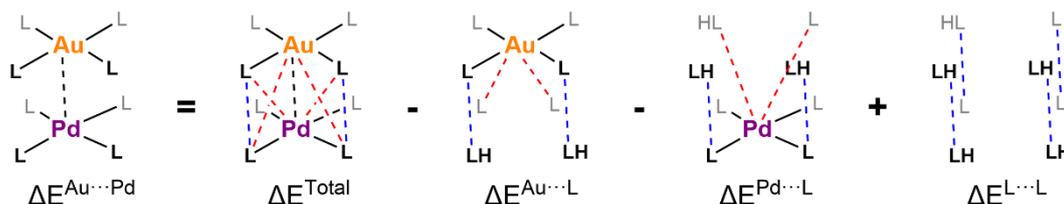
$$\Delta E_{disp} = \Delta E_{XC}^0 + \Delta E_C^{MP2} \quad \text{S6}$$

The ΔE_{XC}^0 term accounts for the exchange-correlation energy, while the ΔE_C^{MP2} represents the additional electron-correlation contribution captured at the MP2 level of theory.

The percentages of the stabilizing components were calculated by dividing the corresponding attractive component by the sum of all the others (**equation S7**).

$$\text{attractive component percentage} = \frac{|\Delta E_{elstat}| \text{ or } |\Delta E_{orb}| \text{ or } |\Delta E_{disp}|}{|\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}|} \cdot 100 \quad \text{S7}$$

The contributions from Au^I/Au^{III}...[ligand], Pd^{II}...[ligand], and [ligand]...[ligand] interactions to the total interaction energy of models **1-5**, were partially removed by subtracting the energies of the calculated monomer and the saturated ligands of the other monomer at the MP2/def2-TZVP minimum-distance geometry. The additional L...L interaction energy removed in this way was restored by adding the corresponding contribution of the saturated ligands. To achieve this, the metal centers were manually removed and replaced with hydrogen atoms attached to the corresponding carbon atoms. The positions of these hydrogen atoms were refined by optimizing the structure at the MP2/def2-TZVP level of theory, while keeping all other atomic positions fixed. Finally, interaction energy calculations and NEDA of the M-M component were carried out using the decomposition shown in the **Scheme 1**.



Scheme S1: Proposed decomposition scheme for isolating the Au...Pd component.

Local Energy Decomposition (LED) analysis was carried out at the DLPNO-CCSD(T)/def2-TZVP level of theory using TightPNO settings.³⁸ The RIJCOSX approximation was employed in conjunction with the def2-TZVP/C and def2/J auxiliary basis sets. In the LED supramolecular approach, the interaction energy (ΔE_{int}) of two fragments can be expressed as **equation S8**.

$$\Delta E_{int} = \Delta E_{int}^{HF} + \Delta E_{int}^C \quad \text{S8}$$

Here, ΔE_{int}^{HF} denotes the Hartree-Fock contribution, which accounts for the (static) electrostatic interaction between the monomers, as well as polarization and donor-acceptor effects. In contrast, ΔE_{int}^C represents the correlation contribution, which corrects all the above components and captures the dispersive attraction arising from instantaneous dipole-dipole interactions. An accurate description of this latter term is essential for a proper treatment of weak noncovalent interactions.

The Hartree-Fock contribution ΔE_{int}^{HF} can be further decomposed into the components presented in **equation S9**.

$$\Delta E_{int}^{HF} = \Delta E_{el-prep} + E_{elstat} + E_{exch} \quad \text{S9}$$

$\Delta E_{el-prep}$ represents the electronic preparation energy, *i.e.*, the repulsive cost of distorting the fragment densities from their isolation to their dimeric states; it includes both Pauli repulsion and polarization. E_{elstat} and E_{exch} denote the electrostatic and exchange interactions, respectively, between the deformed fragment densities.

Conversely, the correlation contribution (ΔE_{int}^C) is described by the expression provided in **equation S10**.

$$\Delta E_{int}^C = \Delta E_{int}^{C-CCSD} + \Delta E_{int}^{C-(T)} \quad \text{S10}$$

Here, ΔE_{int}^{C-CCSD} denotes the DLPNO-CCSD correlation contribution to the interaction energy, while $\Delta E_{int}^{C-(T)}$ corresponds to the perturbative triples correction.

Moreover, ΔE_{int}^{C-CCSD} is partitioned into dispersive and non-dispersive components, as defined in **equation S11**.

$$\Delta E_{int}^{C-CCSD} = \Delta E_{disp}^{C-CCSD} + \Delta E_{no-disp}^{C-CCSD} \quad \text{S11}$$

Accordingly, the total dispersive component of the interaction energy (ΔE_{disp}), associated with London dispersion effects, is evaluated using **equation S12**. The dispersive component of $\Delta E_{int}^{C-(T)}$, weighted by γ (*i.e.* the ratio of strong-pair dispersion to the total intermolecular strong-pair contribution),³⁹ is added to ΔE_{disp}^{C-CCSD} .

$$\Delta E_{disp} = \Delta E_{disp}^{C-CCSD} + \gamma \cdot \Delta E_{int}^{C-(T)} \quad \text{S12}$$

Therefore, non-dispersive correlation energy of the interaction energy ($\Delta E_{no-disp}$) is the remainder of ΔE_{int}^C (**equation S13**). This term represents the sum of all double-excitation contributions that do not conserve the charge within each fragment and includes the electronic preparation associated with strong and weak pairs.

$$\Delta E_{no-disp} = \Delta E_{int}^C - \Delta E_{disp} \quad \text{S13}$$

Finally, topological analyses were carried out on all computational models to gain qualitative insight into the nature of the interactions. The topology and properties of the electron densities obtained at the MP2/def2-TZVP and DLPNO-CCSD(T)/def2-TZVP levels of theory were examined using Quantum Theory of Atoms in Molecules (QTAIM)⁴⁰ and Independent Gradient Model based on Hirshfeld partitioning (IGMH),⁴¹ as implemented in the Multiwfn 3.8 software package. Electron density representations were generated using the VMD 1.9.4a53 visualization program.⁴²

Optimized structures

Table S1 Selected bond lengths (in angstrom) and angles (in degrees) for the MP2, RHF, SCS-MP2 and SCS-MP2-ZORA/def2-TZVP optimized structures.

Model	$D_{Au...Pd}$	$D_{Au...H-X}$ (X = N, C)	$D_{Pd...H-N}$	$A_{N-Pd-Au}$	A_{L-Au-L}
1a ^{MP2}	3.4455	2.9394	2.3851	77.02	178.79
1a ^{RHF}	4.1327	3.5299	2.7290	71.72	178.74
1a ^{SCS-MP2}	3.5807	3.0208	2.4438	76.38	179.17
1a ^{SCS-MP2-ZORA}	3.5805	2.9919	2.4304	75.39	179.10
1b ^{MP2}	3.3751	3.1312	2.5438	92.58	179.94
1b ^{RHF}	4.0737	3.9428	3.2745	89.28	179.76
1b ^{SCS-MP2}	3.4844	3.2097	2.6326	92.28	179.66
1b ^{SCS-MP2-ZORA}	3.4745	3.2196	2.6441	91.76	179.53
2a ^{MP2}	3.2169	2.8032	2.4948	77.54	179.08
2a ^{RHF}	3.9739	3.2979	2.7955	77.18	178.62
2a ^{SCS-MP2}	3.3339	2.8857	2.5491	77.60	178.87
2a ^{SCS-MP2-ZORA}	3.7660	2.7979	2.3414	68.84	178.79
2b ^{MP2}	4.2631	2.3401	2.4608	131.63	179.07
2b ^{RHF}	5.4462	3.0929	-	-	178.87
2b ^{SCS-MP2}	4.3609	2.4316	2.5361	131.48	179.17
2b ^{SCS-MP2-ZORA}	4.4053	2.4764	2.5295	131.56	179.30
3 ^{MP2}	3.1175	2.3657	-	93.11	176.25
3 ^{RHF}	3.6050	2.6910	-	93.37	179.28
3 ^{SCS-MP2}	3.1895	2.4148	-	92.72	176.63
3 ^{SCS-MP2-ZORA}	3.1716	2.4850	-	92.84	175.50
4 ^{MP2}	2.9102	2.8306	-	86.91	173.81
4 ^{RHF}	3.1069	3.1212	-	88.25	177.48
4 ^{SCS-MP2}	2.9414	2.8768	-	87.72	174.39
4 ^{SCS-MP2-ZORA}	2.9046	2.8699	-	88.02	172.88
5a ^{MP2}	4.5861	2.4078	-	-	179.37
5a ^{RHF}	5.0876	2.8741	-	-	179.26
5a ^{SCS-MP2}	4.6707	2.4745	-	-	179.49
5a ^{SCS-MP2-ZORA}	4.6940	2.4943	-	-	179.52
5b ^{MP2}	3.2852	2.5626	-	92.25	176.25
5b ^{RHF}	4.0450	3.0366	-	97.57	179.39
5b ^{SCS-MP2}	3.4117	2.7996	-	91.99	176.94
5b ^{SCS-MP2-ZORA}	3.5871	2.5797	-	98.88	178.24

Table S2 Selected bond lengths (in angstrom) and angles (in degrees) for PBE0-D3(BJ), M06L and M06-2x/def2-TZVP optimized structures.

Model	$D_{Au\cdots Pd}$	$D_{Au\cdots H-X}$ (X = N, C)	$D_{Pd\cdots H-N}$	$A_{N-Pd-Au}$	A_{L-Au-L}
1a ^{PBE0-D3(BJ)}	3.6227	2.9458	2.3303	74.24	177.55
1a ^{M06L}	3.4181	2.9238	2.5253	76.19	178.28
1a ^{M06-2X}	3.4778	3.0505	2.5849	77.32	178.98
1b ^{PBE0-D3(BJ)}	3.4525	3.2515	2.5543	90.77	179.08
1b ^{M06L}	3.4405	3.0095	2.5759	98.38	178.79
1b ^{M06-2X}	3.4720	3.0898	2.6920	97.54	178.98
2a ^{PBE0-D3(BJ)}	3.5846	2.7599	2.3506	71.16	178.04
2a ^{M06L}	3.3187	2.8135	2.5409	75.60	178.50
2a ^{M06-2X}	3.3963	2.9015	2.6010	75.78	178.28
2b ^{PBE0-D3(BJ)}	4.3354	2.4128	2.4450	131.07	178.80
2b ^{M06L}	4.4057	2.4468	2.4565	131.95	178.99
2b ^{M06-2X}	4.2223	2.5485	2.6837	126.86	178.04
3 ^{PBE0-D3(BJ)}	3.3598	2.3197	-	98.47	177.80
3 ^{M06L}	3.3401	2.4301	-	101.95	178.46
3 ^{M06-2X}	3.2633	2.7631	-	96.22	179.036
4 ^{PBE0-D3(BJ)}	2.9397	2.8494	-	86.68	174.54
4 ^{M06L}	2.9703	2.8726	-	86.34	175.69
4 ^{M06-2X}	2.9964	2.8865	-	86.66	177.40
5a ^{PBE0-D3(BJ)}	4.6648	2.4808	-	-	178.84
5a ^{M06L}	4.7875	2.5367	-	-	179.06
5a ^{M06-2X}	4.8436	2.6140	-	-	179.00
5b ^{PBE0-D3(BJ)}	3.5500	2.5667	-	99.24	179.06
5b ^{M06L}	3.5083	2.5626	-	100.76	179.75
5b ^{M06-2X}	3.5624	2.6368	-	100.13	179.80

Table S3 Counterpoise-corrected interaction energies from optimizations obtained at their respective levels of theory with def2-TZVP basis sets.

Models	SCS-MP2	SCS-MP2-ZORA	PBE0-D3(BJ)	M06L	M06-2x
1a	-79.09	-86.12	-87.57	-85.35	-77.82
1b	-64.46	-69.92	-73.35	-68.70	-64.02
2a	-66.50	-74.11	-76.57	-75.14	-68.87
2b	-49.47	-53.71	-60.54	-52.84	-45.31
3	-390.60	-398.91	-410.45	-409.74	-401.12
4	-775.45	-785.90	-802.37	-797.81	-790.02
5a	-100.23	-107.74	-115.77	-107.49	-103.51
5b	-51.44	-57.81	-59.41	-61.92	-58.28

MP2 optimization using THF as solvent

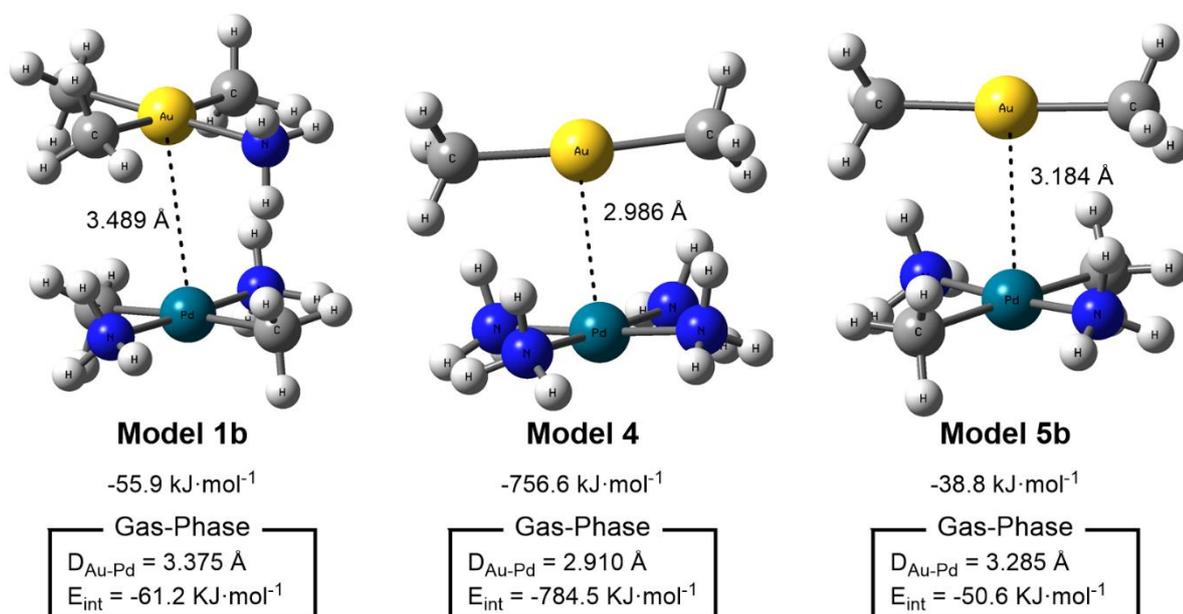


Figure S1 Representations of the MP2/def2-TZVP optimized structures of models **1b**, **4** and **5** using tetrahydrofuran as solvent. Key interatomic distances, and interaction energy values reported in kJ·mol⁻¹ computed at the same level of theory are displayed.

Potential energy curves

Table S4 Absolute energies ($\text{kJ}\cdot\text{mol}^{-1}$) as function of Au(III)-Pd(II) distance (\AA) of the neutral model **1a** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	1a QR		1a NR		1a FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.80	176.359	45.606	182.931	53.555	176.949	46.275
3.00	74.809	-25.146	79.995	-19.916	75.168	-24.727
3.20	17.556	-59.162	21.896	-55.480	17.771	-58.953
3.40	-13.254	-72.551	-9.461	-69.789	-13.129	-72.425
3.60	-28.508	-74.726	-25.108	-72.467	-28.442	-74.643
3.80	-34.821	-71.128	-31.733	-69.203	-34.793	-71.128
4.00	-36.166	-64.894	-33.342	-63.178	-36.161	-64.894
4.20	-34.888	-57.781	-32.302	-56.191	-34.897	-57.781
4.40	-32.346	-50.668	-29.978	-49.204	-32.363	-50.668

Table S5 Absolute energies (kJ·mol⁻¹) as function of Au(III)-Pd(II) distance (Å) of the neutral model **1b** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	1b QR		1b NR		1b FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.80	207.432	68.199	208.930	73.220	207.787	68.534
3.00	86.616	-16.987	87.132	-14.518	86.822	-16.820
3.20	26.025	-51.631	26.084	-50.543	26.148	-51.505
3.40	-2.881	-61.672	-2.987	-61.296	-2.805	-61.588
3.60	-15.396	-60.417	-15.526	-60.375	-15.348	-60.375
3.80	-19.656	-54.559	-19.750	-54.643	-19.624	-54.559
4.00	-19.915	-47.279	-19.936	-47.405	-19.977	-47.279
4.20	-18.447	-40.083	-18.436	-40.166	-18.433	-40.083
4.40	-16.306	-33.598	-16.252	-33.639	-16.296	-33.598

Table S6 Absolute energies (kJ·mol⁻¹) as function of Au(I)-Pd(II) distance (Å) of the neutral model **2a** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	2a QR		2a NR		2a FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.40	283.019	150.624	290.311	176.105	284.460	152.005
2.60	136.958	34.100	140.946	50.250	137.800	34.853
2.80	54.967	-23.974	57.200	-14.644	55.464	-23.514
3.00	8.782	-51.338	10.102	-45.857	9.077	-51.087
3.20	-16.742	-62.342	-15.874	-59.162	-16.568	-62.216
3.40	-30.087	-64.685	-29.440	-62.844	-29.987	-64.601
3.60	-36.191	-62.467	-35.665	-61.505	-36.137	-62.425
3.80	-38.020	-58.032	-37.577	-57.656	-37.995	-58.032
4.00	-37.392	-52.677	-37.016	-52.635	-37.386	-52.677
4.20	-35.432	-47.154	-35.109	-47.279	-35.436	-47.154
4.40	-32.825	-41.798	-32.545	-42.049	-32.836	-41.840

Table S7 Absolute energies (kJ·mol⁻¹) as function of Au(III)-Pd(II) distance (Å) of the neutral model **3** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	3 QR		3 NR		3 FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.40	44.076	-118.575	64.690	-83.64	45.490	-117.319
2.60	-154.366	-279.491	-135.866	-250.914	-153.541	-279.031
2.80	-260.344	-356.017	-243.597	-332.335	-259.862	-355.598
3.00	-314.910	-387.522	-299.905	-368.234	-314.630	-387.313
3.20	-340.378	-395.346	-327.129	-379.782	-340.221	-395.221
3.40	-349.195	-390.744	-337.670	-378.359	-349.119	-390.702
3.60	-348.475	-379.824	-338.592	-370.158	-348.454	-379.865
3.80	-342.371	-366.100	-334.004	-358.694	-342.389	-366.142
4.00	-333.343	-351.330	-326.334	-345.766	-333.386	-351.414
4.20	-322.853	-336.519	-317.028	-332.461	-322.913	-336.603
4.40	-311.777	-322.168	-306.954	-319.323	-311.846	-322.252

Table S8 Absolute energies (kJ·mol⁻¹) as function of Au(I)-Pd(II) distance (Å) of the cationic model **4** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	4 QR		4 NR		4 FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.20	-166.82	-352.544	-135.303	-309.909	-164.160	-351.330
2.40	-462.384	-611.241	-435.115	-574.296	-460.863	-610.404
2.60	-613.143	-730.234	-589.397	-700.025	-612.301	-729.731
2.80	-685.142	-776.383	-664.829	-752.869	-684.710	-776.592
3.00	-713.435	-784.960	-696.489	-767.053	-713.247	-784.960
3.20	-717.271	-766.174	-703.498	-760.651	-717.231	-773.663
3.40	-707.500	-752.158	-696.616	-743.455	-707.553	-752.241
3.60	-690.347	-726.050	-682.035	-721.029	-690.462	-726.217
3.80	-669.433	-698.268	-663.365	-698.477	-669.588	-698.268
4.00	-646.872	-670.444	-642.726	-671.072	-647.054	-670.695
4.20	-623.896	-643.457	-621.365	-646.177	-624.094	-643.708

Table S9 Absolute energies (kJ·mol⁻¹) as function of Au(I)-Pd(II) distance (Å) of the model **5b** calculated at the RHF/def2-TZVP and MP2/def2-TZVP levels of theory with the counterpoise correction for the BSSE and different ECPs (QR = Quasi-Relativistic; NR = Non-Relativistic; FR = Fully-Relativistic).

R	5b QR		5b NR		5b FR	
	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$	$\Delta E_{\text{int}}^{\text{HF}}$	$\Delta E_{\text{int}}^{\text{MP2}}$
2.40	499.624	325.557	500.212	341.749	500.752	326.561
2.60	248.870	117.738	248.404	128.784	249.478	118.240
2.80	114.198	16.694	113.435	23.765	114.518	16.945
3.00	42.616	-29.372	41.837	-24.811	42.779	-29.246
3.20	3.847	-47.530	4.668	-44.643	5.442	-47.530
3.40	-13.242	-52.049	-13.846	-50.292	-13.216	-52.049
3.60	-21.815	-50.250	-22.344	-49.288	-21.818	-50.292
3.80	-25.065	-45.898	-25.545	-45.480	-25.085	-45.940
4.00	-25.562	-40.836	-26.015	-40.794	-25.591	-40.878
4.20	-24.696	-35.899	-25.135	-36.108	-24.731	-35.941
4.40	-23.214	-31.380	-23.643	-31.757	-23.252	-31.422

Interaction energies of the decomposition components

Table S10 Absolute interaction energy (in $\text{kJ}\cdot\text{mol}^{-1}$) calculated at the SCS-MP2/def2-TZVP level of theory, including counterpoise correction for the BSSE, at the MP2 minimum using QR-ECPs of their corresponding potential energy curve.^a

Model	Component		
	$\Delta E^{\text{Au}\cdots\text{L}}$	$\Delta E^{\text{Pd}\cdots\text{L}}$	$\Delta E^{\text{L}\cdots\text{L}}$
1a	-38.39	-35.49	-15.04
1b	-31.95	-28.14	-9.58
2a	-33.33	-21.50	-11.65
3	-22.17	-13.62	1.48
4	-7.15	-36.05	7.21
5b	-27.71	-8.10	0.58

^a Components calculated according to the decomposition shown in **Scheme S1**.

Table S11 Absolute interaction energy (in $\text{kJ}\cdot\text{mol}^{-1}$) calculated at the DLPNO-CCSD(T)/def2-TZVP level of theory, including counterpoise correction for the BSSE, at the MP2 minimum using QR-ECPs of their corresponding potential energy curve.^a

Model	Component		
	$\Delta E^{\text{Au}\cdots\text{L}}$	$\Delta E^{\text{Pd}\cdots\text{L}}$	$\Delta E^{\text{L}\cdots\text{L}}$
1a	-41.91	-38.65	-18.66
1b	-35.51	-31.05	-13.79
2a	-33.20	-23.48	-13.66
3	-23.80	-16.92	-2.20
4	-10.67	-39.96	2.15
5b	-29.09	-10.11	-1.74

^a Components calculated according to the decomposition shown in **Scheme S1**.

EDA-NOCV results

Table S12 EDA-NOCV contributions to the total interaction energy (in $\text{KJ}\cdot\text{mol}^{-1}$) at the MP2 QR-PEC minimum for the neutral model **1a**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-84.9 (29%)	-29.0 (10%)	-130.0	-47.8	-177.8 (61%)	+217.7	-74.0
$\Delta E^{\text{Au}\cdots\text{L}}$	-33.4 (22%)	-10.7 (7%)	-70.2	-36.0	-106.3 (71%)	+114.7	-35.8
$\Delta E^{\text{Pd}\cdots\text{L}}$	-45.4 (23%)	-17.2 (9%)	-98.8	-34.9	-133.7 (68%)	+164.1	-32.2
$\Delta E^{\text{L}\cdots\text{L}}$	-5.9 (6%)	-18.5 (18%)	-54.6	-26.5	-81.1 (77%)	+89.7	-15.8
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-11.9 (24%)	-19.6 (39%)	-15.6	-3.3	-18.9 (48%)	+28.6	-21.9

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

Table S13 EDA-NOCV contributions to the total interaction energy (in $\text{KJ}\cdot\text{mol}^{-1}$) at the MP2 QR-PEC minimum for the neutral model **1b**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-73.4 (25%)	-26.4 (10%)	-137.7	-53.3	-191.0 (66%)	+229.1	-61.7
$\Delta E^{\text{Au}\cdots\text{L}}$	-34.6 (21%)	-12.9 (8%)	-84.6	-37.1	-121.7 (72%)	+140.0	-29.1
$\Delta E^{\text{Pd}\cdots\text{L}}$	-42.9 (21%)	-16.5 (8%)	-106.5	-38.3	-144.9 (71%)	+177.7	-26.6
$\Delta E^{\text{L}\cdots\text{L}}$	-22.7 (17%)	-8.5 (6%)	-74.2	-27.7	-101.9 (77%)	+124.2	-8.8
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-18.7 (37%)	-5.5 (11%)	-20.8	-5.6	-26.3 (52%)	+35.7	-14.8

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

Table S14 EDA-NOCV contributions to the total interaction energy (in KJ·mol⁻¹) at the MP2 QR-PEC minimum for the neutral model **2a**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-94.2 (32%)	-27.6 (9%)	-141.0	-34.3	-175.3 (59%)	+233.5	-63.7
$\Delta E^{\text{Au}\cdots\text{L}}$	-32.2 (24%)	-10.6 (8%)	-67.4	-26.8	-94.2 (69%)	+109.1	-28.0
$\Delta E^{\text{Pd}\cdots\text{L}}$	-31.3 (27%)	-9.6 (8%)	-59.0	-16.4	-75.4 (65%)	+97.0	-19.3
$\Delta E^{\text{L}\cdots\text{L}}$	-10.5 (20%)	-2.8 (5%)	-26.1	-13.8	-39.9 (76%)	+42.5	-10.7
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-41.2 (43%)	-10.2 (11%)	-40.7	-4.8	-45.5 (47%)	+69.9	-27.1

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

Table S15 EDA-NOCV contributions to the total interaction energy (in KJ·mol⁻¹) at the MP2 QR-PEC minimum for the neutral model **3**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-432.8 (55%)	-70.4 (9%)	-229.8	-52.8	-282.6 (36%)	+391.4	-394.4
$\Delta E^{\text{Au}\cdots\text{L}}$	-54.9 (18%)	-34.4 (11%)	-176.3	-41.8	-218.1 (71%)	+285.6	-21.7
$\Delta E^{\text{Pd}\cdots\text{L}}$	-17.8 (15%)	-16.7 (14%)	-60.3	-25.0	-85.4 (71%)	+105.1	-14.8
$\Delta E^{\text{L}\cdots\text{L}}$	-14.9 (14%)	-5.7 (5%)	-64.7	-19.7	-84.5 (80%)	+109.4	+4.3
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-375.1 (81%)	-25.0 (5%)	-57.9	-5.7	-63.6 (14%)	+101.1	-353.6

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

Table S16 EDA-NOCV contributions to the total interaction energy (in $\text{KJ}\cdot\text{mol}^{-1}$) at the MP2 QR-PEC minimum for the neutral model **4**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-821.6 (62%)	-131.2 (10%)	-303.4	-73.8	-377.2 (28%)	+545.5	-784.5
$\Delta E^{\text{Au}\cdots\text{L}}$	-52.3 (14%)	-41.3 (11%)	-228.5	-46.9	-275.3 (75%)	+367.5	+14.0
$\Delta E^{\text{Pd}\cdots\text{L}}$	-29.0 (15%)	-47.1 (24%)	-88.9	-34.3	-123.2 (62%)	+161.4	-1.5
$\Delta E^{\text{L}\cdots\text{L}}$	-26.2 (15%)	-10.0 (6%)	-109.0	-26.3	-135.2 (79%)	+185.5	-37.9
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-766.6 (82%)	-52.8 (6%)	-95.1	-18.8	-113.9 (12%)	+202.2	-731.1

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

Table S17 EDA-NOCV contributions to the total interaction energy (in $\text{KJ}\cdot\text{mol}^{-1}$) at the MP2 QR-PEC minimum for the neutral model **5b**, calculated at the DLPNO-MP2/def2-TZVP level of theory.

Component ^a	$\Delta E_{\text{elstat}}^{\text{b}}$	$\Delta E_{\text{orb}}^{\text{b}}$	ΔE_{XC}	ΔE_{C}	$\Delta E_{\text{disp}}^{\text{b}}$	ΔE_{Pauli}	ΔE_{int}
ΔE^{total}	-65.4 (24%)	-32.4 (12%)	-142.7	-35.8	-178.5 (65%)	+225.0	-51.3
$\Delta E^{\text{Au}\cdots\text{L}}$	-34.3 (19%)	-22.0 (12%)	-98.6	-30.3	-128.9 (70%)	+156.2	-29.1
$\Delta E^{\text{Pd}\cdots\text{L}}$	-12.0 (14%)	-6.1 (7%)	-44.4	-20.6	-65.0 (78%)	+74.7	-8.4
$\Delta E^{\text{L}\cdots\text{L}}$	-10.2 (14%)	-4.1 (6%)	-43.1	-15.5	-58.6 (80%)	+72.6	-0.3
$\Delta E^{\text{Au}\cdots\text{Pd}}$	-29.3 (36%)	-8.4 (10%)	-42.7	-0.4	-43.1 (53%)	+69.7	-14.1

^a Components calculated following the decomposition shown in **Scheme 1**. ^b The percentage contributions are calculated relative to the sum of stabilizing, as defined in **equation S7**.

LED analysis

Table S18 LED contributions to the total interaction energy (in KJ·mol⁻¹) at the MP2 QR-PEC minimum for models **1-5** at the DLPNO-CCSD(T)/def2-TZVP level of theory.

<i>Model</i>	$\Delta E_{el-prep}^{HF}$	E_{elstat}	E_{exch}	ΔE_{int}^C	ΔE_{disp}^{C-CCSD}	$E_{int}^{C-(T)}$	γ
1a	+277.59	-249.37	-56.20	-56.97	-44.34	-6.79	0.9997
1b	+285.88	-235.86	-59.91	-59.70	-45.64	-6.90	0.9739
2a	+283.87	-257.42	-57.19	-43.29	-34.00	-4.88	0.9950
3	+493.02	-744.33	-91.66	-64.39	-41.73	-15.16	0.7781
4	+749.97	-1334.75	-127.72	-81.75	-49.04	-9.40	0.7077
5b	+245.34	-212.00	-50.11	-44.95	-33.21	-5.05	0.9245

Topological analyses

Theoretical background

QTAIM

According to the Quantum Theory of Atoms in Molecules (QTAIM) framework,⁴⁰ a Bond Critical Point (BCP) and an associated bond path appear between atoms whenever electron density connects them. Bond paths do not exclusively represent classical Lewis-type bonds but also encompass weaker interactions such as dispersion or van der Waals interactions.^{43,44}

The local properties at a BCP provide insights into the nature and strength of the bond/interaction. High electron density (ρ_e) combined with a negative Laplacian ($\nabla^2\rho_e < 0$) and negative total energy density ($H < 0$) denotes electron accumulation and is characteristic of shared-shell (covalent) bonds. In contrast, low ρ_e , positive $\nabla^2\rho_e$, and positive H indicate charge depletion typical of closed-shell interactions such as ionic, hydrogen-bonding, or van der Waals interactions.^{45,46}

A more refined characterization of bonding within the QTAIM framework can be obtained from the Lagrangian kinetic energy density, $G(r)$, and the potential energy density, $V(r)$, evaluated at the bond critical point. Dominance of $V(r)$ reflects local charge concentration and is associated with shared-shell (covalent) interactions, whereas dominance of $G(r)$ indicates charge depletion, typical of closed-shell interactions. The $|V|/G$ ratio, based on potential (V) and kinetic (G) energy densities, differentiates interaction types: values < 1 correspond to purely closed-shell interactions; values > 2 imply significant electron sharing (covalency); and intermediate values (from 1 to 2) represent “regular closed-shell” interactions with partial covalent character.⁴⁷

A complementary descriptor, G/ρ , distinguishes metallic from donor-acceptor interactions: metallic bonding is associated with $G/\rho < 1$, whereas donor-acceptor closed-shell interactions exhibit $G/\rho \approx 1$.⁴⁸

Together, these QTAIM parameters enable qualitative classification of bonding interactions, ranging from ionic or van der Waals to partially covalent or metallic in nature.

IGMH

The Independent Gradient Model based on the Hirshfeld partition of the molecular density (IGMH) is a recent real-space approach derived from the Reduced Density Gradient (RDG), enabling visualization and analysis of both covalent and noncovalent interactions.⁴¹

The RDG takes high positive values in regions far from the molecule and approaches zero in areas where interactions, either covalent or noncovalent, occur. The RDG further identifies interaction regions based on electron density and the sign of the second-largest Hessian eigenvalue (λ_2): low gradient and low density indicates weak interactions, while low gradient with high density denotes stronger interactions. In addition, Negative λ_2 corresponds to attractive interactions, and positive λ_2 to repulsive ones.

These features are represented as isosurfaces colored on a blue-green-red (BGR) scale: blue to green for attractive interactions ($\text{sign}(\lambda_2) \cdot \rho < 0$), green for van der Waals contacts ($\text{sign}(\lambda_2) \cdot \rho \approx 0$), and green to red for repulsive interactions ($\text{sign}(\lambda_2) \cdot \rho > 0$). Together, this mapping provides a clear qualitative picture of the nature and relative strength of the interactions present in the computational models.

QTAIM analysis

Table S19 QTAIM descriptors of the (3, -1) Bond Critical Point between gold and palladium atoms calculated with the MP2/def2-TZVP electron density.^a

Model	$r_{\text{Au-Pd}}$	$\text{sign}(\lambda_2) \cdot \rho_e(r)$	$\nabla^2 \rho_e(r)$	$H(r) \cdot 10^3$	$G(r)$	$V(r)$	$ V(r) /G(r)$	$G(r)/\rho_e$	E_{int}^b	E_{int}^c
1a	3.559	-0.0116	+0.0272	-0.0856	0.0069	-0.0070	1.0124	0.5929	9.16	7.76
1b	3.467	-0.0131	+0.0316	-0.2067	0.0081	-0.0083	1.0255	0.6201	10.92	9.14
2a	3.385	-0.0158	+0.0350	-0.8797	0.0096	-0.0105	1.0914	0.6095	13.78	10.84
3	3.219	-0.0205	+0.0473	-1.9146	0.0137	-0.0156	1.1394	0.6695	20.54	15.47
4	2.969	-0.0321	+0.0792	-4.8929	0.0247	-0.0296	1.1982	0.7688	38.84	27.81
5b	3.439	-0.0137	+0.0319	-0.0004	0.0084	-0.0088	1.0480	0.6112	11.53	9.44

^a Distance Au-Pd ($r_{\text{Au-Pd}}$ in Å), product of the sign of second largest eigenvalue of Hessian matrix of electron density ($\text{sign}(\lambda_2) \cdot \rho_e(r)$ in a.u.), Laplacian of electron density ($\nabla^2 \rho_e(r)$ in a.u.), electron energy density ($H(r)$ in a.u.), Lagrangian kinetic energy density ($G(r)$ in a.u.), potential energy density ($V(r)$ in a.u.), ratio $|V(r)|/G(r)$, ratio $G(r)/\rho_e$ in a.u., estimated interaction energies (E_{int} in $\text{kJ} \cdot \text{mol}^{-1}$).^b Espinosa: $E_{\text{int}} = -V(r)/2$.⁴⁹ ^c Vener: $E_{\text{int}} = 0.429G(r)$.⁵⁰

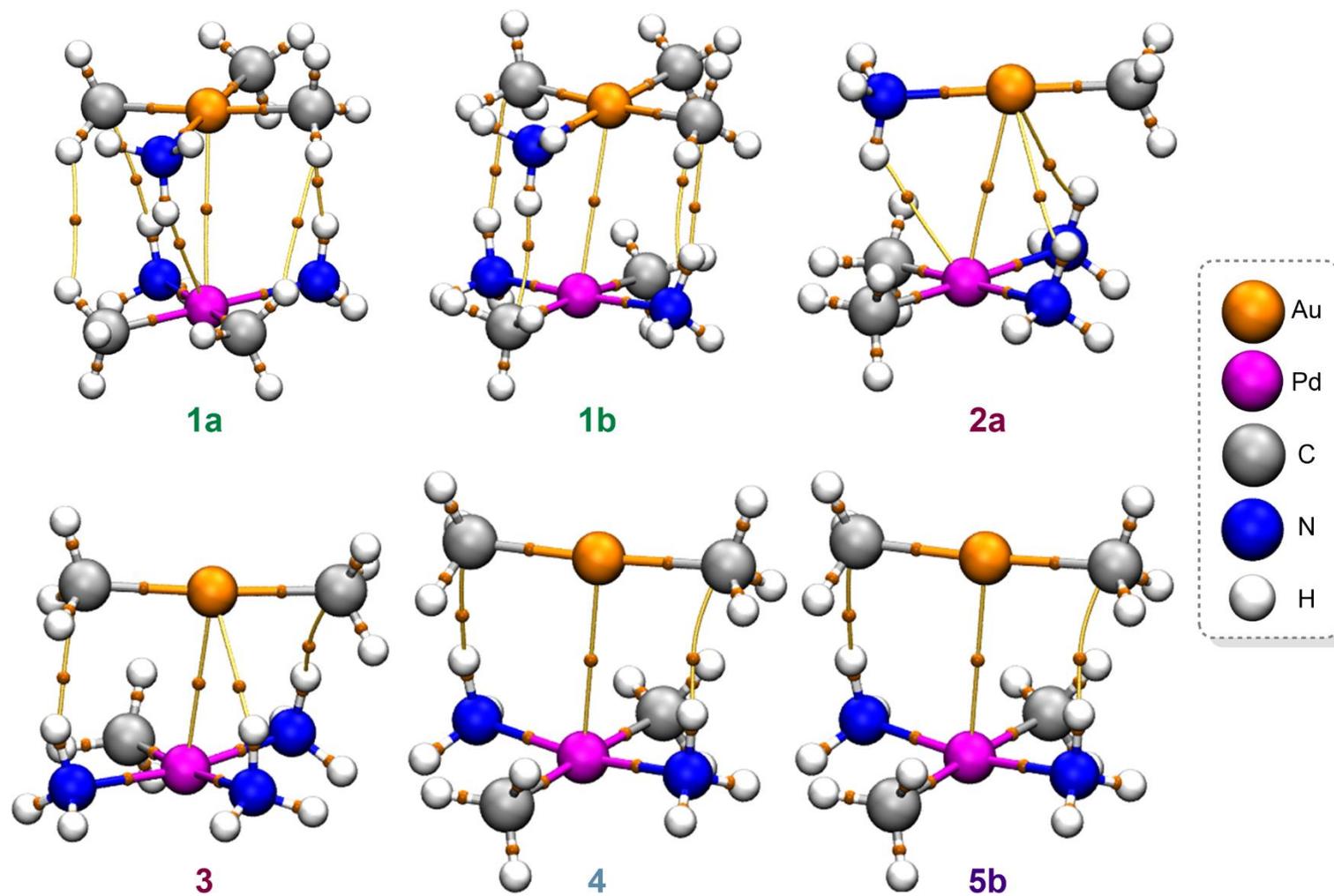


Fig. S2 QTAIM (3, -1) BCPs (orange dots) and bond paths (yellow strings) identified for computational models.

IGMH analysis

Table S20 Results of IGMH analysis for the metal atoms in models **1-5** calculated at the DLPNO-CCSD(T)/def2-TZVP level of theory. Values of IGMH atomic indexes (δg^{atom}) are in a.u.

Model	1a		1b		2a		3		4		5b	
	Au ^{III}	Pd ^{II}	Au ^{III}	Pd ^{II}	Au ^I	Pd ^{II}						
δg^{atom} (a.u.)	0.247	0.263	0.264	0.271	0.324	0.225	0.495	0.206	0.664	0.313	0.334	0.149
δg^{atom} (%)	18.8	20.0	19.6	20.1	34.4	23.9	39.5	16.4	40.2	19.0	36.6	16.4

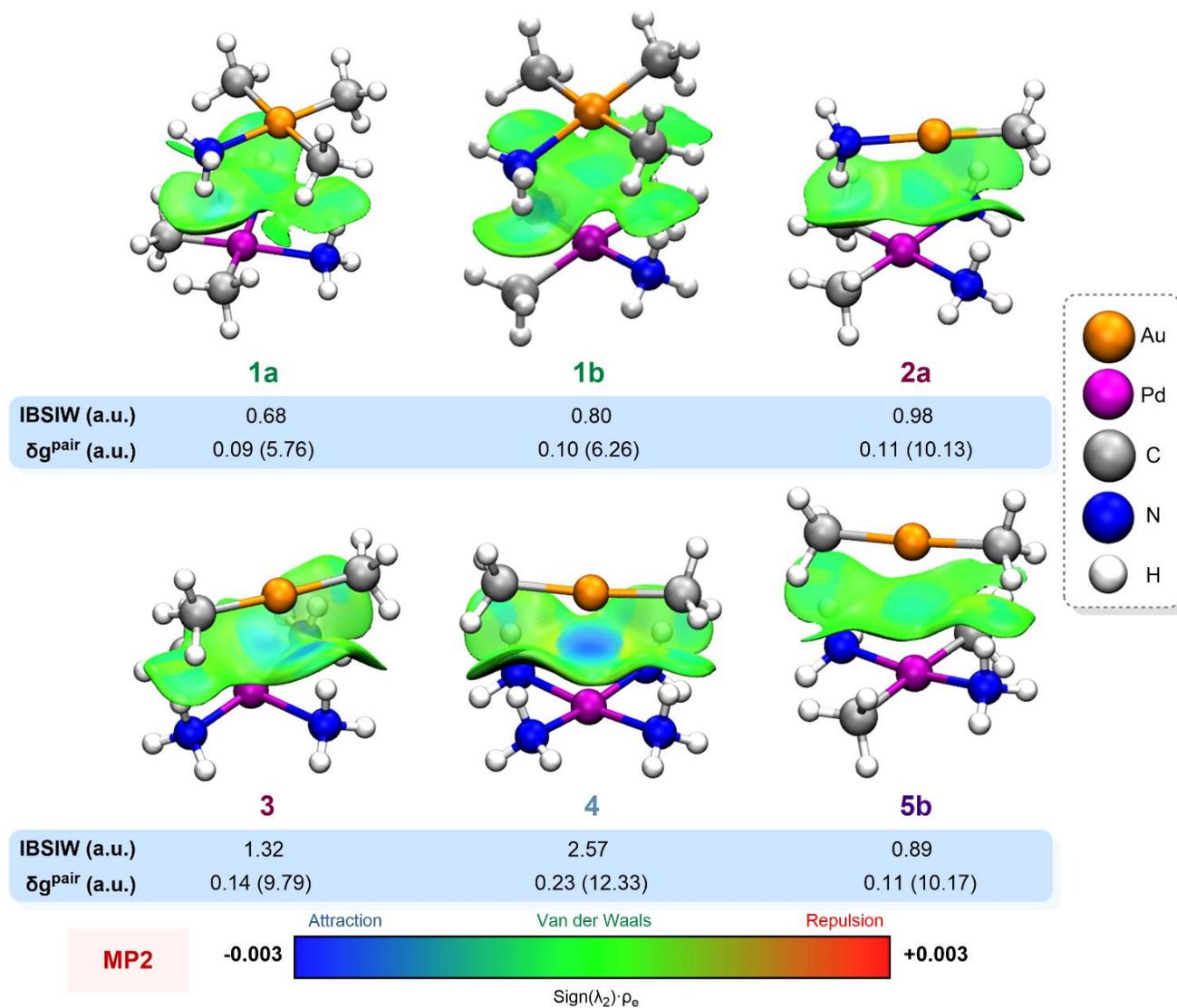


Fig. S3 IGMH map representations of the MP2/def2-TZVP electron density for models **1-5**. The isosurfaces maps correspond to an isovalue of $\delta g^{\text{inter}} = 0.003$ a.u., and are colored according to the color scale, with a range from -0.003 to $+0.003$ a.u. Values of IBSIW and δg^{pair} are in a.u.

Table S21 Results of IGMH analysis for the metal atoms in models **1-5** calculated at the MP2/def2-TZVP level of theory. Values of IGMH atomic indexes (δg^{atom}) are in a.u.

Model	1a		1b		2a		3		4		5b	
Atom	Au ^{III}	Pd ^{II}	Au ^{III}	Pd ^{II}	Au ^I	Pd ^{II}						
δg^{atom} (a.u.)	0.298	0.319	0.315	0.325	0.385	0.271	0.567	0.242	0.763	0.363	0.403	0.186
δg^{atom} (%)	19.9	21.3	20.5	21.1	34.9	24.5	40.5	17.3	41.6	19.8	38.9	17.9

Table S22 IGMH results for additional BCPs in the neutral model **1a** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	Pd(II)···H-N	C···H-N	1a		
			C···H-N	C-H···H-C	C-H···H-C
δg^{pair} (a.u./Å ²)	0.075	0.030	0.033	0.015	0.018
δg^{pair} (%)	5.7	2.3	2.5	1.2	1.4
IBSIW (a.u.)	1.244	0.465	0.507	0.224	0.258

Table S23 IGMH results for additional BCPs in the neutral model **1a** at the MP2/def2-TZVP level of theory.

BCP	Pd(II)···H-N	C···H-N	1a		
			C···H-N	C-H···H-C	C-H···H-C
δg^{pair} (a.u./Å ²)	0.094	0.033	0.033	0.014	0.014
δg^{pair} (%)	6.3	2.2	2.2	1.0	1.0
IBSIW (a.u.)	1.555	0.511	0.511	0.206	0.206

Table S24 IGMH results for additional BCPs in the neutral model **1b** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	Pd(II)···H-N	C···H-N	1b	
			C···H-N	C-H···C
δg^{pair} (a.u./Å ²)	0.072	0.033	0.026	0.017
δg^{pair} (%)	5.33	2.43	1.93	1.26
IBSIW (a.u.)	1.061	0.532	0.396	0.187

Table S25 IGMH results for additional BCPs in the neutral model **1b** at the MP2/def2-TZVP level of theory.

BCP	Pd(II)···H-N	C···H-N	1b	
			C···H-N	C-H···C
δg^{pair} (a.u./Å ²)	0.083	0.037	0.030	0.019
δg^{pair} (%)	5.42	2.4	1.93	1.24
IBSIW (a.u.)	1.232	0.600	0.574	0.211

Table S26 IGMH results for additional BCPs in the neutral model **2a** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	2a		
	Pd(II)···H-N	Au(I)···H-N	Au(I)···H-N
δg^{pair} (a.u./Å ²)	0.064	0.042	0.040
δg^{pair} (%)	6.83	4.5	4.29
IBSIW (a.u.)	0.949	0.501	0.477

Table S27 IGMH results for additional BCPs in the neutral model **2a** at the MP2/def2-TZVP level of theory.

BCP	2a		
	Pd(II)···H-N	Au(I)···H-N	Au(I)···H-N
δg^{pair} (a.u./Å ²)	0.078	0.049	0.049
δg^{pair} (%)	7.08	4.48	4.48
IBSIW (a.u.)	1.153	0.584	0.584

Table S28 IGMH results for additional BCPs in the neutral model **3** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	3		
	Au(I)···H-N	C···H-N	C···H-N
δg^{pair} (a.u./Å ²)	0.085	0.046	0.043
δg^{pair} (%)	6.79	3.65	3.39
IBSIW (a.u.)	1.445	0.837	0.743

Table S29 IGMH results for additional BCPs in the neutral model **3** at the MP2/def2-TZVP level of theory.

BCP	3		
	Au(I)···H-N	C···H-N	C···H-N
δg^{pair} (a.u./Å ²)	0.097	0.054	0.046
δg^{pair} (%)	6.95	3.86	3.26
IBSIW (a.u.)	1.653	0.988	0.798

Table S30 IGMH results for additional BCPs in the cationic model **4** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	4			
	C···H-N	C···H-N	C-H···H-N	C-H···H-N
δg^{pair} (a.u./Å ²)	0.057	0.053	0.03657	0.037
δg^{pair} (%)	3.45	3.23	2.21	2.22
IBSIW (a.u.)	1.106	1.036	0.926	0.929

Table S31 IGMH results for additional BCPs in the cationic model **4** at the MP2/def2-TZVP level of theory.

BCP	4			
	C···H-N	C···H-N	C-H···H-N	C-H···H-N
δg^{pair} (a.u./Å ²)	0.059	0.059	0.040416	0.040
δg^{pair} (%)	3.23	3.23	2.2	2.2
IBSIW (a.u.)	1.151	1.148	1.023	1.022

Table S32 IGMH results for additional BCPs in the anionic model **5b** at the DLPNO-CCDS(T)/def2-TZVP level of theory.

BCP	5b	
	C-H···H-N	C-H···H-N
δg^{pair} (a.u./Å ²)	0.044	0.035
δg^{pair} (%)	4.78	3.85
IBSIW (a.u.)	0.762	0.569

Table S33 IGMH results for additional BCPs in the anionic model **5b** at the MP2/def2-TZVP level of theory.

BCP	5b	
	C-H···H-N	C-H···H-N
δg^{pair} (a.u./Å ²)	0.049	0.038
δg^{pair} (%)	4.73	3.67
IBSIW (a.u.)	0.857	0.616

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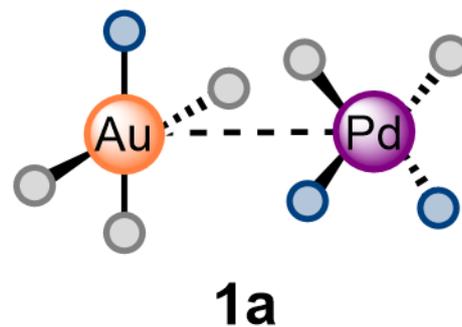
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Cartesian coordinates

Model **1a** (MP2/def2-TZVP optimization)

Au	-0.19824300	-0.15832500	1.68959500
H	1.19872900	-2.38579500	-1.77982200
H	0.38167500	-2.16503500	-0.37852700
H	-0.41961900	-2.62029400	-1.73932200
C	2.19003800	0.14419600	-1.92674500
H	2.41102700	-0.25066000	-2.92552100
H	2.69082200	1.11066200	-1.84157100
H	2.63230200	-0.53377100	-1.18508500
H	1.02146700	2.24559800	1.42287300
H	2.19897000	1.08437900	1.47339700
H	1.25848400	1.25019700	0.11225200
C	-1.67626000	1.31068400	1.68953000
H	-2.68493900	0.92286800	1.51632000
H	-1.68884800	1.78271200	2.67820500
H	-1.47296100	2.09116500	0.94777500
C	-1.58203600	-1.54087300	2.16419100
H	-1.96951800	-1.97420100	1.23658200
H	-1.13653000	-2.33442000	2.76369800
H	-2.40664000	-1.08190000	2.70914300
C	1.28843500	-1.61301900	1.81676600
H	2.09772300	-1.43014700	1.10101900
H	1.71715700	-1.57620400	2.82438100
H	0.92163600	-2.63384100	1.67110000
C	0.23014300	2.07695600	-2.01084300
H	-0.12371400	2.24903500	-3.03430600
H	-0.48514700	2.54047500	-1.31888700
H	1.18539500	2.59524400	-1.90612000
N	0.33044900	-2.03285700	-1.38712900
N	1.26178700	1.29839000	1.14289100
N	-1.94395800	0.21005300	-1.48472400
H	-2.29075100	1.05535300	-1.92956800
H	-2.50573000	-0.56307700	-1.82882400
H	-2.12050700	0.30251000	-0.48589700
Pd	0.22532600	0.12289200	-1.71813300



Model 1a (RHF/def2-TZVP optimization)

Au	-0.25034500	-0.22380400	2.03447500
H	1.25951200	-2.33480300	-2.19596200
H	0.54195900	-2.23986700	-0.75266900
H	-0.32546900	-2.62941700	-2.06308400
C	2.31108600	0.24267100	-2.23929300
H	2.57772100	-0.19025800	-3.20400800
H	2.75654600	1.22998100	-2.20034800
H	2.79144500	-0.36888100	-1.47175200
H	1.06357500	2.14811500	1.57476400
H	2.19056700	0.97935200	1.62102700
H	1.28565800	1.18406500	0.29354200
C	-1.73144600	1.29466000	1.99240300
H	-2.70923600	0.91098500	1.71692300
H	-1.83427600	1.74139400	2.97846100
H	-1.47739300	2.09362300	1.29786700
C	-1.65112200	-1.53840600	2.71572700
H	-2.12997500	-2.00738700	1.86316600
H	-1.18544400	-2.30374700	3.31896900
H	-2.40110500	-1.01953300	3.29440300
C	1.20180800	-1.77156300	2.09856300
H	2.04506500	-1.57256600	1.43923800
H	1.59486600	-1.86807400	3.10779600
H	0.78905500	-2.73941200	1.82899700
C	0.23085100	2.23677000	-2.31494000
H	0.58271100	2.48307500	-3.31337800
H	-0.77635500	2.64328300	-2.21097600
H	0.86712800	2.77766600	-1.61846800
N	0.42079100	-2.05360800	-1.72922200
N	1.27224300	1.20970700	1.29829000
N	-1.99660700	0.20599100	-1.79510400
H	-2.37547000	0.77505700	-2.52499900
H	-2.48650100	-0.66568400	-1.79385900
H	-2.18590900	0.66411300	-0.92504800
Pd	0.27022600	0.20545600	-2.04281000

Model 1a (SCS-MP2/def2-TZVP optimization)

Au	-0.21500000	-0.17310000	1.75230000
H	1.21870000	-2.38400000	-1.82420000
H	0.38740000	-2.17140000	-0.43150000
H	-0.39900000	-2.62180000	-1.80090000
C	2.22480000	0.15230000	-1.99050000
H	2.45480000	-0.24130000	-2.98910000
H	2.72460000	1.11950000	-1.89830000
H	2.66490000	-0.52800000	-1.24750000
H	1.01710000	2.24080000	1.44810000
H	2.19340000	1.08250000	1.49850000
H	1.25970000	1.25280000	0.14000000
C	-1.70530000	1.30210000	1.73750000
H	-2.71050000	0.90720000	1.55330000
H	-1.73230000	1.78180000	2.72340000
H	-1.50080000	2.08150000	0.99300000
C	-1.59860000	-1.55340000	2.27160000
H	-2.00100000	-2.00310000	1.35760000
H	-1.14290000	-2.33620000	2.87880000
H	-2.41410000	-1.08350000	2.82240000
C	1.27710000	-1.64180000	1.86720000
H	2.08660000	-1.45810000	1.14990000
H	1.71230000	-1.62070000	2.87370000
H	0.90290000	-2.65910000	1.70860000
C	0.24000000	2.10970000	-2.07540000
H	-0.11270000	2.29130000	-3.09890000
H	-0.47760000	2.57110000	-1.38200000
H	1.19580000	2.62720000	-1.96330000
N	0.34590000	-2.03240000	-1.43950000
N	1.25500000	1.29270000	1.16820000
N	-1.94210000	0.22260000	-1.53710000
H	-2.28910000	1.07250000	-1.97370000
H	-2.50480000	-0.54650000	-1.89020000
H	-2.12420000	0.30500000	-0.53850000
Pd	0.24500000	0.14040000	-1.78490000

Model 1a (SCS-MP2-ZORA/SARC-TZVP optimization)

Au	-0.22840000	-0.18680000	1.75290000
H	1.21120000	-2.40130000	-1.79130000
H	0.38390000	-2.16660000	-0.40410000
H	-0.40610000	-2.60370000	-1.76960000
C	2.24850000	0.16560000	-2.02900000
H	2.45620000	-0.22210000	-3.03320000
H	2.74610000	1.13310000	-1.94140000
H	2.70390000	-0.51650000	-1.29830000
H	1.00870000	2.23100000	1.46120000
H	2.18290000	1.07490000	1.51120000
H	1.25500000	1.24900000	0.15120000
C	-1.71820000	1.30020000	1.75110000
H	-2.72770000	0.91360000	1.57610000
H	-1.72550000	1.77460000	2.73910000
H	-1.51180000	2.07720000	1.00530000
C	-1.61950000	-1.57530000	2.26220000
H	-2.01500000	-2.01380000	1.34070000
H	-1.16210000	-2.35950000	2.86480000
H	-2.43330000	-1.10450000	2.81310000
C	1.27610000	-1.65370000	1.87990000
H	2.08260000	-1.46730000	1.16060000
H	1.70640000	-1.61300000	2.88710000
H	0.91030000	-2.67510000	1.73100000
C	0.25530000	2.13190000	-2.11690000
H	-0.08960000	2.28910000	-3.14560000
H	-0.46470000	2.60890000	-1.43830000
H	1.21140000	2.64700000	-2.00900000
N	0.34770000	-2.02420000	-1.41090000
N	1.24520000	1.28350000	1.17860000
N	-1.93540000	0.22680000	-1.50930000
H	-2.30770000	1.06750000	-1.94190000
H	-2.48850000	-0.55040000	-1.85930000
H	-2.12110000	0.30340000	-0.51180000
Pd	0.25940000	0.15570000	-1.77760000

Model 1a (PBE0-D3(BJ)/def2-TZVP optimization)

Au	-0.24449100	-0.19915800	1.77194100
H	1.24015700	-2.35097600	-1.77155800
H	0.41471700	-2.10075700	-0.37910900
H	-0.38114300	-2.58305900	-1.73514100
C	2.27800900	0.14703100	-2.04669300
H	2.48384900	-0.26016000	-3.04440900
H	2.76958900	1.12040800	-1.98465400
H	2.74692800	-0.51686200	-1.30660600
H	0.97650800	2.20526100	1.37903900
H	2.15465700	1.04832100	1.43438100
H	1.18949400	1.18105100	0.09101300
C	-1.74173000	1.28360300	1.74891200
H	-2.74350500	0.89035400	1.55012000
H	-1.78085100	1.75017700	2.73865200
H	-1.52934700	2.07260800	1.01833800
C	-1.62641200	-1.57963100	2.32963600
H	-2.04233900	-2.03962600	1.42830800
H	-1.16373100	-2.35669100	2.93722000
H	-2.43490600	-1.10484400	2.88462100
C	1.26267600	-1.66752900	1.88308900
H	2.07933800	-1.47258900	1.17861900
H	1.68496100	-1.65291800	2.89317100
H	0.89611700	-2.68457100	1.71318000
C	0.24418500	2.15645500	-2.14039000
H	-0.10869600	2.31057100	-3.16766100
H	-0.46554400	2.64922700	-1.46086000
H	1.20671200	2.66434900	-2.04744500
N	0.37034600	-1.99884500	-1.38954100
N	1.21428800	1.25534800	1.12008000
N	-1.90855600	0.25149500	-1.49470600
H	-2.25410600	1.09352900	-1.93972500
H	-2.46641400	-0.52679500	-1.82416100
H	-2.05721600	0.34904900	-0.49384800
Pd	0.27262000	0.16512600	-1.79512000

Model 1a (M06L/def2-TZVP optimization)

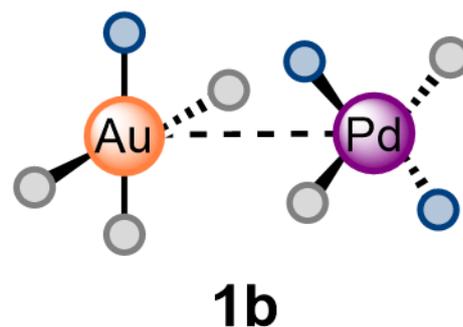
Au	-0.16767900	-0.18070800	1.68694900
H	1.20158600	-2.41664200	-1.71289800
H	0.35890100	-2.22795600	-0.33297700
H	-0.40350500	-2.68970400	-1.70516100
C	2.18550000	0.23498900	-1.95432000
H	2.41649200	-0.21036100	-2.92584600
H	2.62238900	1.23519400	-1.94065900
H	2.67657900	-0.36773300	-1.18047600
H	1.23513100	2.23198100	1.51183700
H	2.35891800	1.02935200	1.50662200
H	1.42564500	1.29144000	0.17158900
C	-1.57152100	1.42183600	1.58590700
H	-2.61467000	1.10438600	1.53810700
H	-1.46858600	2.04567000	2.47671900
H	-1.35745200	2.04333700	0.71158600
C	-1.63959900	-1.55528500	2.08146400
H	-1.75443000	-2.20538600	1.21173800
H	-1.34190000	-2.16943200	2.92830100
H	-2.58840300	-1.06895600	2.29512500
C	1.30634300	-1.72408400	1.85202200
H	2.09699700	-1.59760500	1.10629100
H	1.77097300	-1.66115900	2.83826000
H	0.90489000	-2.73540600	1.75774900
C	0.11346100	2.17092400	-2.02923500
H	0.47265700	2.38926100	-3.03642700
H	-0.91096600	2.54715300	-1.93933300
H	0.73557300	2.74409300	-1.33527800
N	0.32089500	-2.08540000	-1.33800800
N	1.43229300	1.29116200	1.19487600
N	-2.08656500	0.09314600	-1.37558300
H	-2.45682400	1.01955600	-1.55284900
H	-2.63559300	-0.55670800	-1.92451000
H	-2.26222500	-0.10169100	-0.39460500
Pd	0.16085800	0.15968700	-1.69828400

Model 1a (M06-2x/def2-TZVP optimization)

Au	-0.18395200	-0.17974000	1.71534600
H	1.32942200	-2.35930900	-1.67913000
H	0.28935900	-2.30808700	-0.41809400
H	-0.24748500	-2.73431100	-1.91624900
C	2.18541300	0.25887000	-1.96080400
H	2.43341000	-0.19465500	-2.92557100
H	2.61000500	1.26449100	-1.95550200
H	2.68317700	-0.32935500	-1.17849700
H	1.22879500	2.21781400	1.50963700
H	2.35145600	1.00913600	1.59241600
H	1.49930400	1.25486900	0.19820700
C	-1.56320100	1.41372800	1.65281800
H	-2.60700800	1.09975600	1.58017400
H	-1.47387500	2.00015200	2.57135800
H	-1.33793300	2.07576000	0.80988100
C	-1.65413800	-1.49709800	2.12815200
H	-1.96406900	-1.96812500	1.19230500
H	-1.28426000	-2.26792100	2.80026600
H	-2.50907800	-0.99413700	2.57269900
C	1.24145800	-1.73352800	1.82263100
H	2.01581400	-1.60743700	1.05883200
H	1.73104400	-1.69938900	2.79952900
H	0.81406200	-2.73368700	1.71864300
C	0.11015800	2.14869700	-1.99175500
H	0.39818100	2.39479900	-3.01628200
H	-0.90765800	2.51560900	-1.82015000
H	0.77632500	2.70933800	-1.32981500
N	0.38041400	-2.11895000	-1.41258800
N	1.44574700	1.27069200	1.21898000
N	-2.09260900	0.08087200	-1.43719100
H	-2.51056500	0.78209400	-2.03860500
H	-2.58960600	-0.79032900	-1.58094600
H	-2.24056900	0.37120000	-0.47396300
Pd	0.17862300	0.14713100	-1.72804100

Model **1b** (MP2/def2-TZVP optimization)

Au	0.00017000	-0.22591700	1.68705300
H	-1.86215900	-1.46595200	-2.17672500
H	-1.98499600	-0.94284900	-0.62583400
H	-2.57953800	-0.01582400	-1.85613400
C	0.82125600	-1.63089900	-1.60386700
H	1.06879100	-1.93977600	-2.62821500
H	1.74267200	-1.65389900	-1.01130300
H	0.15466300	-2.38989700	-1.17899400
H	-1.70096000	1.87624200	1.56270400
H	-0.16469900	2.46979800	1.61217000
H	-0.74060200	1.79461200	0.20925300
C	-1.92643300	-1.01573700	1.76278800
H	-1.99123600	-1.98612100	1.25816200
H	-2.19966000	-1.19063200	2.80808000
H	-2.68948900	-0.34971500	1.33877800
C	0.70749400	-2.06436500	2.10883400
H	0.85363400	-2.58122700	1.15850500
H	1.65927700	-1.99053500	2.63453800
H	-0.01316300	-2.61081500	2.71721500
C	1.95936700	0.47184200	1.71768600
H	2.05237500	1.49900600	1.34074200
H	2.34312000	0.46986400	2.74244900
H	2.61425000	-0.18190400	1.13187900
N	-1.82464400	-0.63990300	-1.58580000
N	-0.74957900	1.72799200	1.23736200
C	-0.84957900	2.13345600	-1.91775700
H	-0.27125100	2.98712500	-1.53179700
H	-0.89182100	2.27095600	-3.00647100
H	-1.87998900	2.28088100	-1.55934600
N	1.85417900	0.97909500	-1.65437000
H	1.89522600	1.94741100	-1.95947700
H	2.21288500	0.92568200	-0.70235600
H	2.47378200	0.42884800	-2.24304600
Pd	-0.01288000	0.22722000	-1.65743300



Model **1b** (RHF/def2-TZVP optimization)

Au	0.02044100	-0.16389600	2.04934100
H	-1.98816200	-1.51070500	-2.63692100
H	-2.17925100	-1.02635300	-1.10711300
H	-2.65150500	-0.05718600	-2.31947400
C	0.79823200	-1.82575100	-2.19840000
H	0.93161800	-2.09354500	-3.24943400
H	1.77440100	-1.93401800	-1.72352900
H	0.16459200	-2.59737000	-1.75881500
H	-1.73098200	1.96271200	1.91481500
H	-0.23024600	2.58107500	1.94764700
H	-0.82324200	1.96211400	0.57221000
C	-1.93059000	-0.99845100	2.00725800
H	-1.94105700	-1.96319300	1.50904500
H	-2.30150400	-1.15660000	3.01669600
H	-2.64604800	-0.35146000	1.49895000
C	0.77081000	-2.00788100	2.47991600
H	0.99412700	-2.50003400	1.54151000
H	1.67749700	-1.91655500	3.05956400
H	0.04195600	-2.59045900	3.02377900
C	1.99303300	0.61823900	2.09314300
H	2.06372100	1.58916200	1.60205500
H	2.32963500	0.75159600	3.11806600
H	2.69844700	-0.05152200	1.61058200
N	-1.95596000	-0.71498700	-2.03252100
N	-0.79926800	1.85099600	1.56925900
C	-0.83532200	2.12378200	-1.92023400
H	-0.20495700	2.86549200	-1.41969300
H	-0.96622900	2.49553700	-2.93872200
H	-1.82328900	2.19863100	-1.45509500
N	1.96252000	0.89968000	-1.94679600
H	2.00315500	1.86083600	-2.21763500
H	2.30550800	0.82164600	-1.00900100
H	2.56830400	0.36685900	-2.53724600
Pd	-0.00992200	0.12567300	-2.01393300

Model **1b** (SCS-MP2/def2-TZVP optimization)

Au	0.00150000	-0.23190000	1.73960000
H	-1.87770000	-1.48040000	-2.21740000
H	-1.99390000	-0.94340000	-0.67170000
H	-2.59370000	-0.02770000	-1.90600000
C	0.83260000	-1.64610000	-1.65970000
H	1.09410000	-1.96110000	-2.68030000
H	1.74960000	-1.67180000	-1.05730000
H	0.16340000	-2.40920000	-1.24180000
H	-1.70420000	1.89410000	1.59780000
H	-0.16850000	2.48550000	1.65150000
H	-0.74360000	1.81670000	0.25080000
C	-1.94150000	-1.01820000	1.80330000
H	-2.00960000	-1.98760000	1.29510000
H	-2.22840000	-1.19140000	2.84640000
H	-2.69680000	-0.34730000	1.36990000
C	0.70900000	-2.07960000	2.16250000
H	0.85600000	-2.59670000	1.21150000
H	1.66060000	-2.00720000	2.69000000
H	-0.01370000	-2.62600000	2.76990000
C	1.97370000	0.47080000	1.75910000
H	2.06270000	1.50030000	1.38380000
H	2.36950000	0.46600000	2.78040000
H	2.62610000	-0.17660000	1.16140000
N	-1.83640000	-0.64880000	-1.63440000
N	-0.75230000	1.74360000	1.27490000
C	-0.85830000	2.14360000	-1.94830000
H	-0.27680000	2.98990000	-1.54630000
H	-0.91690000	2.31420000	-3.03300000
H	-1.88560000	2.27870000	-1.57160000
N	1.86780000	0.99160000	-1.70140000
H	1.90890000	1.96100000	-2.00350000
H	2.21800000	0.93820000	-0.74630000
H	2.49610000	0.44520000	-2.28470000
Pd	-0.01100000	0.22580000	-1.71460000

Model **1b** (SCS-MP2-ZORA/SARC-TZVP optimization)

Au	0.00930000	-0.22900000	1.72950000
H	-1.89600000	-1.49550000	-2.21440000
H	-2.00610000	-0.95530000	-0.67390000
H	-2.61530000	-0.04880000	-1.90440000
C	0.83470000	-1.65960000	-1.63170000
H	1.10170000	-1.99550000	-2.64310000
H	1.74730000	-1.67290000	-1.02380000
H	0.16450000	-2.41490000	-1.20310000
H	-1.69140000	1.91110000	1.60130000
H	-0.15660000	2.49750000	1.65760000
H	-0.73200000	1.83180000	0.25760000
C	-1.94280000	-1.01220000	1.78640000
H	-2.01270000	-1.98130000	1.27880000
H	-2.23320000	-1.17760000	2.82900000
H	-2.68820000	-0.33520000	1.34620000
C	0.71260000	-2.09110000	2.13450000
H	0.84930000	-2.59170000	1.17480000
H	1.66550000	-2.02400000	2.65890000
H	-0.01290000	-2.63410000	2.74020000
C	1.98920000	0.47120000	1.76600000
H	2.07810000	1.50240000	1.39650000
H	2.37160000	0.45980000	2.79170000
H	2.64240000	-0.17420000	1.16830000
N	-1.85100000	-0.66150000	-1.63590000
N	-0.74000000	1.75640000	1.27960000
C	-0.87520000	2.14600000	-1.96140000
H	-0.29450000	2.98850000	-1.55270000
H	-0.94380000	2.32830000	-3.04220000
H	-1.89810000	2.26970000	-1.57170000
N	1.87140000	1.00090000	-1.69060000
H	1.91550000	1.97150000	-1.98710000
H	2.22940000	0.94640000	-0.73970000
H	2.50430000	0.46350000	-2.27650000
Pd	-0.01660000	0.22330000	-1.71530000

Model **1b** (PBE0-D3(BJ)/def2-TZVP optimization)

Au	0.08045200	-0.20589200	1.71310600
H	-2.00691200	-1.40303400	-2.34941200
H	-2.18527200	-0.89260700	-0.79924500
H	-2.67044000	0.07888400	-2.04476300
C	0.66689300	-1.74273800	-1.68727900
H	0.75707500	-2.11448000	-2.71708100
H	1.65710100	-1.81766800	-1.22145300
H	0.01331200	-2.43185400	-1.13892300
H	-1.69586300	1.84955100	1.55042800
H	-0.18371500	2.50137700	1.56932100
H	-0.74948600	1.77333600	0.18950400
C	-1.83533800	-1.07575800	1.66417000
H	-1.83112900	-1.99634900	1.07120200
H	-2.15504800	-1.34992800	2.67345800
H	-2.60021500	-0.39876700	1.25963300
C	0.85594800	-2.03279300	2.14558600
H	1.09719500	-2.51267000	1.19534600
H	1.76234900	-1.92890300	2.74133100
H	0.12515300	-2.63761400	2.68160200
C	2.02148000	0.60480800	1.82607300
H	2.09080400	1.62116800	1.41476500
H	2.33493200	0.66461800	2.87236500
H	2.75503800	-0.02833300	1.31558300
N	-1.97124800	-0.59013300	-1.74581900
N	-0.74619500	1.73619600	1.21772500
C	-0.84432400	2.18585500	-1.93383300
H	-0.22938600	3.00564100	-1.53086200
H	-0.87809200	2.34490100	-3.02007200
H	-1.86867500	2.36868600	-1.57311100
N	1.84399000	0.90026000	-1.57580200
H	1.92938000	1.86946800	-1.85715300
H	2.12371500	0.81279600	-0.60202300
H	2.47096000	0.33337100	-2.13418000
Pd	-0.07946200	0.20414600	-1.71125600

Model **1b** (M06L/def2-TZVP optimization)

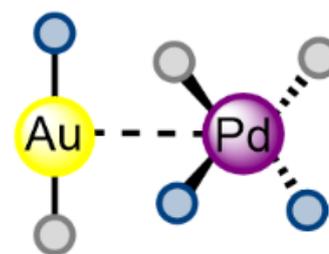
Au	0.20272400	-0.20462000	1.69844800
H	-2.01167100	-1.53254500	-2.50637600
H	-2.35033700	-1.03499800	-0.98497000
H	-2.76717900	-0.09220500	-2.26556400
C	0.68108700	-1.73561000	-1.56147200
H	0.86995500	-2.13285000	-2.56474200
H	1.63205500	-1.73657000	-1.01850900
H	0.01764000	-2.43613500	-1.04352400
H	-1.42981600	2.05633800	1.65128200
H	0.10143100	2.59869300	1.44978300
H	-0.68756700	1.86320600	0.19552700
C	-1.78248900	-0.95750000	1.50325500
H	-1.77633900	-1.87664400	0.91220100
H	-2.22045900	-1.20112300	2.47256800
H	-2.43852300	-0.22634500	1.01805300
C	0.84261100	-2.09991000	2.15395600
H	0.98730300	-2.62767500	1.21292900
H	1.78050700	-2.05960900	2.70174100
H	0.08419800	-2.60883300	2.74391100
C	2.20923600	0.50083000	1.91291100
H	2.34040600	1.54696900	1.61383200
H	2.51406800	0.42994900	2.95774500
H	2.91367000	-0.10960000	1.34100800
N	-2.05915800	-0.71946900	-1.90535000
N	-0.54162700	1.85482600	1.20975700
C	-1.07745400	2.13903500	-1.98103800
H	-0.46683000	3.00999100	-1.70718900
H	-1.26438000	2.23158600	-3.05602300
H	-2.05098400	2.27826200	-1.49062500
N	1.74341500	1.00678300	-1.42292500
H	1.79837000	1.99835100	-1.61958500
H	2.01919900	0.85063700	-0.45651300
H	2.41790300	0.52901000	-2.00763100
Pd	-0.17598700	0.19331700	-1.69794100

Model **1b** (M06-2x/def2-TZVP optimization)

Au	0.18447900	-0.18760200	1.71764000
H	-2.05442500	-1.50772400	-2.51555900
H	-2.35886500	-1.02486400	-0.97600400
H	-2.77163900	-0.04444900	-2.23897400
C	0.63334800	-1.76388100	-1.60355100
H	0.77076000	-2.17428900	-2.61053300
H	1.60442300	-1.79329900	-1.09747100
H	-0.03232500	-2.43855100	-1.05390200
H	-1.53140300	2.00669600	1.68247900
H	-0.00728800	2.61159500	1.55685000
H	-0.73475200	1.91787500	0.24196100
C	-1.75092100	-1.00158600	1.55042900
H	-1.72239500	-1.91839900	0.95554300
H	-2.15247600	-1.26267100	2.53169100
H	-2.44753500	-0.29467900	1.08555500
C	0.87384200	-2.03810800	2.12849300
H	1.04523100	-2.53619800	1.17478200
H	1.80534400	-1.97751400	2.68603200
H	0.12873800	-2.58919100	2.69784600
C	2.15075100	0.55831000	1.91883800
H	2.26415600	1.59031800	1.56699300
H	2.43529800	0.54693800	2.97303100
H	2.87621100	-0.06762200	1.39103200
N	-2.08035000	-0.70321100	-1.89920100
N	-0.62193800	1.86292700	1.25767900
C	-0.99946500	2.14290900	-1.96731300
H	-0.37948500	2.98969700	-1.64072100
H	-1.14014400	2.27672400	-3.04615600
H	-1.98955300	2.29342200	-1.51342600
N	1.80474100	0.93102000	-1.48398100
H	1.87568200	1.91346400	-1.72239600
H	2.07897600	0.80574600	-0.51191000
H	2.45461900	0.40479900	-2.05748200
Pd	-0.15666500	0.16694000	-1.71936600

Model **2a** (MP2/def2-TZVP optimization)

H	2.34475700	-1.36125200	-1.94423400
H	1.49687900	-1.57627800	-0.55482200
H	1.06438400	-2.37986400	-1.92224200
C	1.87997400	1.22400500	-2.51256300
H	2.17761100	0.78130700	-3.47053500
H	1.83385500	2.30552500	-2.65712800
H	2.67112900	1.01254700	-1.78010100
C	-0.77108500	1.97777500	-2.27473600
H	-1.40915200	1.80113500	-3.14877700
H	-1.42282500	2.17655900	-1.41284200
H	-0.19150900	2.88139700	-2.47541500
N	1.41104800	-1.49392900	-1.56614300
N	-1.64216900	-0.62581300	-1.29222800
H	-2.41644900	-0.00752000	-1.51711100
H	-1.87343700	-1.54456600	-1.65865500
H	-1.59035300	-0.69846500	-0.27785300
Au	0.51757900	0.31636100	1.26633200
N	1.00585500	2.24849400	0.58580100
H	1.96122100	2.52855300	0.78968300
C	0.04910100	-1.52551100	1.88143100
H	-0.80303800	-1.50731600	2.56742000
H	-0.21595500	-2.19704300	1.05597700
H	0.88472100	-1.98720100	2.41587900
H	0.38631700	2.97632700	0.93099200
H	0.89578900	2.18274500	-0.43257100
Pd	0.22787900	0.30840800	-1.93749200



2a

Model **2a** (RHF/def2-TZVP optimization)

H	2.30537500	-1.43831100	-2.21199200
H	1.56358100	-1.61062700	-0.78324800
H	1.01335400	-2.40304700	-2.08240300
C	1.95666900	1.34198500	-2.72251100
H	2.05629400	1.34351400	-3.80643500
H	1.99555900	2.38082200	-2.40735500
H	2.84101400	0.84711900	-2.31502500
C	-0.85418600	2.06433000	-2.56528600
H	-1.63995700	1.83733300	-3.28769500
H	-1.35122100	2.40737500	-1.65406600
H	-0.28503100	2.89653900	-2.96090500
N	1.41400700	-1.54116400	-1.77120900
N	-1.70697600	-0.67066300	-1.57140800
H	-2.43175500	0.00826800	-1.68886700
H	-1.96415000	-1.48581900	-2.09079400
H	-1.66967900	-0.91733100	-0.60151200
Au	0.54991200	0.23423500	1.75545400
N	1.05989800	2.17967700	0.85282800
H	1.99434600	2.46607900	1.06710200
C	0.06243700	-1.60983000	2.55695300
H	-0.86125000	-1.55389100	3.12561000
H	-0.07088600	-2.37183200	1.79174800
H	0.84203200	-1.95742700	3.22816500
H	0.44112400	2.90787500	1.14953500
H	0.98301200	2.09805000	-0.14529700
Pd	0.22860500	0.36312200	-2.20332200

Model **2a** (SCS-MP2/def2-TZVP optimization)

H	2.34940000	-1.37730000	-1.98140000
H	1.49750000	-1.61660000	-0.60040000
H	1.06280000	-2.38710000	-1.98440000
C	1.89910000	1.23510000	-2.55320000
H	2.19910000	0.80840000	-3.51900000
H	1.85180000	2.31980000	-2.67910000
H	2.69280000	1.01340000	-1.82430000
C	-0.78540000	1.99490000	-2.30570000
H	-1.42200000	1.83270000	-3.18530000
H	-1.44260000	2.18440000	-1.44380000
H	-0.20410000	2.90210000	-2.49020000
N	1.41280000	-1.50960000	-1.60950000
N	-1.64970000	-0.63570000	-1.32470000
H	-2.42470000	-0.01390000	-1.53920000
H	-1.88310000	-1.54760000	-1.70780000
H	-1.60480000	-0.72840000	-0.31150000
Au	0.51960000	0.31170000	1.34150000
N	1.00880000	2.25470000	0.62650000
H	1.96350000	2.53940000	0.82870000
C	0.04840000	-1.53600000	1.98040000
H	-0.80700000	-1.51210000	2.66370000
H	-0.21410000	-2.21520000	1.15870000
H	0.88390000	-1.99310000	2.52090000
H	0.38930000	2.98500000	0.96770000
H	0.90100000	2.19210000	-0.39070000
Pd	0.22970000	0.31540000	-1.97980000

Model **2a** (SCS-MP2-ZORA/SARC-TZVP optimization)

H	2.41520000	-1.21020000	-1.91020000
H	1.47990000	-1.40120000	-0.58070000
H	1.13310000	-2.21260000	-1.95920000
C	1.91570000	1.35990000	-2.81630000
H	2.21040000	0.83200000	-3.73110000
H	1.84130000	2.42220000	-3.04950000
H	2.71610000	1.23100000	-2.07480000
C	-0.78750000	2.11500000	-2.59200000
H	-1.49630000	1.83400000	-3.38030000
H	-1.36490000	2.42530000	-1.71020000
H	-0.21900000	2.97670000	-2.94210000
N	1.45480000	-1.31930000	-1.59620000
N	-1.59310000	-0.45750000	-1.33060000
H	-2.38650000	0.16170000	-1.47250000
H	-1.86030000	-1.35980000	-1.71510000
H	-1.48700000	-0.58030000	-0.32460000
Au	0.46820000	0.03020000	1.60010000
N	0.93030000	1.91910000	0.72830000
H	1.88950000	2.21770000	0.88610000
C	0.02260000	-1.76840000	2.38470000
H	-0.81050000	-1.68080000	3.08820000
H	-0.26250000	-2.49370000	1.61490000
H	0.88370000	-2.17290000	2.92450000
H	0.32300000	2.67320000	1.03880000
H	0.79890000	1.80460000	-0.28800000
Pd	0.25710000	0.47030000	-2.13410000

Model **2a** (PBE0-D3(BJ)/def2-TZVP optimization)

H	2.37859000	-1.23343600	-1.88039100
H	1.42589700	-1.46141400	-0.56013200
H	1.11130900	-2.26883500	-1.96047000
C	1.93287900	1.29502200	-2.73042000
H	2.19747000	0.82796600	-3.68749000
H	1.86933000	2.37235100	-2.89562000
H	2.75733700	1.10980900	-2.02632000
C	-0.80449400	2.08874800	-2.47827800
H	-1.35951500	1.91505800	-3.40846500
H	-1.53589700	2.28563900	-1.68080700
H	-0.20902300	2.99390000	-2.61559400
N	1.42475300	-1.38614600	-1.57482300
N	-1.60390600	-0.51910000	-1.29601300
H	-2.37244800	0.12393500	-1.44529800
H	-1.86808000	-1.41634000	-1.68499700
H	-1.47437500	-0.62992900	-0.29285600
Au	0.48505400	0.12716100	1.49726800
N	0.94432000	2.04769500	0.65791400
H	1.89969800	2.34480900	0.81950600
C	0.03790300	-1.71129200	2.22619400
H	-0.79712500	-1.65310400	2.93058900
H	-0.24351300	-2.42145200	1.43982500
H	0.89523600	-2.13326800	2.75890000
H	0.32649800	2.78792200	0.97012900
H	0.81152000	1.91922400	-0.35648900
Pd	0.24271200	0.41145300	-2.06779600

Model **2a** (M06L/def2-TZVP optimization)

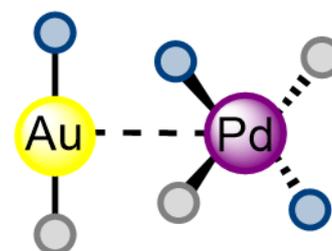
H	2.36261500	-1.46936600	-1.97584600
H	1.55908600	-1.55172900	-0.55353600
H	1.06591000	-2.44561900	-1.83022700
C	1.95857000	1.26653700	-2.56157500
H	2.29013700	0.81808000	-3.50228400
H	1.89008400	2.34450400	-2.71679700
H	2.72920000	1.07583500	-1.80389900
C	-0.82613600	2.05449000	-2.31385600
H	-1.49213000	1.88773400	-3.16513100
H	-1.44638000	2.25801600	-1.43170700
H	-0.23353100	2.94519300	-2.52884600
N	1.44100300	-1.54396200	-1.56325500
N	-1.69149200	-0.65619200	-1.28496300
H	-2.49426000	-0.10116500	-1.55451400
H	-1.88431400	-1.61249300	-1.55565700
H	-1.63312300	-0.63488200	-0.27028600
Au	0.50904000	0.27178900	1.31230000
N	1.02219600	2.30123200	0.58715500
H	1.97297300	2.59099300	0.77831900
C	0.02584400	-1.61960500	1.93204500
H	-0.82921400	-1.60453700	2.60924600
H	-0.23186000	-2.27430900	1.09348500
H	0.85725900	-2.08303000	2.46484900
H	0.40585400	3.03490800	0.91324800
H	0.91234500	2.22213300	-0.42611900
Pd	0.23245300	0.34182200	-1.99408600

Model **2a** (M06-2x/def2-TZVP optimization)

H	2.39138300	-1.39012000	-1.89359300
H	1.45472300	-1.67044900	-0.57350300
H	1.13555400	-2.43863400	-1.99330300
C	1.94237000	1.25564400	-2.57522100
H	2.28313400	0.79189800	-3.50652400
H	1.88858100	2.33130600	-2.74653200
H	2.70645400	1.06946600	-1.80872300
C	-0.81413800	2.04301700	-2.33283700
H	-1.49384300	1.87033300	-3.17353800
H	-1.42560000	2.25095900	-1.44464900
H	-0.23254300	2.93676800	-2.56124900
N	1.44092000	-1.56306500	-1.58478800
N	-1.71387000	-0.66036400	-1.30785700
H	-2.46951700	-0.00609000	-1.47976900
H	-1.97748900	-1.55278100	-1.70892300
H	-1.62340900	-0.77770200	-0.30173500
Au	0.51751600	0.27863800	1.36077900
N	1.02140900	2.31343300	0.61387800
H	1.96858400	2.60339100	0.83012100
C	0.04934100	-1.59816900	1.98527400
H	-0.77898000	-1.57682300	2.69580700
H	-0.24535500	-2.25417500	1.15941000
H	0.90005900	-2.06529400	2.48516800
H	0.38947000	3.03395600	0.94491400
H	0.92921100	2.25051400	-0.40198400
Pd	0.22816300	0.34072400	-2.02255800

Model **2b** (MP2/def2-TZVP optimization)

N	4.57418900	1.05516000	1.70601400
H	4.76023800	1.61058200	0.87582200
H	4.94675900	1.54425300	2.51509700
H	5.08306700	0.18168300	1.59805200
C	2.63584800	-0.25634100	0.04989500
H	3.58279100	-0.15974900	-0.49556500
H	2.44337700	-1.33045900	0.16713500
H	1.85210300	0.15220800	-0.59894900
C	2.58782200	1.48510400	3.79202100
H	1.59550900	1.75829300	4.17482700
H	2.98598400	0.72604000	4.47864800
H	3.22455000	2.37408400	3.91829100
N	0.66081400	0.19058200	2.02287600
H	0.44562200	-0.21045500	2.93252000
H	0.07376400	1.02927300	1.92582800
H	0.36886600	-0.46955300	1.30613000
Au	-0.81594900	3.19209100	1.84404100
C	-2.70506500	2.60044700	1.63090700
H	-3.32119800	3.42467200	1.26089600
H	-2.79124300	1.77606300	0.91756500
H	-3.12524200	2.26943600	2.58450900
N	1.19470500	3.78594600	2.07112000
H	1.33229600	4.37506300	2.88851000
H	1.78618100	2.95125800	2.19540100
H	1.53619200	4.29503100	1.26034800
Pd	2.60839000	0.65309300	1.88234700



2b

Model **2b** (RHF/def2-TZVP optimization)

N	4.92261000	0.11134400	1.73114000
H	5.26059400	-0.72829900	1.30677400
H	5.40105100	0.89231700	1.32961900
H	5.14067700	0.09141600	2.70689200
C	2.82928000	-1.51676200	0.38867400
H	3.19987900	-2.33649700	1.00896700
H	1.85302700	-1.83359900	0.01989000
H	3.48247000	-1.46721700	-0.48594700
C	2.84687600	2.18169600	2.54262100
H	2.19304300	2.11652700	3.41617800
H	3.82657400	2.49440000	2.90966400
H	2.47789600	2.99270400	1.90940200
N	0.73803500	0.49087000	1.16075200
H	0.27647400	-0.30549200	1.55284400
H	0.33281600	1.31323800	1.56234200
H	0.53583000	0.49226300	0.18091600
Au	-1.23534000	3.73592100	2.67468600
C	-2.82088600	2.74324400	1.79772600
H	-3.74414100	3.29543800	1.94430100
H	-2.67353200	2.62631700	0.72766500
H	-2.95694800	1.75447800	2.22696300
N	0.48799300	4.76653100	3.59975000
H	0.37015800	4.87309300	4.58754600
H	1.31685800	4.22394300	3.44092600
H	0.63106700	5.67566800	3.20734700
Pd	2.82801000	0.32026400	1.45664800

Model **2b** (SCS-MP2/def2-TZVP optimization)

N	4.61360000	1.04160000	1.70540000
H	4.79880000	1.60530000	0.88010000
H	4.98750000	1.52510000	2.51760000
H	5.12710000	0.17150000	1.58930000
C	2.66600000	-0.28160000	0.03370000
H	3.61380000	-0.17830000	-0.51250000
H	2.48050000	-1.35950000	0.14280000
H	1.88080000	0.12140000	-0.61990000
C	2.61230000	1.47030000	3.80350000
H	1.61810000	1.73510000	4.19170000
H	3.02140000	0.71990000	4.49570000
H	3.23990000	2.36830000	3.92550000
N	0.67100000	0.15950000	2.02710000
H	0.45890000	-0.24320000	2.93690000
H	0.07890000	0.99100000	1.93040000
H	0.38140000	-0.50330000	1.31180000
Au	-0.86940000	3.22850000	1.84550000
C	-2.77440000	2.64290000	1.62950000
H	-3.37950000	3.45810000	1.22020000
H	-2.86080000	1.79130000	0.94690000
H	-3.21000000	2.35190000	2.59050000
N	1.16470000	3.82160000	2.07550000
H	1.30420000	4.40550000	2.89650000
H	1.75910000	2.99160000	2.19060000
H	1.50300000	4.33830000	1.26790000
Pd	2.63340000	0.63110000	1.88210000

Model **2b** (SCS-MP2-ZORA/SARC-TZVP optimization)

N	4.64030000	1.03960000	1.71990000
H	4.83210000	1.59150000	0.88870000
H	5.01710000	1.53460000	2.52310000
H	5.16000000	0.17210000	1.61710000
C	2.69140000	-0.27310000	0.02290000
H	3.65230000	-0.19290000	-0.50230000
H	2.47060000	-1.34510000	0.11040000
H	1.93370000	0.16680000	-0.63740000
C	2.61560000	1.46320000	3.82390000
H	1.61710000	1.72760000	4.19760000
H	3.02660000	0.73050000	4.53150000
H	3.23220000	2.36970000	3.92990000
N	0.67530000	0.13850000	2.03550000
H	0.46100000	-0.25010000	2.95030000
H	0.06740000	0.95520000	1.92100000
H	0.39280000	-0.54260000	1.33540000
Au	-0.89950000	3.23330000	1.83160000
C	-2.82130000	2.67630000	1.64580000
H	-3.43140000	3.53250000	1.34450000
H	-2.93240000	1.89510000	0.88840000
H	-3.20770000	2.29580000	2.59550000
N	1.14930000	3.80000000	2.03110000
H	1.30440000	4.39560000	2.84050000
H	1.73720000	2.96820000	2.15310000
H	1.48780000	4.29900000	1.21290000
Pd	2.64860000	0.62290000	1.89360000

Model **2b** (PBE0-D3(BJ)/def2-TZVP optimization)

N	4.61610100	0.99383200	1.70504900
H	4.80436000	1.44986500	0.82009900
H	4.96786400	1.56802000	2.46240100
H	5.11292200	0.11001000	1.70599800
C	2.60651300	-0.37647600	0.06643100
H	3.56152400	-0.33890100	-0.47448700
H	2.36523900	-1.43928900	0.20408500
H	1.84785800	0.05047900	-0.60210800
C	2.62431900	1.54506300	3.81822100
H	1.64395500	1.86782600	4.19365100
H	3.00210900	0.80408300	4.53558700
H	3.29080700	2.41825600	3.89989000
N	0.61447800	0.17505300	2.09186400
H	0.41468400	-0.19894700	3.01264100
H	0.03739600	1.01527700	1.97477600
H	0.32544400	-0.50099900	1.39382100
Au	-0.82091600	3.26291800	1.79357200
C	-2.77642400	2.75497000	1.69176600
H	-3.39695200	3.65421200	1.63529000
H	-2.98064600	2.14724700	0.80543300
H	-3.08448500	2.18748800	2.57481400
N	1.26652500	3.75879100	1.90481000
H	1.45498500	4.44556100	2.62631600
H	1.80778300	2.91240300	2.13098800
H	1.60686500	4.12441800	1.02312100
Pd	2.60806200	0.61264200	1.91026000

Model **2b** (PBE0-D3(BJ)/def2-TZVP optimization)

N	4.68323300	0.95261800	1.69863100
H	4.89927800	1.40308800	0.81824700
H	5.04905900	1.52043700	2.45294400
H	5.17247400	0.06594300	1.70515400
C	2.61559700	-0.40314300	0.01972300
H	3.57399200	-0.37423300	-0.50934800
H	2.35726500	-1.45909300	0.15479300
H	1.86713700	0.03536000	-0.64827700
C	2.62492300	1.54143300	3.81982600
H	1.63686800	1.87179700	4.16154300
H	2.98919400	0.82342500	4.56209100
H	3.28784800	2.41525200	3.88271400
N	0.57630700	0.16301200	2.07134500
H	0.37178700	-0.23317200	2.98077400
H	0.00262500	1.00810600	1.98108600
H	0.26846700	-0.49250900	1.36304900
Au	-0.86115300	3.29209800	1.82565600
C	-2.83705400	2.80095600	1.72219500
H	-3.39093300	3.57713200	1.19309800
H	-2.98749000	1.86059300	1.19027200
H	-3.26444900	2.69940100	2.72014500
N	1.29178900	3.78736200	1.94120200
H	1.52053600	4.30969100	2.77842200
H	1.84149000	2.92021100	1.98109600
H	1.61214800	4.32615000	1.14661800
Pd	2.61943700	0.59188800	1.89128900

Model **2b** (M06L/def2-TZVP optimization)

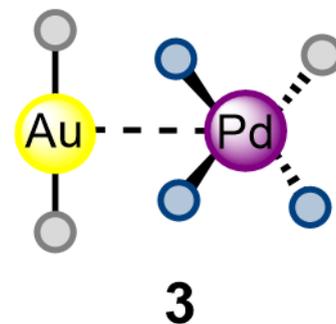
N	4.68323300	0.95261800	1.69863100
H	4.89927800	1.40308800	0.81824700
H	5.04905900	1.52043700	2.45294400
H	5.17247400	0.06594300	1.70515400
C	2.61559700	-0.40314300	0.01972300
H	3.57399200	-0.37423300	-0.50934800
H	2.35726500	-1.45909300	0.15479300
H	1.86713700	0.03536000	-0.64827700
C	2.62492300	1.54143300	3.81982600
H	1.63686800	1.87179700	4.16154300
H	2.98919400	0.82342500	4.56209100
H	3.28784800	2.41525200	3.88271400
N	0.57630700	0.16301200	2.07134500
H	0.37178700	-0.23317200	2.98077400
H	0.00262500	1.00810600	1.98108600
H	0.26846700	-0.49250900	1.36304900
Au	-0.86115300	3.29209800	1.82565600
C	-2.83705400	2.80095600	1.72219500
H	-3.39093300	3.57713200	1.19309800
H	-2.98749000	1.86059300	1.19027200
H	-3.26444900	2.69940100	2.72014500
N	1.29178900	3.78736200	1.94120200
H	1.52053600	4.30969100	2.77842200
H	1.84149000	2.92021100	1.98109600
H	1.61214800	4.32615000	1.14661800
Pd	2.61943700	0.59188800	1.89128900

Model **2b** (M06-2x/def2-TZVP optimization)

N	4.57070900	1.02174300	1.52812200
H	4.68241900	1.56623400	0.68024600
H	4.99405100	1.51965400	2.30299100
H	5.06231800	0.14495600	1.39284400
C	2.42975000	-0.42549700	0.05818700
H	3.33007000	-0.32566600	-0.55795700
H	2.27511400	-1.49690600	0.22959500
H	1.58844300	-0.05956900	-0.53955600
C	2.62041900	1.55115900	3.81037600
H	1.65651000	1.92924600	4.17533100
H	2.95054500	0.79628100	4.53344000
H	3.33561700	2.38229100	3.89390900
N	0.50375100	0.07087000	2.21066100
H	0.33160100	-0.12179200	3.19151000
H	-0.10348500	0.84625000	1.94361100
H	0.23966200	-0.74057900	1.66238500
Au	-0.69279700	3.32240700	1.81615600
C	-2.56798000	2.62525000	1.49966900
H	-3.23813700	3.44813000	1.24567800
H	-2.59192500	1.90860100	0.67615800
H	-2.96225400	2.13397600	2.39127800
N	1.38845300	4.01548300	2.16951700
H	1.47308800	4.58505900	3.00443500
H	1.95621100	3.17720500	2.31100900
H	1.76293400	4.54005500	1.38748700
Pd	2.52528300	0.58896200	1.88720700

Model 3 (MP2/def2-TZVP optimization)

H	0.68055800	-2.52208800	-1.03270500
H	0.18570300	-1.41329800	0.08040600
H	-0.91149900	-2.34626100	-0.73809500
C	0.11725900	1.81605700	-2.84838300
H	-0.85900300	2.28843600	-2.96638400
H	0.73593300	2.45211300	-2.21107700
H	0.57311400	1.70078800	-3.83480500
N	-0.03938000	-1.83356800	-0.83197600
N	-1.98619900	0.39578400	-1.69299300
H	-2.43478600	0.94863400	-2.41721300
H	-2.54224700	-0.44498200	-1.56717600
H	-2.02169600	0.92759100	-0.81882400
Au	0.69485100	0.70564100	1.00094100
C	2.48060700	-0.34054200	1.05310500
H	2.71657000	-0.58662000	2.09461700
H	2.51486100	-1.29944300	0.51345700
H	3.34072200	0.24572600	0.69623100
N	2.03227700	0.02877300	-2.10199100
H	2.44302500	-0.84466000	-2.42020800
H	2.42303700	0.77458900	-2.67132700
H	2.32235000	0.18096300	-1.12902100
C	-1.05131100	1.79012100	1.07288600
H	-1.95604200	1.16725200	1.14880600
H	-1.07383800	2.43268800	1.96032400
H	-1.17223800	2.46550500	0.21333400
Pd	0.00208300	0.07345900	-1.97212500



Model 3 (RHF/def2-TZVP optimization)

H	0.27534200	-2.27529400	-0.67914100
H	-0.63719300	-1.23452700	0.12879500
H	-1.29997600	-2.19581700	-1.01014100
C	0.36617400	1.73688100	-3.30504900
H	-0.52352500	2.23567000	-3.67695400
H	0.95245600	2.46687000	-2.75332100
H	0.94083800	1.41928700	-4.17165700
N	-0.49658200	-1.64600800	-0.77766600
N	-2.03994800	0.84239700	-1.81408400
H	-2.21636800	1.67822600	-2.33304200
H	-2.76333900	0.18821600	-2.03736800
H	-2.11470500	1.06687500	-0.83697100
Au	0.85000600	0.64231100	1.35641300
C	2.93336100	0.21739400	1.13318800
H	3.42930500	0.33796300	2.09436900
H	3.16223200	-0.80380400	0.81289700
H	3.44984600	0.89232900	0.44590400
N	2.02326600	-0.34049100	-2.15401200
H	2.24831900	-1.27586100	-2.42888700
H	2.53509100	0.27970400	-2.74852700
H	2.35470800	-0.20251100	-1.21298700
C	-1.23955200	1.06831400	1.60757600
H	-1.93798600	0.28215100	1.29656200
H	-1.45934000	1.24211500	2.65904900
H	-1.53569700	1.98352900	1.08745800
Pd	-0.04202200	0.15674100	-2.10260000

Model 3 (SCS-MP2/def2-TZVP optimization)

H	0.67620000	-2.52670000	-1.04830000
H	0.17960000	-1.43550000	0.07700000
H	-0.91550000	-2.35440000	-0.75380000
C	0.11500000	1.82150000	-2.91060000
H	-0.86300000	2.28650000	-3.05260000
H	0.72400000	2.47840000	-2.28310000
H	0.58420000	1.68900000	-3.88990000
N	-0.04350000	-1.83920000	-0.84100000
N	-2.00320000	0.40600000	-1.70070000
H	-2.45510000	0.96880000	-2.41560000
H	-2.56320000	-0.43380000	-1.58180000
H	-2.03700000	0.92760000	-0.82100000
Au	0.70270000	0.71090000	1.05200000
C	2.50420000	-0.34180000	1.09010000
H	2.74670000	-0.59070000	2.13070000
H	2.53470000	-1.30200000	0.54860000
H	3.36360000	0.24400000	0.72710000
N	2.04500000	0.02330000	-2.11460000
H	2.45420000	-0.85240000	-2.42990000
H	2.44430000	0.76580000	-2.68270000
H	2.33580000	0.17500000	-1.14290000
C	-1.06390000	1.79280000	1.12830000
H	-1.96790000	1.16450000	1.18990000
H	-1.09530000	2.42570000	2.02380000
H	-1.18680000	2.47820000	0.27510000
Pd	-0.00120000	0.08130000	-1.99450000

Model 3 (SCS-MP2-ZORA/SARC-TZVP optimization)

H	0.66230000	-2.54980000	-1.06210000
H	0.13980000	-1.50810000	0.08990000
H	-0.93130000	-2.38220000	-0.80720000
C	0.11340000	1.83180000	-2.90690000
H	-0.86690000	2.28940000	-3.04870000
H	0.71830000	2.48630000	-2.27550000
H	0.58250000	1.69920000	-3.88490000
N	-0.05780000	-1.86420000	-0.85090000
N	-2.01750000	0.40330000	-1.69490000
H	-2.47260000	0.96110000	-2.41100000
H	-2.58020000	-0.43310000	-1.56930000
H	-2.05410000	0.93000000	-0.82050000
Au	0.71140000	0.72020000	1.02970000
C	2.52000000	-0.33060000	1.09260000
H	2.75310000	-0.55900000	2.13900000
H	2.54760000	-1.29840000	0.56560000
H	3.37690000	0.25230000	0.72040000
N	2.06060000	0.02670000	-2.10840000
H	2.47570000	-0.84970000	-2.41240000
H	2.46970000	0.76300000	-2.67670000
H	2.34490000	0.18590000	-1.13750000
C	-1.05780000	1.80830000	1.12180000
H	-1.95790000	1.17520000	1.18500000
H	-1.07830000	2.43230000	2.02280000
H	-1.18600000	2.49690000	0.27280000
Pd	-0.00100000	0.07590000	-1.99290000

Model 3 (PBE0-D3(BJ)/def2-TZVP optimization)

H	0.11861800	-2.48105100	-0.97107800
H	-0.03819900	-1.25625200	0.13813400
H	-1.36491300	-1.93330400	-0.56915800
C	0.27550700	1.77178500	-3.13502300
H	-0.63675600	2.24579000	-3.50962400
H	0.81011700	2.49307300	-2.50909000
H	0.89100200	1.50986900	-4.00144900
N	-0.40866700	-1.64661300	-0.74245700
N	-2.06197300	0.70111900	-1.83214400
H	-2.28562200	1.50732100	-2.40358000
H	-2.73972400	-0.02407600	-2.03545200
H	-2.15026800	0.97098700	-0.85008000
Au	0.88235400	0.61456400	1.15489200
C	2.90452200	0.04985800	1.07618500
H	3.29981100	0.10991000	2.09666300
H	3.10163100	-0.98076800	0.74581100
H	3.54395200	0.70995500	0.47223200
N	1.95044700	-0.19363600	-2.01385000
H	2.25441300	-1.11925500	-2.29246300
H	2.45580500	0.48300500	-2.57398500
H	2.19998900	-0.04532800	-1.02534000
C	-1.12874600	1.18955800	1.31280200
H	-1.84811700	0.38712900	1.07889500
H	-1.37509000	1.50907700	2.33149700
H	-1.35115800	2.05123200	0.66499400
Pd	-0.08422400	0.13870700	-2.02753000

Model 3 (M06L/def2-TZVP optimization)

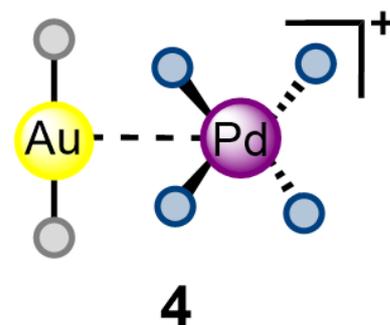
H	-0.03090600	-2.56710200	-0.97007400
H	-0.05884700	-1.35740500	0.15366500
H	-1.44688000	-1.93003100	-0.49391600
C	0.28348000	1.82669500	-3.05847400
H	-0.62380300	2.34352500	-3.37533500
H	0.86110500	2.48707700	-2.40856900
H	0.86544300	1.57473400	-3.94679700
N	-0.48611000	-1.69869300	-0.71637000
N	-2.14164400	0.72284500	-1.86413700
H	-2.36261400	1.51913300	-2.44953000
H	-2.81303800	-0.00509000	-2.07399400
H	-2.26479900	1.00466600	-0.89019000
Au	0.95439600	0.62631800	1.12492500
C	3.01600900	0.10989600	1.08951300
H	3.40991800	0.20840700	2.10377600
H	3.23643900	-0.92151200	0.78716000
H	3.64005600	0.76111900	0.46555100
N	1.96175200	-0.22815600	-1.99623200
H	2.24524800	-1.17332000	-2.22372000
H	2.48871700	0.39880700	-2.59202100
H	2.22682200	-0.03901200	-1.02057100
C	-1.10649400	1.15170900	1.21675300
H	-1.78718300	0.32997000	0.94749500
H	-1.41183400	1.46499100	2.21842500
H	-1.32558200	2.00145500	0.55607500
Pd	-0.11494100	0.15163200	-2.00360600

Model 3 (M06-2x/def2-TZVP optimization)

H	0.72978200	-1.79265600	-0.22167100
H	-0.85063000	-1.63174100	-0.01039700
H	-0.30671300	-2.69154900	-1.15077000
C	0.11322000	1.84409600	-3.02872600
H	-0.85618900	2.29636700	-3.23996000
H	0.70035100	2.53967700	-2.42540100
H	0.62165300	1.64881700	-3.97525200
N	-0.15160400	-1.78021400	-0.73324600
N	-2.13410500	0.51790400	-1.72510600
H	-2.55424300	1.08938800	-2.44904500
H	-2.70110300	-0.31575900	-1.61881700
H	-2.16644200	1.03824900	-0.84603700
Au	0.81153700	0.65636700	1.10960400
C	2.66405300	-0.38826200	1.08735900
H	2.92739200	-0.64949200	2.11618100
H	2.70463600	-1.33900300	0.53194400
H	3.50419700	0.21267500	0.71464600
N	2.08356500	0.00964400	-2.09567600
H	2.45809000	-0.88751300	-2.38427300
H	2.50554900	0.72594200	-2.67665800
H	2.36492600	0.17102800	-1.12334200
C	-1.03324700	1.67597200	1.16219900
H	-1.90356600	1.00294600	1.17192900
H	-1.12473700	2.28091600	2.06839800
H	-1.14651600	2.37397200	0.32097700
Pd	-0.04514500	0.15488400	-1.99905700

Model 4 (MP2/def2-TZVP optimization)

H	2.24085500	-1.49177400	-1.89225700
H	1.22139800	-1.69952900	-0.62487500
H	0.92567000	-2.42771500	-2.09156900
N	1.25709600	-1.57458000	-1.64374300
N	-1.48005000	-0.96706000	-1.33347600
H	-2.38581100	-0.58808200	-1.60206800
H	-1.49692700	-1.94416200	-1.62060600
H	-1.41117800	-0.94793500	-0.30609800
Au	0.61191400	0.61052600	0.91484600
C	-0.13713500	-1.22661600	1.49069400
H	-1.22480400	-1.21734100	1.65982500
H	0.06239200	-2.12593100	0.88546900
H	0.28861400	-1.46139300	2.47185200
C	1.39695200	2.48728100	0.55570300
H	0.96702600	3.13185500	-0.22823400
H	1.28668900	3.07074700	1.47573300
H	2.48160600	2.47442700	0.36844900
N	1.80001300	1.19336000	-2.27480300
H	2.05823800	1.53392400	-1.33785200
H	2.59592000	0.69349200	-2.66575700
N	-0.92683000	1.81250000	-1.90141000
H	-1.93248500	1.70559100	-1.78468700
H	-0.58116200	2.27944100	-1.05441100
H	-0.80179200	2.43793700	-2.69603100
H	1.66992900	2.00866300	-2.87130300
Pd	0.14227600	0.09373600	-1.91028000



Model 4 (RHF/def2-TZVP optimization)

H	2.25860800	-1.58195300	-2.01941800
H	1.31180100	-1.82411600	-0.73688300
H	0.94669500	-2.49050300	-2.17361100
N	1.30224800	-1.66353200	-1.73166800
N	-1.56159500	-1.04138800	-1.40218000
H	-2.44858700	-0.62432200	-1.61004600
H	-1.60121300	-1.97145500	-1.77450300
H	-1.49280200	-1.12107600	-0.39835200
Au	0.63587900	0.63640800	1.06058700
C	-0.17015000	-1.27445400	1.59156200
H	-1.25666900	-1.26406700	1.70910400
H	0.06020600	-2.14528800	0.96733900
H	0.21707800	-1.52964200	2.57390500
C	1.45707900	2.56394800	0.62100100
H	0.99351000	3.17858200	-0.15899800
H	1.38297300	3.16312700	1.52408300
H	2.52449600	2.53258600	0.38844100
N	1.85216900	1.23623200	-2.38465900
H	2.09668900	1.66012100	-1.50188900
H	2.65178400	0.72317700	-2.70293000
N	-1.00145900	1.86959400	-1.99370100
H	-1.99351800	1.74879300	-1.92086100
H	-0.70817100	2.36285200	-1.16535600
H	-0.85005900	2.47230800	-2.78073700
H	1.72002800	1.97761000	-3.04656200
Pd	0.13492100	0.08603300	-1.95584300

Model 4 (SCS-MP2/def2-TZVP optimization)

H	2.26260000	-1.48990000	-1.88860000
H	1.23180000	-1.74470000	-0.64330000
H	0.95600000	-2.42840000	-2.13140000
N	1.27580000	-1.58550000	-1.65590000
N	-1.48670000	-0.98030000	-1.33420000
H	-2.39110000	-0.60870000	-1.61900000
H	-1.49400000	-1.95930000	-1.61640000
H	-1.43940000	-0.95980000	-0.30700000
Au	0.61320000	0.61490000	0.95130000
C	-0.16070000	-1.23100000	1.52370000
H	-1.25170000	-1.21650000	1.67830000
H	0.04270000	-2.12730000	0.91230000
H	0.25230000	-1.47460000	2.50910000
C	1.41970000	2.49670000	0.57700000
H	0.98530000	3.13720000	-0.21030000
H	1.32250000	3.08980000	1.49320000
H	2.50330000	2.47230000	0.37800000
N	1.80850000	1.20880000	-2.29650000
H	2.08460000	1.56210000	-1.37120000
H	2.60100000	0.70820000	-2.69420000
N	-0.94290000	1.81890000	-1.90550000
H	-1.94650000	1.70410000	-1.77550000
H	-0.59760000	2.30920000	-1.07290000
H	-0.83390000	2.43240000	-2.71210000
H	1.66730000	2.01760000	-2.89980000
Pd	0.14620000	0.09520000	-1.90590000

Model 4 (SCS-MP2-ZORA/SARC-TZVP optimization)

H	2.26900000	-1.50520000	-1.90780000
H	1.26270000	-1.75500000	-0.64430000
H	0.95620000	-2.43670000	-2.12340000
N	1.28690000	-1.59430000	-1.65570000
N	-1.50860000	-0.96800000	-1.32650000
H	-2.39920000	-0.66000000	-1.71160000
H	-1.46940000	-1.97000000	-1.50230000
H	-1.53460000	-0.85290000	-0.30760000
Au	0.60500000	0.60890000	0.92600000
C	-0.14670000	-1.24460000	1.52560000
H	-1.22740000	-1.21220000	1.73050000
H	0.01290000	-2.13170000	0.88960000
H	0.31990000	-1.49640000	2.48310000
C	1.40200000	2.50730000	0.57780000
H	1.00140000	3.13010000	-0.23980000
H	1.25050000	3.10170000	1.48430000
H	2.49220000	2.48050000	0.42900000
N	1.83370000	1.20000000	-2.29570000
H	2.18400000	1.46110000	-1.36800000
H	2.57740000	0.72100000	-2.79930000
N	-0.95270000	1.82980000	-1.90620000
H	-1.95790000	1.71360000	-1.79680000
H	-0.62640000	2.32240000	-1.06930000
H	-0.83150000	2.44460000	-2.70940000
H	1.68020000	2.06950000	-2.80250000
Pd	0.14860000	0.09800000	-1.89670000

Model 4 (PBE0-D3(BJ)/def2-TZVP optimization)

H	2.21232500	-1.58376300	-2.00666600
H	1.25939100	-1.68930200	-0.66455900
H	0.85902800	-2.48596900	-2.06755900
N	1.24966900	-1.62850000	-1.68874900
N	-1.52314200	-0.98534500	-1.36868500
H	-2.41692300	-0.52742500	-1.51400400
H	-1.61302500	-1.91766500	-1.76075500
H	-1.36519000	-1.06454300	-0.35457400
Au	0.60725800	0.60693200	0.89151100
C	-0.12024600	-1.28275700	1.45982000
H	-1.21351100	-1.31344600	1.58960400
H	0.14133400	-2.18697200	0.88516800
H	0.27679800	-1.47691600	2.46135600
C	1.36689400	2.53256300	0.51771900
H	0.88712700	3.19896900	-0.21858300
H	1.29315800	3.08005300	1.46283700
H	2.44207100	2.54430500	0.27935500
N	1.82949000	1.19623200	-2.32069500
H	1.99006500	1.62923900	-1.40061500
H	2.65870900	0.66666800	-2.56888000
N	-0.93402300	1.84731500	-1.95718100
H	-1.94320800	1.75200600	-1.91006800
H	-0.61667600	2.26040100	-1.07304700
H	-0.73886500	2.49457900	-2.71503200
H	1.73953400	1.92920300	-3.01760900
Pd	0.13389800	0.08371200	-1.96228400

Model 4 (M06L/def2-TZVP optimization)

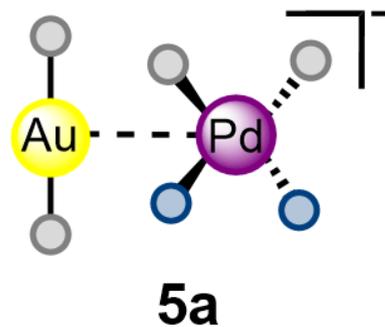
H	2.20953000	-1.64781100	-2.10302000
H	1.23221300	-1.74024500	-0.77957100
H	0.86028900	-2.55069000	-2.17912500
N	1.24167400	-1.68848900	-1.80400000
N	-1.58056700	-1.02079900	-1.48852100
H	-2.47730100	-0.59426800	-1.69274500
H	-1.63869800	-1.97675500	-1.82310800
H	-1.45573000	-1.04408600	-0.46930200
Au	0.58897500	0.58475400	0.78006700
C	-0.13527000	-1.34143300	1.33124300
H	-1.22568400	-1.37918700	1.45783400
H	0.12050100	-2.22805900	0.73170800
H	0.25996300	-1.56395200	2.32389700
C	1.33778500	2.54018200	0.38436000
H	0.85153400	3.18615600	-0.36232500
H	1.26733400	3.10561400	1.31519600
H	2.40728000	2.55970500	0.13484300
N	1.84402300	1.18725500	-2.45651000
H	2.03688700	1.57270700	-1.52412600
H	2.65815200	0.66620400	-2.76219100
N	-0.96407200	1.86539300	-2.08037000
H	-1.97145400	1.78069800	-2.00414000
H	-0.61897800	2.27381700	-1.20483400
H	-0.78556200	2.51453600	-2.83955000
H	1.74181400	1.96004300	-3.10580000
Pd	0.11047000	0.05849600	-2.10379000

Model 4 (M06-2x/def2-TZVP optimization)

H	2.13649900	-1.73772200	-2.30853400
H	1.44923400	-1.64084600	-0.80213400
H	0.76949900	-2.55948000	-1.98574800
N	1.25380500	-1.68337000	-1.80817800
N	-1.58834200	-1.00825300	-1.48270000
H	-2.47491100	-0.52568700	-1.59882500
H	-1.70885600	-1.92848300	-1.89765000
H	-1.42842900	-1.12538300	-0.47390600
Au	0.59613100	0.58982200	0.81907100
C	-0.11020600	-1.33819800	1.33656500
H	-1.18077700	-1.33699700	1.58190000
H	0.04160900	-2.18729000	0.65149100
H	0.38549700	-1.64158500	2.26168500
C	1.31797700	2.53443600	0.39482500
H	0.90686800	3.10566100	-0.45253400
H	1.12561100	3.16369000	1.26698500
H	2.40921800	2.55522700	0.27186500
N	1.85356400	1.17957300	-2.45635300
H	2.00584100	1.65714600	-1.55885100
H	2.68773900	0.63555300	-2.65775200
N	-0.98060100	1.86208900	-2.07983100
H	-1.97522800	1.79369500	-2.27610500
H	-0.85763700	2.17198300	-1.10985900
H	-0.62001600	2.59914700	-2.68018800
H	1.78838900	1.88209100	-3.18834400
Pd	0.11263300	0.06296300	-2.09077500

Model **5a** (MP2/def2-TZVP optimization)

Au	2.70697200	1.06312900	1.35636900
C	-1.33842700	1.93984700	-3.24759700
H	-1.29474000	2.97002400	-2.87146100
H	-0.84585200	1.91216600	-4.22678000
H	-2.38979000	1.67574700	-3.39442400
N	0.66547400	2.36059100	-1.06795500
H	0.00195000	2.99560900	-0.63439600
H	1.33719200	2.08142000	-0.34198600
H	1.18530800	2.89646900	-1.75677200
C	1.53945300	-0.12671500	2.56956500
H	0.46573600	0.07527200	2.45677700
H	1.68311100	-1.19877500	2.37784100
H	1.77622800	0.03417600	3.62932600
C	3.88984500	2.25463600	0.15979300
H	4.93650500	2.23365200	0.49010100
H	3.88907100	1.93551500	-0.89118200
H	3.58063800	3.30865000	0.17220300
Pd	-0.39558900	0.72492500	-2.00405500
N	0.60578700	-0.68592000	-0.70622600
H	1.24078000	-0.26431000	-0.01687800
H	-0.06766800	-1.23853000	-0.18378700
H	1.15515700	-1.33339000	-1.26341500
C	-1.42733800	-0.70524300	-2.89931100
H	-2.44263800	-0.73445100	-2.48638700
H	-1.51004800	-0.56484500	-3.98103200
H	-0.95543400	-1.67922500	-2.71677700



Model **5a** (RHF/def2-TZVP optimization)

Au	2.90304000	1.00623000	1.61315100
C	-1.23145100	2.05933600	-3.57262100
H	-2.30319100	1.95769300	-3.72290400
H	-1.03556300	3.10201200	-3.30929300
H	-0.75312200	1.87491400	-4.53521200
N	0.84503400	2.36360800	-1.34659800
H	0.27934400	3.07252000	-0.92508400
H	1.53470600	2.09019600	-0.67013300
H	1.32483800	2.78725200	-2.11461700
C	1.84683800	-0.51295300	2.69058800
H	0.77326300	-0.32400000	2.76607700
H	1.96189000	-1.50821500	2.25501000
H	2.21810200	-0.58061800	3.71443300
C	3.97775100	2.52677300	0.55612700
H	4.95254900	2.69354400	1.01724500
H	4.17267200	2.27312300	-0.48868600
H	3.46786400	3.49296500	0.55612000
Pd	-0.50961500	0.75503200	-2.15171400
N	0.26067300	-0.69713900	-0.61266000
H	0.84505000	-0.32992700	0.11649500
H	-0.52175400	-1.14311500	-0.17854600
H	0.78278500	-1.40922200	-1.08231000
C	-1.76162700	-0.69456100	-2.90827500
H	-2.77731400	-0.54977200	-2.53839500
H	-1.81042300	-0.67531600	-3.99399600
H	-1.45065500	-1.69994000	-2.61264500

Model **5a** (SCS-MP2/def2-TZVP optimization)

Au	1.39100000	1.34410000	1.14280000
H	-1.24860000	-1.51770000	-1.51830000
H	-1.07780000	-0.49510000	-0.23600000
H	-2.15550000	-0.13140000	-1.43640000
C	1.50330000	-1.17980000	-1.98490000
H	1.02090000	-2.07370000	-1.55960000
H	1.81750000	-1.44540000	-3.00780000
H	2.41160000	-1.01250000	-1.38920000
N	-1.24770000	-0.54110000	-1.24240000
C	-0.84160000	2.24950000	-2.05440000
H	-0.39760000	3.02600000	-1.41660000
H	-0.89400000	2.64700000	-3.08140000
H	-1.88170000	2.12590000	-1.71310000
N	1.94720000	1.62830000	-2.39830000
H	1.75360000	2.50920000	-2.86460000
H	2.29840000	1.83880000	-1.45900000
H	2.66920000	1.12800000	-2.90740000
C	0.14870000	-0.18040000	1.81090000
H	-0.92170000	0.07660000	1.73200000
H	0.31060000	-1.12190000	1.26310000
H	0.31530000	-0.41440000	2.87230000
C	2.64260000	2.91200000	0.57700000
H	2.97930000	3.46130000	1.46780000
H	3.56740000	2.60980000	0.05740000
H	2.14290000	3.65420000	-0.06550000
Pd	0.30550000	0.51960000	-1.98470000

Model **5a** (SCS-MP2-ZORA/SARC-TZVP optimization)

Au	2.75250000	1.06710000	1.40700000
C	-1.37500000	1.96180000	-3.28910000
H	-1.32250000	2.99340000	-2.91580000
H	-0.89850000	1.93480000	-4.27640000
H	-2.43060000	1.70530000	-3.42000000
N	0.65420000	2.37720000	-1.08720000
H	-0.00330000	3.01570000	-0.64900000
H	1.32280000	2.10140000	-0.36090000
H	1.17940000	2.91980000	-1.76680000
C	1.56740000	-0.13290000	2.62900000
H	0.49320000	0.07040000	2.51300000
H	1.71250000	-1.20530000	2.43330000
H	1.80510000	0.02790000	3.68950000
C	3.94810000	2.27070000	0.19830000
H	4.99380000	2.25090000	0.53440000
H	3.94940000	1.95010000	-0.85320000
H	3.63390000	3.32450000	0.21040000
Pd	-0.41730000	0.72130000	-2.03780000
N	0.59830000	-0.70490000	-0.72270000
H	1.23160000	-0.28600000	-0.03430000
H	-0.06720000	-1.26250000	-0.19500000
H	1.15420000	-1.35500000	-1.27070000
C	-1.46590000	-0.73560000	-2.93170000
H	-2.48430000	-0.76340000	-2.52580000
H	-1.54130000	-0.60480000	-4.01540000
H	-0.99900000	-1.71130000	-2.74160000

Model **5a** (PBE0-D3(BJ)/def2-TZVP optimization)

Au	2.95919700	1.03297400	1.69142500
C	-0.99700300	2.07179800	-3.08946200
H	-2.08791200	2.09088800	-2.98345000
H	-0.62578200	3.09773000	-2.95024900
H	-0.76988800	1.76823500	-4.11823100
N	1.04195200	2.38033100	-0.90310800
H	0.42724700	3.08115600	-0.50705000
H	1.69406500	2.08865800	-0.16674300
H	1.58876500	2.83087900	-1.62691100
C	1.78116500	-0.23790200	2.87309700
H	0.70967300	0.00129400	2.82344900
H	1.88537100	-1.29797100	2.60188400
H	2.07056800	-0.15555200	3.92937300
C	4.16601500	2.30566000	0.54112800
H	5.18800600	2.33040700	0.94259700
H	4.24993100	1.98509800	-0.50674100
H	3.80893800	3.34514100	0.53015300
Pd	-0.16393400	0.78844600	-1.76492000
N	0.69628600	-0.64939600	-0.37007100
H	1.32415800	-0.24869200	0.33550400
H	-0.03917500	-1.13783800	0.12621600
H	1.22453500	-1.34191400	-0.88698100
C	-1.29728400	-0.68618700	-2.56653300
H	-1.98592700	-1.07282300	-1.80145300
H	-1.89566900	-0.37579600	-3.42812700
H	-0.65184500	-1.51683600	-2.88692100

Model **5a** (M06L/def2-TZVP optimization)

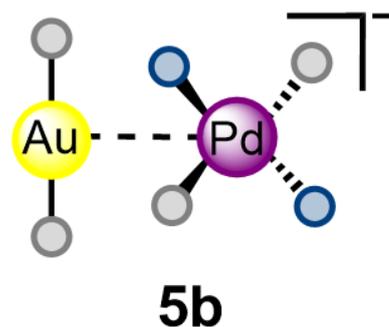
Au	3.00027700	1.03035300	1.73307600
C	-0.97788100	2.06447700	-3.20768300
H	-2.06084200	2.16361500	-3.09195200
H	-0.53143800	3.06160900	-3.11572400
H	-0.78677500	1.69781700	-4.22004400
N	1.11247700	2.39095500	-0.95449400
H	0.55515000	3.17733600	-0.64496700
H	1.68883700	2.10197500	-0.15789500
H	1.75600600	2.75047600	-1.64890500
C	1.88398300	-0.37866600	2.86687200
H	0.81160800	-0.15046800	2.89410200
H	1.97615700	-1.40547000	2.49240700
H	2.22032400	-0.39978900	3.90891900
C	4.14035000	2.44066100	0.62488600
H	5.14103500	2.56056300	1.05344300
H	4.28679900	2.14340400	-0.42056200
H	3.69123500	3.44114000	0.60593900
Pd	-0.20852200	0.79114300	-1.81187200
N	0.61298000	-0.65036900	-0.29166900
H	1.33199500	-0.26618800	0.32936500
H	-0.11552800	-1.00709200	0.31474500
H	1.02160700	-1.45376300	-0.75261300
C	-1.39946200	-0.68182300	-2.57154200
H	-2.04204300	-1.06948100	-1.77245100
H	-2.03957500	-0.36947700	-3.39907300
H	-0.76730100	-1.50515000	-2.92443400

Model **5a** (M06-2x/def2-TZVP optimization)

Au	3.05393500	1.02566200	1.74204300
C	-0.95580200	2.01584300	-3.23311100
H	-2.03741100	1.92543600	-3.35766700
H	-0.72447000	3.05917600	-2.98726500
H	-0.48835700	1.78182200	-4.19507800
N	1.15999900	2.38476600	-1.01428000
H	0.60208600	3.11364800	-0.58354000
H	1.84976100	2.08814600	-0.32054000
H	1.66735300	2.81087200	-1.78159600
C	2.02838800	-0.47421300	2.82520500
H	0.95090200	-0.28443000	2.91042800
H	2.14119600	-1.47409200	2.38766500
H	2.41323200	-0.53712700	3.84921100
C	4.10496400	2.52679900	0.68533600
H	5.08951200	2.69373100	1.13641400
H	4.28581500	2.26765100	-0.36557500
H	3.59160000	3.49651500	0.68964200
Pd	-0.23387700	0.77589000	-1.80594500
N	0.55416100	-0.66384700	-0.23618100
H	1.16910300	-0.26673500	0.47734400
H	-0.21957600	-1.10803900	0.24528000
H	1.07699000	-1.39738700	-0.70162000
C	-1.50610800	-0.61873900	-2.53525500
H	-2.51532100	-0.43090400	-2.15452800
H	-1.55499400	-0.61133200	-3.62661500
H	-1.20162900	-1.62132300	-2.21189900

Model **5b** (MP2/def2-TZVP optimization)

Au	1.36690100	1.32384600	1.06154200
H	-1.29712700	-1.44942400	-1.51676500
H	-1.07230600	-0.46293900	-0.21319400
H	-2.14614200	-0.02857300	-1.39692300
C	1.46554200	-1.18390600	-1.92288300
H	0.96055500	-2.05789400	-1.48681000
H	1.77427900	-1.46553000	-2.94111900
H	2.37186100	-1.02454000	-1.32492500
N	-1.25573400	-0.48071800	-1.21835700
C	-0.77835800	2.27386900	-2.04063100
H	-0.28936300	3.05750700	-1.44887800
H	-0.85697000	2.62929000	-3.07934000
H	-1.80488900	2.18921100	-1.65462000
N	1.97015200	1.58849800	-2.35827400
H	1.80501700	2.44785700	-2.87265100
H	2.27815400	1.83635100	-1.41097200
H	2.70455300	1.05447600	-2.81172900
C	0.21710900	-0.25195700	1.72336200
H	-0.86147000	-0.02430000	1.72249700
H	0.37560500	-1.15874300	1.12211900
H	0.45476600	-0.52688300	2.75957000
C	2.53700000	2.94410900	0.52598300
H	2.80762900	3.51046200	1.42675000
H	3.49529900	2.69326200	0.04421900
H	2.02068700	3.65457700	-0.13613400
Pd	0.31611800	0.52930200	-1.94793700



Model **5b** (RHF/def2-TZVP optimization)

Au	1.65971100	1.57708900	1.46779100
H	-1.28121400	-1.77840500	-1.71600800
H	-1.21817000	-0.81428500	-0.40898900
H	-2.26669800	-0.47650000	-1.60412500
C	1.55820900	-1.22792800	-2.21828700
H	1.09835000	-2.20804700	-2.06148300
H	2.05161000	-1.27971100	-3.19495700
H	2.34462200	-1.13587300	-1.46837500
N	-1.35639100	-0.83384900	-1.40264700
C	-1.19951200	2.05107700	-2.14225000
H	-1.61731500	2.22472000	-1.14908700
H	-0.78308900	3.00707700	-2.46768600
H	-2.04186000	1.84336600	-2.81230800
N	1.82740500	1.74166400	-2.43716200
H	1.58682000	2.56901700	-2.94120200
H	2.09740500	2.00930000	-1.50580500
H	2.61054200	1.29947900	-2.87134000
C	0.10319500	0.25495900	2.11742000
H	-0.87952700	0.59250200	1.77598200
H	0.25224900	-0.75862300	1.73424900
H	0.04048400	0.16875800	3.20380300
C	3.21458500	2.89701800	0.79499200
H	3.74278400	3.33639500	1.64299300
H	3.97557600	2.39513600	0.19027100
H	2.84148400	3.73705000	0.20179500
Pd	0.19761400	0.42582600	-2.12368700

Model **5b** (SCS-MP2/def2-TZVP optimization)

Au	2.74220000	1.06660000	1.39640000
C	-1.36650000	1.95420000	-3.27530000
H	-1.31340000	2.98820000	-2.90620000
H	-0.88750000	1.92140000	-4.26250000
H	-2.42280000	1.69720000	-3.40860000
N	0.65710000	2.37200000	-1.08570000
H	-0.00640000	3.00900000	-0.65360000
H	1.32650000	2.09670000	-0.35900000
H	1.17830000	2.90850000	-1.77360000
C	1.56230000	-0.13460000	2.61430000
H	0.48700000	0.07090000	2.50620000
H	1.70020000	-1.20830000	2.41830000
H	1.80090000	0.01910000	3.67630000
C	3.93520000	2.26790000	0.19160000
H	4.98200000	2.25270000	0.52710000
H	3.94310000	1.94520000	-0.86010000
H	3.62390000	3.32300000	0.19610000
Pd	-0.41590000	0.72380000	-2.02770000
N	0.59660000	-0.69520000	-0.71870000
H	1.23120000	-0.27740000	-0.02970000
H	-0.07550000	-1.25020000	-0.19610000
H	1.14640000	-1.34300000	-1.27610000
C	-1.45140000	-0.72630000	-2.92060000
H	-2.47240000	-0.75260000	-2.51800000
H	-1.52440000	-0.59560000	-4.00560000
H	-0.98510000	-1.70270000	-2.72740000

Model **5b** (SCS-MP2-ZORA/SARC-TZVP optimization)

Au	1.54590000	1.49040000	1.16540000
H	-1.24700000	-1.68830000	-1.65700000
H	-1.16870000	-0.72290000	-0.32790000
H	-2.22030000	-0.35620000	-1.54030000
C	1.51430000	-1.20120000	-2.03970000
H	1.03430000	-2.15870000	-1.78360000
H	1.96190000	-1.33730000	-3.03660000
H	2.33170000	-1.06290000	-1.32010000
N	-1.29700000	-0.72580000	-1.34010000
C	-1.00910000	2.12840000	-2.01240000
H	-0.70550000	2.82410000	-1.21980000
H	-0.94950000	2.66330000	-2.97310000
H	-2.07620000	1.90960000	-1.84970000
N	1.83740000	1.66370000	-2.28350000
H	1.62690000	2.56510000	-2.70030000
H	2.14700000	1.83340000	-1.31970000
H	2.60920000	1.24060000	-2.78920000
C	0.12340000	0.08480000	1.74320000
H	-0.89140000	0.41350000	1.46770000
H	0.31170000	-0.88840000	1.26490000
H	0.10750000	-0.09490000	2.82750000
C	2.97020000	2.92650000	0.64440000
H	3.40760000	3.35780000	1.55540000
H	3.81630000	2.53530000	0.05780000
H	2.54890000	3.76920000	0.07490000
Pd	0.22940000	0.44790000	-2.00430000

Model **5b** (PBE0-D3(BJ)/def2-TZVP optimization)

Au	1.55798700	1.49507600	1.14295200
H	-1.11550000	-1.75859600	-1.58423900
H	-1.14216900	-0.72436600	-0.29159100
H	-2.17950400	-0.48052700	-1.55886500
C	1.58911000	-1.15723300	-2.02783900
H	1.11540200	-2.15157700	-1.99837300
H	2.20732300	-1.13893000	-2.93894400
H	2.26116700	-1.09506600	-1.16258700
N	-1.25293500	-0.79640900	-1.30342000
C	-1.10788000	2.07888000	-1.97115000
H	-0.91388100	2.70861800	-1.09365300
H	-0.99110200	2.70485800	-2.86955100
H	-2.17080900	1.79106800	-1.93388700
N	1.77928500	1.74694100	-2.29599900
H	1.50520200	2.60743300	-2.75244000
H	2.06100800	1.96111500	-1.33040500
H	2.56570200	1.33203200	-2.77901100
C	0.01580700	0.19935100	1.72392400
H	-0.95357900	0.56220800	1.34867300
H	0.19017600	-0.81152800	1.32402700
H	-0.08988000	0.09188200	2.81174800
C	3.11346200	2.80211600	0.59270200
H	3.59720500	3.18776100	1.50028900
H	3.91123100	2.32725900	0.00137400
H	2.77873500	3.68555900	0.02782900
Pd	0.22730500	0.44928400	-1.97766300

Model **5b** (M06L/def2-TZVP optimization)

Au	1.53064000	1.49252600	1.13864400
H	-1.27277300	-1.70472100	-1.68132100
H	-1.23814600	-0.74486000	-0.34203700
H	-2.24614000	-0.37234200	-1.59350900
C	1.57826800	-1.21653900	-1.99057400
H	1.07488100	-2.17457700	-1.80262900
H	2.10039900	-1.31538600	-2.95160300
H	2.33454600	-1.09620800	-1.20680100
N	-1.33788200	-0.74916200	-1.35709800
C	-1.06422100	2.13734200	-1.95049200
H	-0.56803500	3.10101500	-2.11795600
H	-1.84665600	2.03982000	-2.71581600
H	-1.55571300	2.20621400	-0.97264800
N	1.92039500	1.71883900	-2.26682500
H	1.71185000	2.58900600	-2.73840600
H	2.18355800	1.93644800	-1.29930100
H	2.70726600	1.27246100	-2.71928200
C	0.02704700	0.06504300	1.60576600
H	-0.95885000	0.42948500	1.28429800
H	0.23224000	-0.88054400	1.08516300
H	-0.06359900	-0.17614900	2.67059200
C	3.03719400	2.93065800	0.67675100
H	3.43751900	3.36452500	1.59909100
H	3.90223300	2.52127200	0.13775200
H	2.66824900	3.77603300	0.08049400
Pd	0.26459800	0.46701300	-1.96835600

Model **5b** (M06-2x/def2-TZVP optimization)

Au	3.05393500	1.02566200	1.74204300
C	-0.95580200	2.01584300	-3.23311100
H	-2.03741100	1.92543600	-3.35766700
H	-0.72447000	3.05917600	-2.98726500
H	-0.48835700	1.78182200	-4.19507800
N	1.15999900	2.38476600	-1.01428000
H	0.60208600	3.11364800	-0.58354000
H	1.84976100	2.08814600	-0.32054000
H	1.66735300	2.81087200	-1.78159600
C	2.02838800	-0.47421300	2.82520500
H	0.95090200	-0.28443000	2.91042800
H	2.14119600	-1.47409200	2.38766500
H	2.41323200	-0.53712700	3.84921100
C	4.10496400	2.52679900	0.68533600
H	5.08951200	2.69373100	1.13641400
H	4.28581500	2.26765100	-0.36557500
H	3.59160000	3.49651500	0.68964200
Pd	-0.23387700	0.77589000	-1.80594500
N	0.55416100	-0.66384700	-0.23618100
H	1.16910300	-0.26673500	0.47734400
H	-0.21957600	-1.10803900	0.24528000
H	1.07699000	-1.39738700	-0.70162000
C	-1.50610800	-0.61873900	-2.53525500
H	-2.51532100	-0.43090400	-2.15452800
H	-1.55499400	-0.61133200	-3.62661500
H	-1.20162900	-1.62132300	-2.21189900