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Supporting Information

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Additional Computational Details

Natural Orbitals for Chemical Valence and Charge Displacement analysis.

Natural Orbitals for Chemical Valence (NOCVs)^{1,2} analysis can be especially useful for a description of the bonding in transition metal complexes, since they allow for separation of the deformation density contributions originating from donation (ligand-to-metal) and back-donation (metal-to-ligand) electron-transfer processes.

When a chemical bond occurs generating an adduct, an electron density difference between the formed adduct (AB) and the sum of the densities of the two non-interacting fragments (A and B) frozen in the geometry they have in the adduct is obtained. In the NOCV scheme, this density rearrangement is defined from the occupied orbitals of A and B suitably orthogonalized to each other and renormalized. The resulting electron density rearrangement ($\Delta\rho$) can be expressed in terms of NOCV pairs, as shown in Equation (1).

$$\Delta\rho = \sum_k v_k (|\phi_k|^2 - |\phi_{-k}|^2) = \sum_k \Delta\rho_k \quad (1)$$

The NOCV pairs orbitals, $\phi_{\pm k}$, and the associated $v_{\pm k}$ values are, respectively, the eigenfunctions and the eigenvalues of the “valence operator” (defined in Equation (2)) that comes from the valence theory of Nalewajski and Mrozek.²⁹

$$\hat{V} = \sum_i (|\psi_i^{(AB)}\rangle\langle\psi_i^{(AB)}| - |\psi_i^0\rangle\langle\psi_i^0|) \quad (2)$$

where $\psi_i^{(AB)}$ represent occupied orbitals of the AB molecule, and the set of spin-orbitals ψ_i^0 is the reference density, obtained from the occupied orbitals of A and B suitably orthogonalized to each other and renormalized. In other words, rather than two separate A and B wavefunctions (two separate A and B determinants), their antisymmetrized product is taken as reference (the so called “promolecule”).

On a physical view of the NOCVs it is possible to say that when the adduct AB forms from the promolecule, a fraction v_k of electrons moves from the ϕ_{-k} orbital to the ϕ_{+k} one, where k ranges from 1 to the total number of occupied orbitals. The advantage of calculating the NOCVs is that usually only a small subset of these NOCV pairs contributes to the overall charge rearrangement $\Delta\rho$, because a large part of them presents values of v_k close to zero.

When the NOCV scheme is coupled with the framework of the Charge Displacement³ (CD) analysis (CD-NOCV), it becomes possible to quantify the amount of electronic charge that is transferred between the two fragments upon the formation of the bond. In this scheme, each $\Delta\rho_k$ of Eq. (1) represents a different bond component and can be integrated, using the CD equation (Equation (3)), in order to obtain

the Charge Transfer (CT) associated to σ donation, π back-donation and, in general, to each bond component coming out from the analysis.

As said above, only few of the NOCV pairs contributes to the chemical bond, allowing to investigate only the first $\Delta\rho_k$ components in order to understand which significant chemical contribution to the bond they represent.

The Charge Displacement (CD) function, $\Delta q(z)$ (Equation (3)), is defined as a practical progressive integration on the electron density rearrangement:

$$\Delta q(z) = \int_{-\infty}^z dz' \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Delta\rho(x, y, z') dx dy \quad (3)$$

The integration of the difference between the electron density of the adduct and that of its non-interacting fragments, frozen in the same position they have in the adduct, $\Delta\rho$, is performed along a suitable z axis. The chosen z axis is commonly the bond axis between the fragments. At a given z point, the CD function quantifies the amount of electron charge that is transferred. This flux of charge is called “Charge Transfer” (CT): it is greater than zero (positive) from the right to the left (the direction in which z decreases), while negative CT values identify the donation of charge in the opposite direction. A numerical value of CT can be estimated by considering the CD function value at a specific point between the fragments on the z axis. More specifically, the CT is often calculated at the “isodensity boundary”, i.e. the point, in the space, where equal-valued isodensity surfaces of the isolated and non-interacting fragments become tangent.

Energy Decomposition Analysis.

The EDA⁴ is a powerful method for a quantitative interpretation of chemical bonds. It allows to partition the fragments interaction energy (known as instantaneous interaction, ΔE_{int}) into four components, as shown in Equation (4).

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} \quad (4)$$

The first term, ΔE_{elstat} , corresponds to the classical electrostatic interaction between the charge distribution of the non-perturbed fragments as they are brought together at their final positions. ΔE_{Pauli} represents the repulsive exchange interactions between occupied orbitals and is responsible for any steric repulsion between fragments. It is also possible to consider a unique term for the sum of the electrostatic interaction and the Pauli repulsion, which is the total steric interaction ΔE_{st} ($\Delta E_{\text{st}} = \Delta E_{\text{Pauli}} + \Delta E_{\text{elstat}}$). The orbital interaction energy contribution, ΔE_{oi} , comes from the orbital relaxation and orbital mixing between the fragments. It accounts for the electron pair bonding, charge transfer (for example from HOMO to LUMO) and polarization, i.e. for what can be associated with “covalency” in chemical bonds.

Finally, the ΔE_{disp} term accounts for the attractive dispersion interaction between fragments. This partition allows to identify the amount of each of these contributions to the interaction energy in the adducts.

Using a combined Extended Transition State ETS-NOCV¹ approach, it is possible to decompose the orbital interaction energy ΔE_{oi} into components corresponding to each NOCV, associating an energy contribution k (ΔE_{oi}^k) to each NOCV deformation density ($\Delta \rho_k$), as follows:

$$\Delta E_{\text{oi}} = \sum_k \Delta E_{\text{oi}}^k \quad (5)$$

This method allows to separate contributions arising from σ and π bonding components to the interaction energy. The result is that a quantitative energy contribution can be associated to each NOCV and, if the NOCVs have been assigned to specific types of interaction, the relative energy contributions of these interactions can be quantified.

Table S1. Energy Decomposition Analysis (EDA) of the interaction energy between [LAu] (L= PMe₃, PPh₃, PF₃, PMe₂[−], experimental ligand **1'**, **CH₂_PP**, NMe₂[−], and **NONAl**[−]) and [H] fragments in the [LAuH] complexes with two possible fragmentations of the LAu-H bond, i.e. closed shell fragments [LAu]^{+0...}[H][−] dative bond, (reported in DAT columns) or open shell fragments ([LAu]^{•0/...}[H][•] covalent bond (listed in the COV columns).

Energies are given in kcal/mol.

	[Me ₃ PAuH]		[Ph ₃ PAuH]		[F ₃ P-AuH]		[Me ₂ PAuH] [−]		1'		[CH ₂ _PPAuH]		[NONAl-AuH] [−]	
	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV
ΔE_{Pauli}	233.4	74.2	237.3	76.5	233.2	73.7	230.2	79.1	241.2	80.0	238.6	78.0	223.6	72.6
ΔE_{Elstat}	-344.3	-86.4	-332.8	-84.7	-379.0	-85.4	-234.8	-84.9	-311.9	-85.4	-336.2	-84.9	-244.8	-78.0
ΔE_{oi}	-94.8	-77.2	-102.0	-79.4	-101.7	-77.7	-79.8	-79.1	-101.7	-80.1	-104.6	-79.2	-80.4	-75.6
ΔE_{Disp}	-0.6	-0.6	-0.7	-0.7	-0.6	-0.6	-0.6	-0.6	-0.9	-0.9	-0.8	-0.8	-0.6	-0.6
ΔE_{Int}	-206.3	-90.0	-198.3	-88.3	-248.1	-90.0	-85.0	-85.6	-173.3	-86.5	-203.0	-86.9	-82.2	-81.7

Table S2. Energy Decomposition Analysis (EDA) of the interaction energy between [LAu] (L= **NHC**, **O_NHC**[−], **Me₃B_NHC**[−], **H₃B_NHC**[−], **F₃B_NHC**[−], and **ox_NHC**) and [H] fragments in the [LAuH] complexes with two possible fragmentations of the LAu-H bond, i.e. closed shell fragments [LAu]^{+0...}[H][−] dative bond, (reported in DAT columns) or open shell fragments ([LAu]^{•0/...}[H][•] covalent bond (listed in the COV columns).

Energies are given in kcal/mol.

	[NHCAuH]	[O_NHCAuH] [−]	[Me ₃ B_NHCAuH] [−]	[H ₃ B_NHCAuH] [−]	[F ₃ B_NHCAuH] [−]	[ox_NHCAuH]

	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV
ΔE_{Pauli}	230.2	71.1	226.7	70.0	227.1	69.7	226.6	69.7	227.0	69.8	231.6	80.3
ΔE_{Elstat}	-342.3	-89.8	-261.6	-89.3	-271.9	-89.5	-271.4	-89.5	-279.6	-89.7	-359.4	-72.2
ΔE_{oi}	-90.7	-76.2	-83.5	-75.7	-86.0	-75.3	-83.9	-75.3	-83.7	-75.3	-98.2	-92.7
ΔE_{Disp}	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6
ΔE_{Int}	-203.5	-95.6	-119.0	-95.6	-131.5	-95.7	-129.4	-95.7	-136.9	-95.8	-226.6	-85.2

Table S3. Energy Decomposition Analysis (EDA) of the interaction energy between [LAu] (L= **4H_NHC**, **H_H_NHC**, CN₂Me₄, NMe₂⁻, CO, Cl⁻, and CN⁻) and [H] fragments in the [LAuH] complexes with two possible fragmentations of the LAu-H bond, i.e. closed shell fragments [LAu]^{+0...}[H]⁻ dative bond, (reported in DAT columns) or open shell fragments ([LAu]^{0/-...}[H][•] covalent bond (listed in the COV columns).

Energies are given in kcal/mol.

	[4H_NHCAuH]		[H_H_NHCAuH] ⁻		[CN ₂ Me ₄ AuH]		[NMe ₂ AuH] ⁻		[COAuH]		[ClAuH] ⁻		[CNAuH] ⁻	
	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV
ΔE _{Pauli}	232.2	72.0	230.7	71.4	236.0	74.0	236.9	79.5	230.9	70.8	234.2	77.2	221.5	67.4
ΔE _{Elstat}	-342.2	-89.7	-346.5	-90.2	-338.2	-90.1	-257.7	-93.6	-386.4	-89.5	-238.6	-95.5	-271.7	-91.1
ΔE _{oi}	-91.2	-76.8	-90.4	-76.6	-94.0	-77.5	-84.0	-79.8	-99.4	-77.2	-78.2	-75.6	-74.9	-74.8
ΔE _{Disp}	-0.6	-0.6	-0.6	-0.6	-0.7	-0.7	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6
ΔE _{Int}	-201.8	-95.2	-206.8	-95.9	-196.9	-94.2	-105.4	-94.4	-255.5	-96.3	-128.1	-94.8	-125.7	-99.1

Table S4. Energy Decomposition Analysis (EDA) of the interaction energy between [L] (L= **NONAI**⁻, CO, CN⁻, **1'**, **4H_NHC**, and PF₃) and [AuH] fragments in the [LAuH] complexes with two possible fragmentations of the L-AuH bond, i.e. closed shell fragments [L]^{0/+...}[AuH]^{0/-} dative bond, (reported in DAT columns) or open shell fragments ([L]^{0/-...}[AuH][•] covalent bond (listed in the COV columns).

Energies are given in kcal/mol.

	[NONAI AuH] ⁻		[COAuH]		[CNAuH] ⁻		1'		[4H_NHCAuH]		[F ₃ PAuH]	
	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV	DAT	COV
ΔE _{Pauli}	233.7	197.3	160.4	147.5	176.2	163.3	188.6	399.5	187.7	271.4	140.1	209.8
ΔE _{Elstat}	-237.3	-203.2	-124.5	-233.3	-185.9	-140.8	-171.1	-275.1	-184.0	-276.2	-109.2	-273.7
ΔE _{oi}	-68.7	-81.5	-69.9	-258.4	-64.7	-164.6	-66.9	-287.8	-57.4	-210.8	-60.7	-221.3
ΔE _{Disp}	-6.0	-6.0	-1.8	-1.8	-2.0	-2.0	-13.1	-13.1	-6.2	-6.2	-3.5	-3.5
ΔE _{Int}	-78.3	-93.4	-35.8	-346.0	-76.4	-144.2	-62.5	176.4	-59.9	-221.7	-33.3	-288.7

Table S5. Solvent effect (COSMO model) on the activation ($\Delta G^\ddagger$) and reaction (ΔG_{rxn}) Gibbs free energy of the reaction LAuH + CO₂. Free energies are given in kcal/mol.

Hydride ligand	$\Delta G^\ddagger$ (gas)	$\Delta G^\ddagger$ (solvent)	ΔG_{rxn} (gas)	ΔG_{rxn} (solvent)
1'	24.0	22.3	1.3	1.0
[O_NHC]⁻	20.8	22.9	1.0	1.8
[Me₃B_NHC]⁻	23.9	24.3	2.8	3.8
[H₃B_NHC]⁻	24.0	24.0	2.6	3.0
[F₃B_NHC]⁻	24.4	24.9	3.4	3.4
NONaI⁻	3.9	2.6	-7.1	-8.1
NHC	32.3	30.5	11.8	7.5
PMe₂⁻	10.1	11.8	-4.9	-3.0
PF₃	38.2	35.9	19.3	15.8

Table S6. O-Ĉ-O bond angles (degrees), Au-H and Au-O bond distances (Angstrom) in the transition states for the [LAuH(CO₂)]^{0/-} hydrides.

Hydride ligand	OĈO angle (degrees)	d _{Au—H} (Å)	d _{Au—O} (Å)	d _{H—C} (Å)
CN ⁻	135.0	1.909	2.527	1.241
[O_NHC] ⁻	134.3	1.940	2.535	1.230
[Me ₃ B_NHC] ⁻	134.8	1.917	2.518	1.214
[H ₃ B_NHC] ⁻	135.1	1.917	2.518	1.241
[F ₃ B_NHC] ⁻	135.6	1.900	2.509	1.250
ox_NHC	142.2	1.786	2.367	1.366
CN ₂ Me ₄	137.7	1.864	2.416	1.285
4H_NHC	137.8	1.859	2.415	1.289
NHC	137.4	1.871	2.417	1.282
H_H_NHC	137.7	1.863	2.409	1.288
PMe ₂ ⁻	134.0	1.979	2.657	1.220
1'	133.4	2.014	2.505	1.215
PMe ₃	137.9	1.881	2.418	1.292
PPh ₃	137.6	1.884	2.422	1.288
CH ₂ _PP	137.3	1.893	2.401	1.283
PF ₃	140.5	1.842	2.331	1.347
NONaI ⁻	136.0	1.936	2.858	1.246
NMe ₂ ⁻	133.0	1.969	2.568	1.211
Cl ⁻	133.4	1.933	2.525	1.224
CO	141.2	1.820	2.312	1.359

Table S7. Atomic Charges (e) for the Au and H atoms in the [LAuH] hydrides computed with various methods. The correlation factors (R^2) with the corresponding activation barriers are reported, as well.

Hydride ligand	Voronoi		Hirshfeld		Mulliken	
	H (e)	Au (e)	H (e)	Au (e)	H (e)	Au (e)
CN ⁻	-0.30	0.15	-0.25	-0.17	-0.47	0.04
[O_NHC] ⁻	-0.30	0.16	-0.25	-0.14	-0.46	0.05
[Me ₃ B_NHC] ⁻	-0.28	0.16	-0.24	-0.11	-0.43	0.08
[H ₃ B_NHC] ⁻	-0.29	0.16	-0.24	-0.12	-0.44	0.08
[F ₃ B_NHC] ⁻	-0.28	0.16	-0.23	-0.11	-0.43	0.08
ox_NHC	-0.18	0.19	-0.17	-0.03	-0.32	0.16
CN ₂ Me ₄	-0.23	0.14	-0.19	-0.04	-0.35	0.10
4H_NHC	-0.22	0.15	-0.19	-0.06	-0.35	0.12
NHC	-0.23	0.15	-0.19	-0.07	-0.36	0.10
H_H_NHC	-0.22	0.15	-0.19	-0.11	-0.35	0.13
PMe ₂ ⁻	-0.33	0.11	-0.27	-0.22	-0.46	-0.07
1'	-0.23	0.08	-0.19	0.00	-0.34	-0.07
PMe ₃	-0.19	0.09	-0.17	-0.07	-0.31	0.02
PPh ₃	-0.19	0.08	-0.17	-0.03	-0.31	0.05
CH ₂ _PP	-0.17	0.07	-0.15	0.00	-0.30	0.09
PF ₃	0.13	0.11	-0.13	0.02	-0.27	0.05
NONaI ⁻	-0.32	0.13	-0.29	-0.26	-0.48	-0.14
NMe ₂ ⁻	-0.32	0.07	-0.24	-0.20	-0.44	0.06
Cl ⁻	-0.28	0.05	-0.21	-0.25	-0.41	0.07
CO	-0.14	0.22	-0.14	0.07	-0.28	0.25
R ²	0.505	0.00	0.838	0.588	0.737	0.502

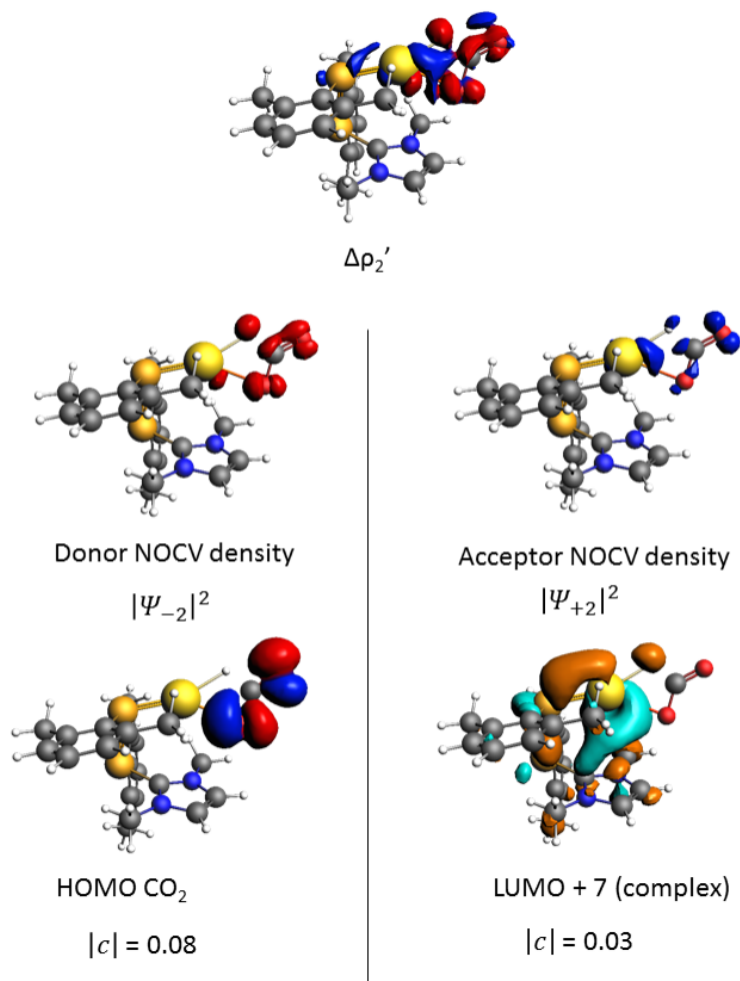


Figure S1. Breakdown of the donor ($|\Psi_{-2}|^2$) and acceptor ($|\Psi_{+2}|^2$) NOCV densities associated with the NOCV deformation density $\Delta\rho_2$ in the transition state TS involving the **1'** complex into the most important MOs of the **1'** and CO₂ fragments frozen at their TS geometry. The molecular orbitals mixing coefficients (c) are given. Isodensity values are 0.001 e au⁻³ for $\Delta\rho_2$, 0.002 e au⁻³ for NOCV densities and 0.03 e au⁻³ for MOs.

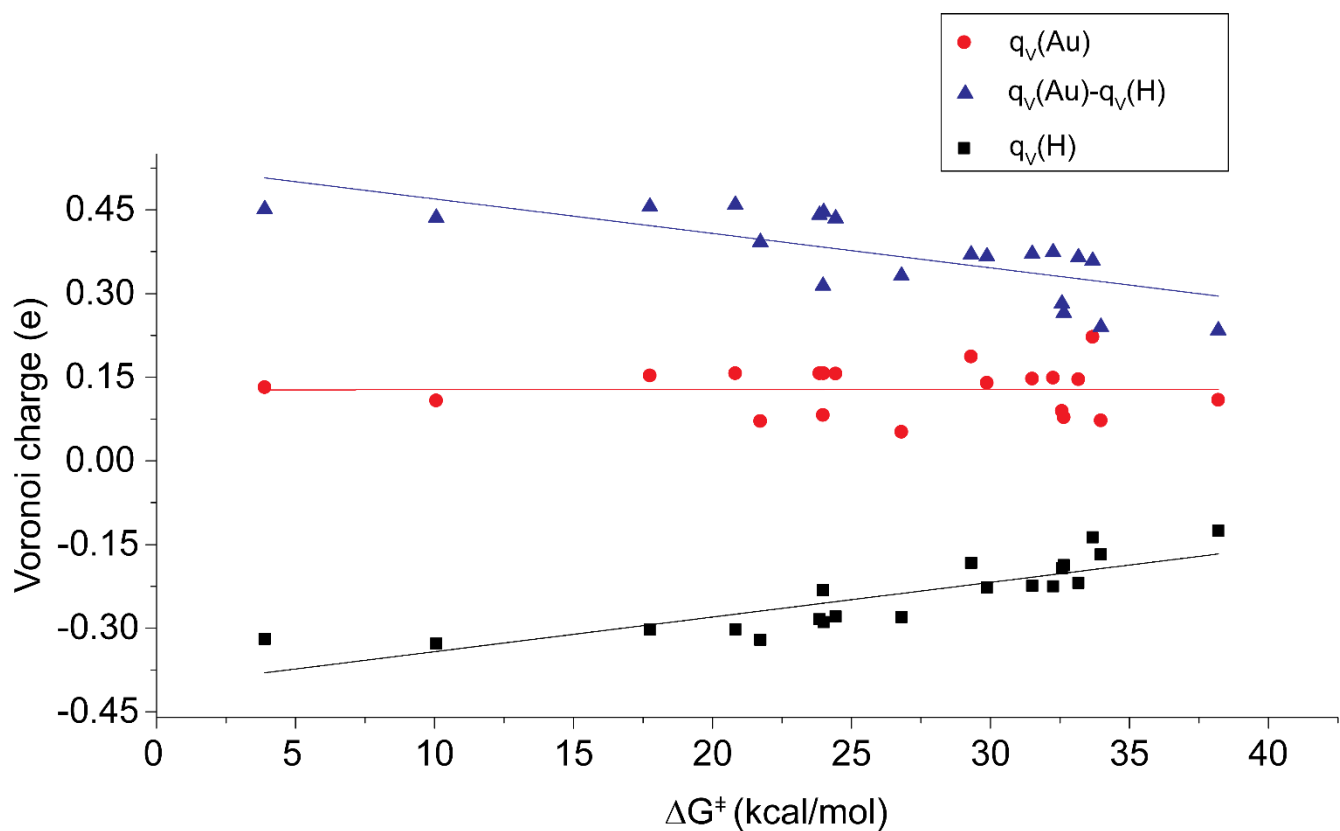


Figure S2. Correlation between the Voronoi atomic charges on Au and H and $\Delta G^\ddagger$. The correlation factors r^2 are 0.6994, 0.055 and 0.4951 for the hydrogen charge $q_v(\text{H})$, gold charge $q_v(\text{Au})$ and the Au-H polarization $q_v(\text{Au})-q_v(\text{H})$, respectively.

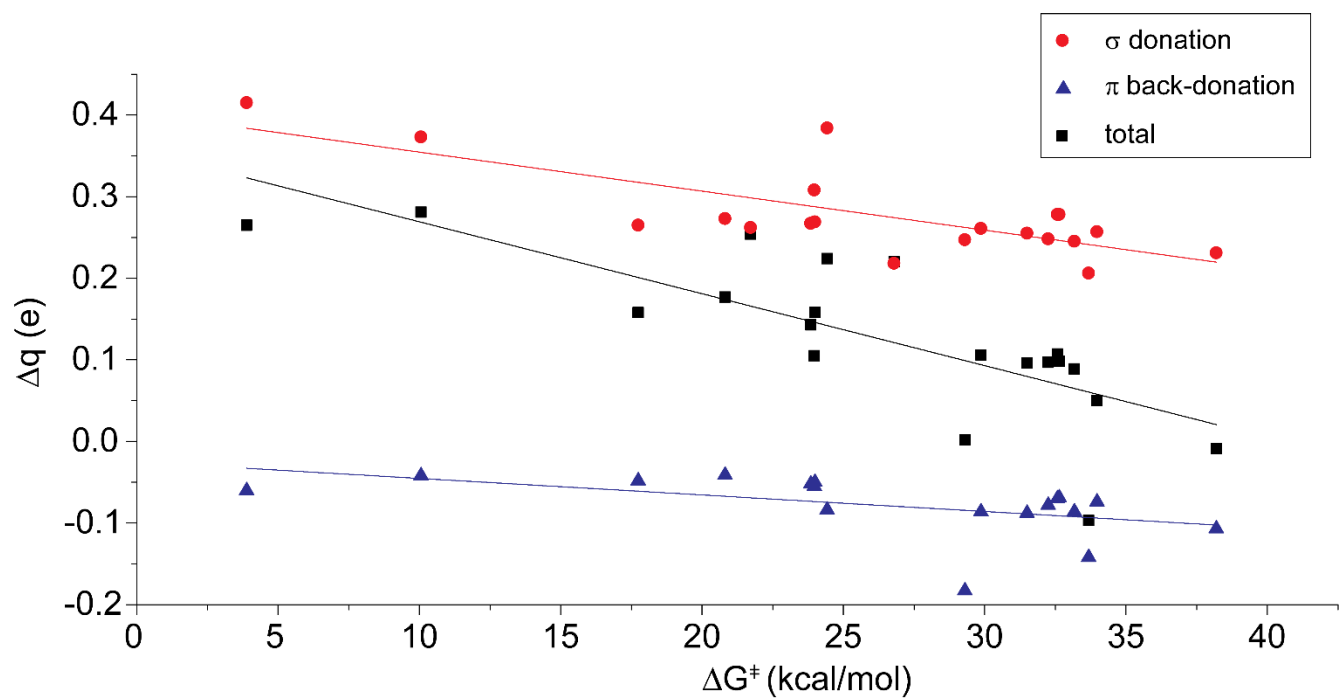


Figure S3. Correlation between the L-AuH bond components and $\Delta G^\ddagger$. The correlation factors r^2 are 0.5405, 0.2032 and 0.5812 for σ donation, π back-donation and the sum of all the components (total), respectively.

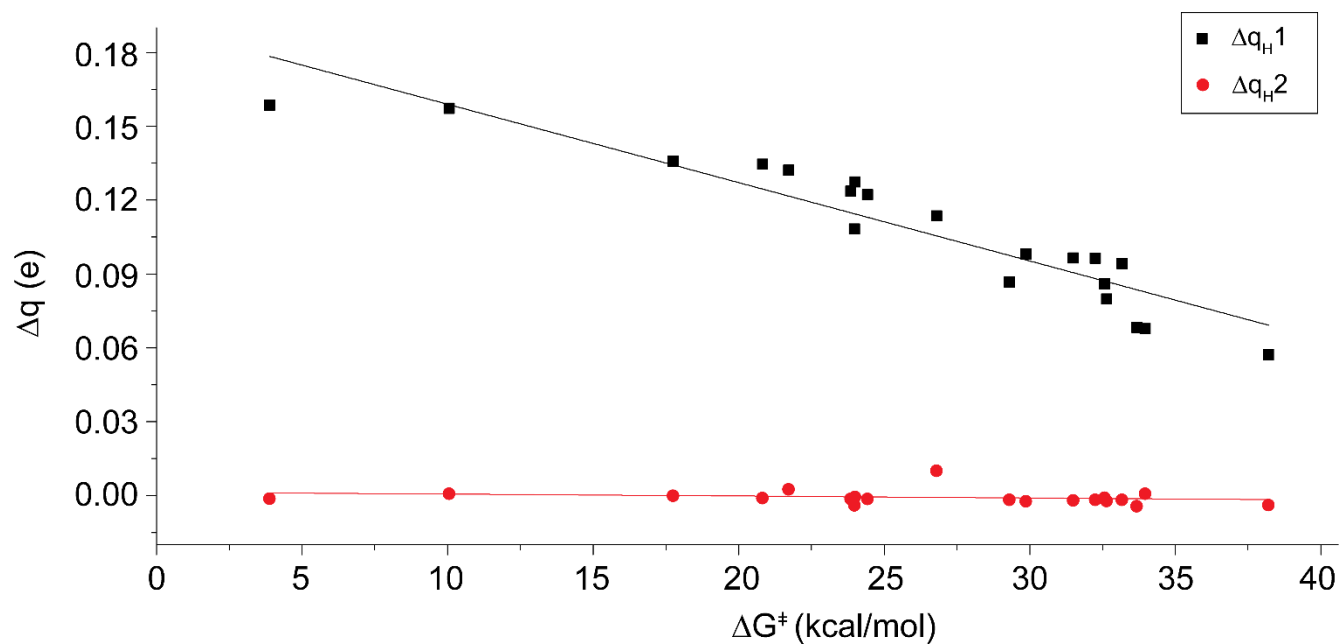


Figure S4. Correlation between Δq_{H1} and Δq_{H2} and $\Delta G^\ddagger$. The correlation factors r^2 are 0.8766 and 0.005 for Δq_{H1} and Δq_{H2} , respectively.

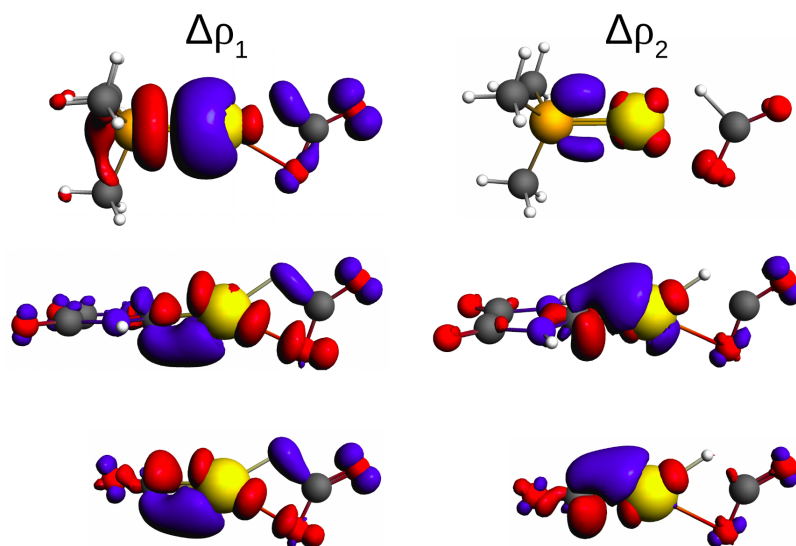


Figure S5. Comparison between NOCV deformation maps (3 me a.u.^{-3}) for three different ligands: PMe_3 (top) that is well described by the correlation in Figure S4, ox_NHC (middle) which shows a negative deviation, and CO (bottom) showing the same negative deviation as ox_NHC .

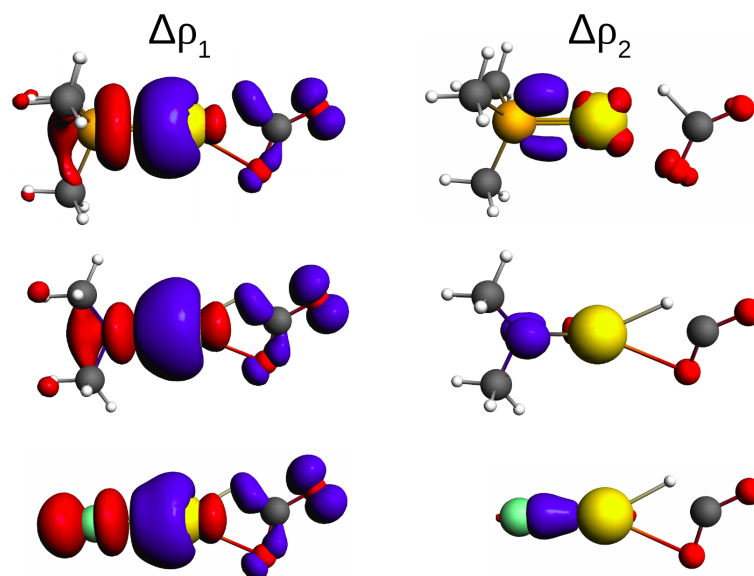


Figure S6. Comparison between NOCV deformation maps (3 me a.u.^{-3}) for three different ligands: PMe_3 (top) that is well described by the correlation in Figure S4, NMe_2^- (middle) which shows a positive deviation, and Cl^- (bottom) showing the same positive deviation as NMe_2^- .

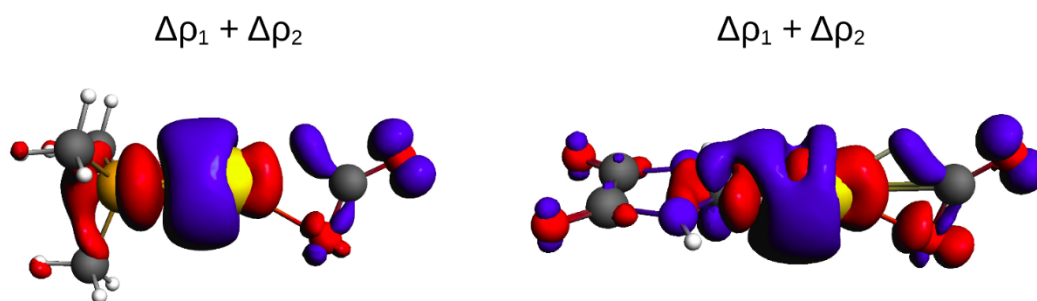


Figure S7. Similarities between the sum of the first two NOCV ($\Delta\rho_1 + \Delta\rho_2$) for the TS of $(\text{PMe}_3)\text{AuH} + \text{CO}_2$ (left) and of $(\text{ox_NHC})\text{AuH} + \text{CO}_2$.

Table S8. Eigenvalues ($|v_k|$) associated to the first four NOCV deformation densities ($k=1-4$) in terms of the [L]-[AuHCO₂] interaction (L=hydride ligand) in the transition states for the [LAuH] complexes reacting with CO₂.

Hydride ligand	$ v_1 $	$ v_2 $	$ v_3 $	$ v_4 $
CN ⁻	0.75	0.28	0.25	0.21
[O_NHC] ⁻	0.76	0.32	0.24	0.17
[Me ₃ B_NHC] ⁻	0.73	0.32	0.24	0.18
[H ₃ B_NHC] ⁻	0.74	0.32	0.23	0.17
[F ₃ B_NHC] ⁻	0.73	0.35	0.23	0.16
ox_NHC	0.84	0.62	0.20	0.17
CN ₂ Me ₄	0.72	0.51	0.23	0.15
4H_NHC	0.69	0.47	0.23	0.16
NHC	0.68	0.44	0.23	0.18
H_H_NHC	0.68	0.47	0.22	0.18
PMe ₂ ⁻	0.90	0.24	0.23	0.20
1'	0.88	0.33	0.25	0.20
PMe ₃	0.70	0.34	0.25	0.21
PPh ₃	0.72	0.34	0.25	0.23
CH ₂ _PP	0.71	0.39	0.26	0.23
PF ₃	0.61	0.45	0.31	0.21
NONaI ⁻	0.97	0.28	0.19	0.17
NMe ₂ ⁻	0.92	0.28	0.25	0.14
Cl ⁻	0.73	0.19	0.15	0.14
CO	0.64	0.52	0.39	0.23

Table S9. EDA components, in kcal/mol of the [L]-[AuH] interaction (L = hydride ligand). The correlation factors (R^2) with the corresponding activation barriers are reported, as well.

Hydride ligand	Pauli	electrostatic	orbital	dispersion
CN ⁻	176.2	-185.9	-64.7	-2.0
[O_NHC] ⁻	207.9	-217.2	-62.2	-6.1
[Me ₃ B_NHC] ⁻	203.3	-210.0	-60.2	-6.3
[H ₃ B_NHC] ⁻	204.2	-211.9	-60.5	-6.1
[F ₃ B_NHC] ⁻	267.9	-278.3	-90.9	-6.8
ox_NHC	187.8	-175.7	-61.9	-4.2
CN ₂ Me ₄	193.7	-190	-58.6	-6.7
4H_NHC	187.7	-184	-57.4	-6.2
NHC	186.8	-183.4	-57.2	-6.1
H_H_NHC	182.4	-179.7	-55.1	-4.1
PMe ₂ ⁻	213.5	-224.3	-63.3	-4.7
1'	188.6	-171.1	-66.9	-13.1
PMe ₃	165	-153.6	-55.2	-6
PPh ₃	156.3	-139.7	-57	-9.8
CH ₂ _PP	141	-118.8	-56.8	-11.6
PF ₃	140.1	-109.2	-60.7	-3.5
NONaI ⁻	233.7	-237.3	-68.7	-6
NMe ₂ ⁻	132.8	-145.6	-57.2	-4.1
Cl ⁻	90.6	-99	-44.1	-1.8
CO	160.4	-124.5	-69.9	-1.8
R^2	0.227	0.372	0.086	0.00

DFT optimized geometries (xyz format, in Å)

3

CO₂

C	-0.00000000363078	0.00000000394876	-0.00000000002205
O	0.00000000181539	-0.00000000197438	1.17140601721511
O	0.00000000181539	-0.00000000197438	-1.17140601719305

Hydrides

15

[Me₃PAuH]

C	2.395737	1.379531	-1.728214
P	1.253457	-0.053855	-1.682416
C	0.576548	-0.101728	-3.385630
Au	-0.320557	0.004784	0.011582
C	2.390213	-1.491934	-1.645964
H	3.122998	1.293562	-2.548511
H	1.811267	2.300327	-1.852636
H	2.929804	1.443801	-0.771359
H	3.115510	-1.454653	-2.471593
H	2.926412	-1.502382	-0.688242
H	1.802939	-2.416606	-1.716431
H	1.377856	-0.122564	-4.138273
H	-0.053720	-0.993418	-3.497598
H	-0.054099	0.782068	-3.547046
H	-1.419015	0.043576	1.199490

36

[Ph₃PAuH]

C	-2.43267452166297	0.17116406139112	-3.49470396613363
C	-1.23156790595365	0.64878415119803	-2.95340211692513
C	-0.79391525719968	1.94508515495625	-3.26717481828314
C	-1.54182532218518	2.74584091981819	-4.12954948953831
C	-2.73697270049378	2.26433076514042	-4.67269105390632
C	-3.18252782222911	0.98013166925017	-4.35126589909020
P	-0.17782092640498	-0.35886691051507	-1.85752633245757
C	0.99914521595582	-1.17135111445540	-2.98934210530153
C	0.78391832047062	-1.26166601565882	-4.37101211334810
C	1.71301651736595	-1.91934402307039	-5.18024934080553
C	2.85609571677795	-2.49002332194594	-4.61544286564884
C	3.07639199848678	-2.39647397734551	-3.23787688774583
C	2.15599187773351	-1.73367444995705	-2.42691520928279
Au	0.83160088206738	0.81025538724806	-0.13178151542998
H	3.97407458616536	-2.83053776640572	-2.79565479897393
H	3.58181599336269	-3.00034084983861	-5.25023241759367
H	1.54394368437740	-1.98304408897078	-6.25616673358954
H	-0.10578182454192	-0.81142996221318	-4.81300148983645
H	-1.19735316793533	3.75265377163282	-4.36924920532478
H	-3.32599338985845	2.89500454666215	-5.34003569628159
H	-4.11917968732228	0.60592752776261	-4.76711234200426

H	0.12942092483572	2.32216751177893	-2.82238282034974
H	1.54117381392577	1.61932779330383	1.07610699082686
H	-2.78276579732139	-0.83001215326591	-3.24069085258044
H	2.33176063733715	-1.63631356466955	-1.35355089234187
C	-1.27144536835881	-1.71014875330854	-1.30439517432293
C	-2.06908904321572	-1.47896289788141	-0.17255553793236
C	-2.95008366383837	-2.46300171974209	0.27431306083481
C	-3.03001435016065	-3.68783162349164	-0.39538109362857
C	-2.22681573788598	-3.92668209016032	-1.51295640828759
C	-1.34924253531994	-2.94093763359939	-1.96985091395587
H	-3.56753852433745	-2.27855511659192	1.15437849402803
H	-3.71288079550434	-4.46054306454265	-0.03947762087369
H	-2.28082375635073	-4.88522499059507	-2.03118600195887
H	-0.71843763883645	-3.12817721235614	-2.83958949812158
H	-1.98418043194492	-0.52826995956145	0.35791466616504

6

[F₃PAuH]

Au	-0.159283	-0.120744	-0.061268
H	-1.742640	-0.117230	0.243383
P	2.058284	-0.120971	-0.509737
F	2.509284	-0.286769	-2.009241
F	2.958957	-1.229313	0.153573
F	2.899218	1.154417	-0.128410

11

[Me₂PAuH]⁻

P	1.42716987331240	0.68739727026538	-0.83557898168215
Au	-0.77066694304320	0.35832397513503	0.01594685879257
C	2.26963009337474	-0.98142252588920	-0.57691167482288
H	1.80841561969436	-1.71990140501813	-1.24963189717061
H	2.17090942347178	-1.35498836775819	0.45546435647451
H	3.34407379405009	-0.91875062282126	-0.82506914587800
C	2.31592624478071	1.59784861063051	0.55854375900442
H	1.88665316391274	2.60656892003556	0.65320105327338
H	3.39182266342631	1.70503473267344	0.33276633611769
H	2.21226520660138	1.09314353384621	1.53314891698501
H	-2.31662913958132	0.15214587890064	0.55919041890606

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1'

Au	5.63771085368128	6.75692985614596	17.35501632677537
P	3.32614136880500	6.65598577061777	16.93136143634363
P	2.84251233653903	5.19092726964023	15.33839492536429
H	7.22767949263516	6.99489055354066	17.58807491771896
N	5.14687522856120	3.46162403255305	15.85300679474978
N	3.25977839667030	2.77601859124245	16.70039485573309
C	3.81607771367587	3.76258470108173	15.93242589536747
C	4.41099265929780	7.89328898756383	14.17786774715532
C	4.24053636175585	4.78899638990665	19.48628991288141
C	5.41780210341248	2.33001459976594	16.59754389216085
C	3.68695045605663	5.46535794724292	13.71712917649577
C	2.25514813494958	5.73942934457982	18.14451956736911

C	4.31485545579709	6.67010953479089	13.31095948888128
C	4.23739203324093	1.90045400579057	17.13065897544457
C	2.77055761952633	4.97912615389683	19.22949585237583
C	0.84362621479366	5.87845300051073	18.00648427651254
C	6.16411443479858	4.25462220849038	15.17223801052300
H	5.95860087855228	4.30116158663647	14.09782213438671
H	7.13669192292436	3.78887865761455	15.35818528271651
H	6.16339953284625	5.27425224612017	15.60994643268934
C	3.58788777503781	4.38093151596230	12.80084296801971
C	0.49727153655616	4.46768395890270	19.95791634205190
H	-0.17842344519158	3.97435768133578	20.65867480071999
C	1.87700331155959	4.35968641262253	20.11746097654732
H	2.28181076790697	3.77812025217122	20.94881856510570
C	-0.00975339258419	5.22936668032311	18.90750802246393
H	-1.08932410898830	5.34290354200051	18.78735557527719
C	2.85827945759306	3.10004432286814	13.12458200657144
C	4.89258884578542	6.72982013701864	12.03476497725373
H	5.38630109262960	7.65553895621376	11.73326123260045
C	0.22741497209110	6.71383540688139	16.91653624097222
C	4.18502086997279	4.48942175302911	11.53900108317362
H	4.10952175695373	3.64813349645821	10.84681289170098
C	1.83580938629209	2.61905927120966	16.98890334528681
H	1.62990370339445	2.86943991391149	18.03668741530867
H	1.54328170736100	1.58331744926122	16.77549012772892
H	1.28038119487938	3.30914993668031	16.34508450923349
C	4.84990368909341	5.65053021203626	11.15706582611602
H	5.31234527445355	5.72276294174253	10.17166127910628
H	4.01228049233170	1.06021697311335	17.77466764246817
H	6.42200505862899	1.93579794399870	16.68732290165626
H	4.80997287821688	8.73816461931150	13.60224424900968
H	5.08334283369220	7.72454924452969	15.03919618245904
H	3.43932527598432	8.18407358259249	14.59750426726707
H	2.60445003837859	2.56532766677732	12.19986718758683
H	1.92890049389458	3.29633027840617	13.68094948942834
H	3.46463759138014	2.41708532789244	13.74071027933809
H	0.71656911563964	7.69630406931422	16.85026053328183
H	-0.84733274299628	6.85128077425598	17.09578253162531
H	0.35297876823082	6.24181592324102	15.92886066062491
H	4.78163201951301	4.47605410807610	18.58165483100262
H	4.39888912288558	4.03956488608831	20.27432760115560
H	4.72441146090374	5.72576532404166	19.80160755621115

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[CH₂PPAuH]

Au	0.74290157424396	0.24110528702608	-0.42738800581970
P	0.49499038176164	-1.39604256625570	-2.03550064834713
P	2.07659353540390	-2.17323265543207	-3.34729650016169
H	1.90629229718809	-3.15593104515543	-0.97045580206969
H	0.70296352819905	-3.90991406450202	-2.12875073905438
C	-2.07935848942769	-2.44134911424975	-2.08276924750570
C	3.73230507741710	0.02107948211475	-2.65304121988834
C	-1.44579455606250	-1.13704207058991	-4.07324222252417
C	1.29858874360086	-3.03273599601855	-1.86736046319664

C	-1.12184574981048	-1.70155309995174	-2.81882759402751
C	3.54235867270810	-1.37832053208199	-2.55796170365921
C	4.52815646233760	-2.19477596396535	-1.95263419726966
C	-1.79686284021820	-2.94967352949911	-0.69298062851258
C	2.75866752920763	0.91585328751296	-3.36714370301969
C	-0.48524752303334	-0.25669364514796	-4.82359715655778
C	-2.71217943791424	-1.39475068644477	-4.61285920383527
H	-2.96734204490475	-0.97047351296139	-5.58573350877232
C	-3.33411861982285	-2.66776737990392	-2.65992431862034
H	-4.07858789927424	-3.23649778341132	-2.09933772272008
C	4.44079301217466	-3.70115196357179	-1.93838897077744
C	5.80287228315217	-0.19953411240277	-1.39788633328685
H	6.67535715455336	0.26118277328764	-0.93256622591104
C	5.64407047558109	-1.58296061058039	-1.36932177118917
H	6.40357288342131	-2.20981103129528	-0.89721202795856
C	-3.64573746588191	-2.16330756499154	-3.92113965477206
H	-4.62852384808823	-2.35069050651152	-4.35624475868202
C	4.86096693458285	0.59014566277175	-2.05191268087153
H	4.99764543190961	1.67174377609690	-2.10661730444102
H	-1.09860923025670	-3.80018025814048	-0.69731161374255
H	-2.72461153575983	-3.28009693242055	-0.20913667920982
H	-1.34104571811585	-2.16824536779329	-0.06464019822819
H	-0.09964529301918	0.54928706179682	-4.18248667956489
H	-0.97652794241420	0.20188878360847	-5.69074349694958
H	0.38734433922215	-0.82499801191370	-5.17985474114139
H	5.44648740964676	-4.13874788232869	-1.88588101185860
H	3.94509437091718	-4.09561660308271	-2.83696883495917
H	3.87787492575844	-4.07579289007265	-1.06943369204673
H	3.22917209867297	1.87301656405989	-3.62514406488698
H	1.88803017921324	1.13224964028365	-2.72296090493675
H	2.37731391740295	0.45774326337939	-4.29033702157454
H	0.86394497572743	1.36854179873814	0.71894325255095

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[NHCAuH]

N	0.06470756097913	-1.07443486324586	2.89861167675726
C	0.03910863428451	-0.68155268298704	4.22791250123106
C	-0.04410302088312	0.67875952386479	4.22867573996824
N	-0.06699268101421	1.07328709174953	2.89978328708809
C	0.00008094620540	0.00000835785138	2.05642823757339
C	-0.14182359746540	2.45378613261376	2.44073332989087
Au	-0.00027864076718	0.00052710472685	0.00099505047209
C	0.14920563995129	-2.45376695548240	2.43762150316497
H	-0.08826278121001	1.38484170178675	5.04900721657699
H	0.07965514952013	-1.38880416324067	5.04742510399461
H	1.07998524377341	-2.91682760022607	2.79136639378233
H	-0.71141159106388	-3.03029420811371	2.80193233246802
H	0.14171954487782	-2.43371658589861	1.34134899403591
H	0.75124151256934	3.00997233392168	2.75575482121813
H	-0.19293544183890	2.43289682680085	1.34568017827277
H	-1.04010053238486	2.93941866939649	2.84423404664760
H	-0.00230594553346	0.00059931648228	-1.61119041314233

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[O₂NHCAuH]⁻

N	0.07239191956496	-1.12726791215558	2.82642820808697
C	0.01460846314146	-0.77955021686204	4.18189662594336
C	-0.08337511246373	0.62197495401918	4.26750640291758
N	-0.07497192902276	1.01262411518536	2.86972698253726
C	0.01908483037720	-0.04527742989959	2.00899635653754
C	-0.15901520535211	2.39782233040463	2.47670129761891
Au	0.06445911296334	-0.02694751254940	-0.05544943164524
C	0.17813957961946	-2.48292449784962	2.34696441028308
O	-0.16397820039101	1.46092143078642	5.19781413970072
H	0.04569007233491	-1.52397422609585	4.96753407208918
H	1.10119406085586	-2.95888655582886	2.71944232207301
H	-0.68412855076198	-3.08444916135718	2.68146950487378
H	0.19914497259093	-2.45018385655140	1.24903619067656
H	0.67662506562824	2.97015923991279	2.90773823662992
H	-0.12521490234613	2.44685136730771	1.38080337477401
H	-1.09361076212115	2.84686555702888	2.84661232808241
H	0.09064658538250	-0.00997762549544	-1.68360102117908

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[Me₃B₂NHCAuH]⁻

N	0.04162226908588	-1.15310955302997	2.75142054277888
C	-0.01150375128564	-0.73774639617991	4.08055235867904
C	-0.06791878758053	0.63462045444687	4.11863254649931
N	-0.04275703011100	0.98960216698955	2.75394535374506
C	0.02385103494057	-0.08329075550487	1.91031415514830
C	-0.05013369873626	2.35536310777649	2.25613392950101
Au	0.08838424365461	-0.12029485837149	-0.15289695833019
C	0.10127146541307	-2.53086445044447	2.31011403844483
B	-0.17533664131015	1.62475663023524	5.41098004701963
H	-0.01005125690244	-1.44962076610575	4.89757137301033
H	1.00973398208699	-3.02144011058306	2.69219656621403
H	-0.77952953858187	-3.08867848235406	2.66345638204104
H	0.11949153076341	-2.53329601485923	1.21266005639772
H	0.91080902019710	2.84554953232315	2.46149373965784
H	-0.21901305088075	2.31667614982485	1.17264343309925
H	-0.84532762887007	2.92636685839272	2.74886263209486
H	0.13517721972271	-0.15930685744814	-1.77627386781592
C	1.04481453937204	2.73812405482133	5.41776933398159
C	-1.64716351522400	2.37774318450639	5.42551364068869
C	-0.04892997978797	0.68821123523770	6.76183669121705
H	-0.84931595831227	-0.07238178351880	6.84054649168625
H	-0.12212951555289	1.31142779376954	7.67201277840368
H	0.91564008378345	0.14942454332022	6.82582923218782
H	0.97374473133929	3.50109070902145	4.62162130285955
H	2.04495053961118	2.27486026624027	5.32762755773011
H	1.04004987144831	3.29401264559069	6.37408210060650
H	-1.82136047381364	3.06624828104973	4.57764824060359
H	-1.75338058693331	2.98934645572073	6.34126235576510
H	-2.48598911753580	1.65773595913280	5.42356394608498

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[H₃B_NHCAuH]⁻

N	0.07274477034195	-1.14059851957638	2.81055285436078
C	0.01229179530082	-0.76666091636576	4.15391796300446
C	-0.08326053994068	0.60276099277185	4.22788407272805
N	-0.07539503397474	0.99484346364989	2.87489909384865
C	0.01915008643225	-0.04784558526024	1.99891722944906
C	-0.15773153836954	2.38306183875407	2.46269840346341
Au	0.06595793335435	-0.02415943098377	-0.06468186536640
C	0.18063980006391	-2.50024005034436	2.32725864145611
B	-0.17893741581619	1.62616434952608	5.45331849989853
H	0.04280199326374	-1.50113643251597	4.95071412415600
H	1.10342869883573	-2.97285055987551	2.69858945916197
H	-0.68241950353080	-3.09975460688156	2.65650745391654
H	0.20410257612598	-2.46609165276853	1.23032386375745
H	0.68064619987190	2.94758213992966	2.89295063178528
H	-0.12691757039163	2.41830716416479	1.36670017597137
H	-1.08927243695748	2.82780344874496	2.83860063832459
H	0.08987488678524	-0.01339290525118	-1.68952558243313
H	0.76883570862394	2.42191854039901	5.40063616576383
H	-1.22676854638022	2.28130261597620	5.36817706219952
H	-0.15265186363853	1.00101610590676	6.51367111455391

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[F₃B_NHCAuH]⁻

N	0.07203908666990	-1.14095256637985	2.80105294192716
C	0.01074832334559	-0.76337636714705	4.14000157972813
C	-0.08597852083908	0.60020914396204	4.19634705631325
N	-0.07921686299952	0.99744216602549	2.85433244737489
C	0.01671855875569	-0.04837125999593	1.98456944760584
C	-0.16440169150073	2.38865325732770	2.43336925463396
Au	0.06423624172295	-0.03725560604924	-0.07822995505047
C	0.18460166726067	-2.50393442648849	2.32211682973870
B	-0.17463611019348	1.61663056970184	5.47311527800415
H	0.04258872040172	-1.48690847958165	4.94606522133051
H	1.11040901285976	-2.96925662512276	2.69286818438092
H	-0.67557053154749	-3.10376723919358	2.65560715961459
H	0.20535617560882	-2.47293318516773	1.22529136174391
H	0.66969219139751	2.95391534281191	2.86747984105422
H	-0.12318543054243	2.41433967457520	1.33782597242538
H	-1.10276864565352	2.82605182061902	2.79665727839626
H	0.09274067991151	-0.04039196579953	-1.70101522292314
F	0.94424522554102	2.50249178679037	5.45878984501830
F	-1.37187090296885	2.38931232433474	5.39787068409364
F	-0.16862718723004	0.85013163477749	6.66799479458975

11

[ox_NHCAuH]

N	0.06712451687645	-1.13174416110420	2.83615778475671
C	-0.04351613722599	0.70388797425824	4.24840588401512
N	-0.06400870175097	1.05040691308488	2.88906562763806
C	0.00064208475950	-0.02077478091223	2.03980439867810
Au	-0.00152873268311	0.02722793163465	0.02422924302748
H	0.12327148775019	-2.06948857659688	2.44716073677625

H	-0.00334096586138	0.06536474924624	-1.58964609348617
C	0.04973093335362	-0.85149877675762	4.21062213735589
O	0.09573439035200	-1.62615637552041	5.13147877987241
O	-0.08751055160158	1.43307207667034	5.20574258756265
H	-0.12110832396874	2.00585302599697	2.54598891380350

19

[4H_NHCAuH]

N	2.21524862593436	-1.37300266707333	-0.22209165722952
C	3.66739174985640	-1.19363389863082	-0.06856538194409
C	3.79513952303700	0.33589718530950	-0.00835352207976
N	2.40405424106695	0.74958196753768	0.23337518673195
C	1.51962828363621	-0.24678045783127	0.03055567082173
C	2.05658495538048	2.14793200942488	0.36329132017067
Au	-0.53298524825551	-0.07969173906061	0.09770028921790
C	1.63608682920294	-2.69477128038351	-0.32525748677485
H	2.02406907790163	-3.21432094517968	-1.21445192512159
H	1.86712093924118	-3.30110452246490	0.56704132875920
H	0.54834759161087	-2.58273639080623	-0.41031770780077
H	2.33645369681707	2.71241915659242	-0.54236493692713
H	0.97135991350630	2.21639396315793	0.50687440213432
H	2.57153909162336	2.59246781170727	1.22843356568532
H	-2.13992524154518	0.05062937422579	0.15227462125735
H	4.21331094047391	-1.64085558140934	-0.91106354763233
H	4.01087129815859	-1.68105699290811	0.86065089052135
H	4.15602573831102	0.76478822726181	-0.95962976971153
H	4.45780799404239	0.68384478053053	0.79637865992177

11

[H_H_NHCAuH]

N	-0.13500827192440	-1.05469780647734	-2.87540394601197
C	-0.08232072664919	-0.67733991171970	-4.20982133108223
C	0.09582881849403	0.67298809647280	-4.21030169103691
N	0.14292571604094	1.05203322336726	-2.87615157779698
C	0.00208631884324	-0.00078069156829	-2.02189782399261
H	0.26692681165847	1.99852325004684	-2.53591997018631
Au	-0.00086405807014	0.00022058275861	0.02249936615323
H	-0.26074810425693	-2.00070077084195	-2.53449590522332
H	0.19018856085185	1.37476744104168	-5.02903483038397
H	-0.17296471221057	-1.38018988103587	-5.02805560212097
H	-0.00170035277731	0.00076646795596	1.63357331168207

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[CN₂Me₄AuH]

N	0.08703815317166	-1.37168413483292	2.91547410698402
N	0.15950419600461	0.92209157167431	2.59355661405507
C	0.38782043783644	-0.32354289675655	2.11079726976477
C	0.05647885760759	-2.72088888588958	2.35550842850931
H	0.14240902323011	-2.65421825737416	1.26375564851387
H	-0.89107188699380	-3.21466753604876	2.62153974834717
H	0.89166019736737	-3.32212824888194	2.74985357468828
C	0.08919882617835	-1.34528637791143	4.37982513245488
H	0.56753196541998	-0.43027158851496	4.74187381040547

H	0.68052277630436	-2.20332372199892	4.73274621070112
H	-0.91804109912899	-1.42781231855414	4.81768414778828
C	-0.85490725165251	1.27426788553348	3.58968058140275
H	-1.54313359153378	0.43761898423285	3.74234466078601
H	-1.43220346359031	2.12483789742923	3.19749612532687
H	-0.42574735162151	1.57593306202055	4.55800321873955
C	0.71226896215656	2.07687955857829	1.88954703883558
H	1.38879723941744	1.72172851094764	1.10208322075185
H	1.26966824691486	2.71324302205440	2.59449039644678
H	-0.09412116371674	2.67462804014786	1.43469330363397
Au	1.16851156256371	-0.61527126412661	0.19705167667642
H	1.76273536406459	-0.84114330172865	-1.28553491481211

41

[NONAlAuH]⁻

C	-2.14630311111654	-0.53864918210174	-0.29274491611081
C	-3.54971225903732	-0.40162391872115	-0.28405725573137
C	-4.03893400899404	0.87573640212270	-0.10370744713432
C	-3.29691918665291	2.03385483641809	0.21338313345733
C	-1.89026117574350	1.86249970511941	0.16419489620316
C	-1.35010957824429	0.59553951282761	-0.09227019722668
O	-5.43106725046025	1.08103195506422	-0.05329647354518
C	-6.06382739029222	0.10930711894938	0.74533232207338
C	-5.69618350516591	-1.21428661932418	0.61836628990697
C	-4.58713590513555	-1.53266402319036	-0.39950906619020
C	-6.34702580790179	-2.12932495419918	1.47125169566594
C	-7.28358746900646	-1.65085153530035	2.39550814864011
C	-7.57162788125998	-0.28772721422059	2.54280764252898
C	-6.91294963558244	0.66576986715829	1.72597603070978
N	-6.96304184311903	2.02748900872906	1.76668582715814
C	-7.90635731340299	2.64919251879026	2.67364847786039
C	-3.95655185302816	-2.90252958896853	-0.13584529305356
C	-5.19291805037450	-1.51939578338724	-1.82560143103271
Al	-5.96663120702942	3.07544478167878	0.47099577222727
Au	-7.09063104337478	4.98116433328694	-0.52472286327025
H	-7.86184667816339	6.33133869547996	-1.18060008443635
N	-4.02708771832773	3.13713205203193	0.54150042681996
C	-3.32167128226056	4.38304359488982	0.76275931568847
H	-8.26260162186320	0.04347385898416	3.31818267564967
H	-6.11427020834100	-3.19257870303314	1.42883048342621
H	-1.68336192867012	-1.51447975361567	-0.43405407636171
H	-1.23134757018782	2.70483421962851	0.37548015778690
H	-3.17173781818147	-3.11103242184815	-0.87655175089677
H	-4.71178169322955	-3.69632906322775	-0.22305665539482
H	-3.51173641976629	-2.95222686555287	0.86747582497041
H	-4.40906353130987	-1.71682889178584	-2.57228846190244
H	-5.64563607087209	-0.54534048404979	-2.04960752213200
H	-5.97194956257135	-2.29163013582738	-1.91320921762393
H	-7.63151863785856	2.50620862621719	3.73768527083104
H	-7.93166630696292	3.72893966669589	2.46248503588307
H	-8.93290832939507	2.25810288809718	2.54002048807924
H	-4.06292188044400	5.19280482179783	0.84090246759384
H	-2.71643784906599	4.37074386194983	1.69106180953258

H	-2.64171462313582	4.63160752495785	-0.07413994216823
H	-7.79312609278998	-2.36547767675122	3.04676940085106
H	-0.26291870168095	0.48547696423021	-0.11097093933260

11

[Me₂NAuH]⁻

N	0.42842589719943	-0.28029527375200	1.94790905575583
Au	0.13131141712209	0.02087974301823	-0.09692152305884
C	-0.03568160365394	0.71773034974332	2.86819325028022
H	-1.13167381710781	0.65054072061636	3.12246702636622
H	0.13807078550332	1.72842979648730	2.46561253891783
H	0.49533300268674	0.65186092445383	3.85492334760377
C	0.21548518621889	-1.59142043538078	2.49055676173224
H	0.57994141191123	-2.36381470217988	1.79467585426289
H	-0.86053000303572	-1.83704860129199	2.71875931083192
H	0.75732786539009	-1.73087419109342	3.46362515658261
H	-0.02261014223434	0.26095166937905	-1.67342077927471

4

[CNAuH]⁻

Au	0.08696953238615	-0.10196595298538	-0.09192145660294
H	-1.51484111350373	-0.13112326929472	0.18362675723079
C	2.07927494870350	-0.06541208924066	-0.43414727006558
N	3.23663663241408	-0.04398868847924	-0.63274803056228

4

[COAuH]

Au	0.12453759215642	-0.10122467919300	-0.09827604884433
H	-1.46101195879151	-0.13016729760378	0.17431625845583
C	2.04984669978502	-0.06595871662388	-0.42909975091511
O	3.17466766685007	-0.04513930657933	-0.62213045869639

3

[ClAuH]⁻

Au	-0.20619236610123	-0.12016059843226	-0.05397052210122
H	-1.76247812074722	-0.11749501925878	0.24839174328068
Cl	2.12503048684846	-0.12128438230896	-0.52205122117946

Reactant complex 1'

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RC_1'

Au	5.308396	6.840680	17.993358
P	3.039465	6.606696	17.421647
P	2.738494	5.137516	15.786496
N	5.068605	3.500606	16.462794
N	3.152090	2.718256	17.142347
C	2.436764	4.834144	19.637680
C	4.280091	6.696685	13.873258
C	0.542690	5.692640	18.338176
C	3.723769	3.741429	16.437074
C	1.949095	5.608723	18.550875
C	5.329668	2.367037	17.207181

C	3.680308	5.462483	14.229349
C	6.099544	4.343958	15.869131
H	5.966460	4.401725	14.783988
H	7.073209	3.914848	16.119737
C	4.130470	1.876496	17.635360
C	3.690153	4.382940	13.302046
C	3.897683	4.695465	19.966873
C	4.267983	7.912675	14.755112
C	-0.047589	6.531268	17.236364
C	-0.329456	4.983185	19.173212
H	-1.404814	5.055772	18.996945
C	1.524714	4.152299	20.458508
H	1.909299	3.561656	21.293017
C	2.997672	3.069367	13.570463
C	1.718497	2.490916	17.307334
H	1.185774	3.192551	16.656833
H	1.420311	2.676698	18.346683
H	1.487181	1.457798	17.018910
H	3.891249	1.015430	18.245877
C	4.999339	5.721348	11.752775
H	5.521924	5.822814	10.800595
C	4.363282	4.528677	12.083086
H	4.370753	3.690716	11.382821
C	0.152102	4.212120	20.228848
H	-0.539007	3.671973	20.878149
C	4.936972	6.793293	12.638205
H	5.408603	7.742201	12.375927
H	6.026960	5.354790	16.319450
H	6.863905	7.190168	18.318178
H	4.498132	4.476148	19.072723
H	4.050654	3.899216	20.708620
H	4.311353	5.628763	20.377160
H	0.384513	7.542178	17.236670
H	-1.138221	6.600274	17.345097
H	0.172818	6.104045	16.245056
H	2.825697	2.531688	12.628751
H	2.027689	3.222445	14.067943
H	3.592179	2.408139	14.220820
H	4.656105	8.783134	14.211143
H	4.900727	7.764498	15.649684
H	3.262101	8.150818	15.124417
H	6.341399	2.025733	17.382164
C	7.422468	4.788409	19.779411
O	7.582684	4.126164	18.822723
O	7.293455	5.391535	20.772402

Transition states

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TS_[Me₃PAuH]

H	0.42782327146499	0.72778406857348	-1.58551678706945
C	-0.05860937674436	-0.07592763143124	-2.47266509906131
O	-0.66568335794229	-1.04659815554921	-1.95407775297111

O	0.20520467239790	0.32844908584592	-3.58197128478160
C	-0.66378332530401	1.53730657696438	3.06405847246910
P	-0.01429267337467	0.00192413958269	2.31784301788705
C	1.64513300954007	-0.20362128212361	3.05253768253554
Au	0.00130010895926	0.02766812143071	0.10747933527563
C	-1.01044777854286	-1.32176664597758	3.09425563291227
H	-0.64101335572413	1.47600612816840	4.16159070656126
H	-0.05801074341405	2.38784332648039	2.72812743160233
H	-1.69661267003309	1.69390191659944	2.72818441106535
H	-0.96141297566752	-1.26042107857802	4.19125981843432
H	-2.05367025145500	-1.22755225199287	2.76720590719988
H	-0.63399399669206	-2.29772242965927	2.76281846171806
H	1.58457114379407	-0.20973031803283	4.15030065459177
H	2.08053881279798	-1.14897929012178	2.70524465091601
H	2.29261948593977	0.61814571982102	2.72276474071485

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TS_[Ph₃PAuH]

C	-1.24051282859003	1.60817007800876	-1.96429468680677
C	-0.58333262235359	1.57637720403031	-0.72560762131084
C	-0.34947884433641	2.76912516214831	-0.02589757192151
C	-0.75359835869502	3.98701909977317	-0.57244989080360
C	-1.40079421271397	4.01834711352736	-1.81089193005231
C	-1.64692338147408	2.82965169766828	-2.50333370062527
P	0.01406504374408	0.01487887082744	-0.00296001454700
C	1.65126774785143	-0.26900119221954	-0.74489261619066
C	2.09583911874225	0.45923595272990	-1.85617906866904
C	3.34582794334754	0.18181317028999	-2.41397829644244
C	4.15067234979002	-0.82059753207608	-1.86884046051380
C	3.70987356637385	-1.54521155696747	-0.75675530745511
C	2.46693071817535	-1.26813714586806	-0.19056845786553
H	4.34136832599028	-2.32092703096924	-0.32216215502021
H	5.12783367738951	-1.03276297125736	-2.30463078422764
H	3.69218576073558	0.75448703463369	-3.27526740330429
H	1.46895851447028	1.24484238090326	-2.27846245892606
H	-0.57400716528938	4.91195705927291	-0.02339045011337
H	-1.72480129102770	4.97091945407107	-2.23217561027424
H	-2.16283223712561	2.85218968247173	-3.46417993718700
H	0.13280563594584	2.73377536157230	0.95328767123802
H	-1.44088426941728	0.67906200507453	-2.49953313289703
H	2.12317345252032	-1.81456093524984	0.68978745627824
C	-1.06840110617077	-1.26386664912721	-0.71286836537056
C	-2.31882695303849	-1.48143074793970	-0.11427334234637
C	-3.19608181011609	-2.41911740846131	-0.65539750956308
C	-2.82732681963677	-3.15130493727549	-1.78864968863676
C	-1.57936916878059	-2.94356651819817	-2.37950028408760
C	-0.69814236488656	-2.00021735740404	-1.84577452679675
H	-4.16608509133580	-2.58693800990061	-0.18605918263413
H	-3.51181773240442	-3.89100827672801	-2.20581669826749
H	-1.28639658458835	-3.51935348936157	-3.25839907233336
H	0.27850842495827	-1.84169914824507	-2.30436987400406
H	-2.59457621409110	-0.92026631781354	0.78085865068016
H	0.31386532016833	-0.79475577466374	3.90822426222390

C	0.09640520847941	0.11867508124910	4.79026224701306
O	-0.19346916114915	1.22660332714318	4.27130976683123
O	0.23101849049475	-0.34017196666357	5.90224215655354
Au	0.07089891804408	-0.01609476900566	2.20952788837573

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TS__[F₃PAuH]

Au	-0.04731012997787	-0.01449321542281	0.02533099925659
H	0.58372953829212	0.64160108032857	-1.57614295623962
C	-0.09269936756272	-0.04805992374877	-2.51436265474553
O	-0.90194047760763	-0.84496218920381	-1.97834932752304
O	0.27837017759315	0.30349860130286	-3.59857592792833
P	-0.02713588197828	-0.02271121366834	2.18274470028635
F	1.29703149148317	-0.52425998827089	2.85294619442355
F	-1.06879972418399	-0.84976453496896	3.02119466103969
F	-0.20176562605796	1.36839138365215	2.88223431143034

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TS__{[Me₂PAuH]⁻}

P	-1.01279089733808	0.00238715221478	1.99660320154207
Au	-0.42294267875039	0.01118469913523	-0.20456336744544
H	-0.04582077581328	0.76985578121884	-1.99290424155942
C	0.15153215553299	-0.04675379155262	-2.87747810606934
O	0.11048716657076	-1.23998050815303	-2.48666742281143
O	0.35148649226592	0.49099040668877	-3.96955550573331
C	-0.06190976235905	1.45325736466544	2.72086311839035
H	-0.46380221033255	2.38814383074762	2.30703353147301
H	1.01588968329838	1.41293008884941	2.50703928147642
H	-0.20715952968077	1.46689131854082	3.81447668321041
C	0.04971645875653	-1.35902475748621	2.74118940234225
H	-0.09292837067377	-1.36834645133704	3.83521301270076
H	1.12097839910126	-1.23803544739869	2.52480035201106
H	-0.27767613057795	-2.32845968613332	2.34151006047252

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TS_1'

Au	-0.11019760790895	-0.38553564722339	2.16707511701649
H	-0.49084918439173	-0.10893063578025	4.12526291053176
C	-0.10889817583227	-1.07107708426151	4.76183634884501
O	0.41309132620588	-1.97333509773363	4.03249049406458
O	-0.30317960513100	-0.97282877116700	5.96060279341592
P	-0.00992378000784	0.01345284835471	-0.05042798068137
P	1.61267806479233	-1.36315614130068	-0.83422828687849
N	1.86991971371595	-2.97572883016098	1.57290871844071
N	0.60090462439661	-3.83106633584568	0.02331270241027
C	-2.28691100610750	-1.82281976165808	-0.36947720732086
C	3.73866135704850	0.39714574360926	0.09121303265227
C	-1.34537984414649	-0.74484789207374	-2.36441899341901
C	1.42266471540345	-2.77669776655961	0.29964776059797
C	-1.31486833280577	-0.96713958333969	-0.95572731474843
C	1.28908607731272	-4.10700912388134	2.10434432534827
C	3.34218123415295	-0.85980269857381	-0.42972140894533
C	2.78689842163486	-2.11125979754858	2.31127322111204

H	3.80888072602390	-2.23538560806028	1.93390350841533
H	2.70441757002683	-2.36863631011912	3.36978107205835
C	0.49532660148471	-4.64831748284038	1.13452432204163
C	4.33003135195350	-1.82147809704494	-0.77975793211312
C	-2.40401711978898	-2.10586754418690	1.10505280979274
C	2.77306491019871	1.48768930605801	0.46354689232311
C	-0.40671627035132	0.21408526460832	-3.05035800294461
C	-2.27995811660046	-1.42434685742381	-3.15440085829101
H	-2.28317965524421	-1.25113581334802	-4.23252133981399
C	-3.21827145426024	-2.46258722516148	-1.20368142626769
H	-3.96538024252985	-3.11490514245302	-0.74664801754011
C	3.98627785754887	-3.16014375516777	-1.38408141174924
C	-0.02191117942762	-4.11414964837828	-1.26727136810255
H	0.27394652251571	-3.32984835966020	-1.97205754743690
H	-1.11322790961340	-4.10150581138162	-1.17186455066445
H	0.32144516649692	-5.09297567101050	-1.62633753456446
H	-0.13819471288459	-5.52578909707220	1.14207327032804
C	6.07236368992371	-0.31237757265988	-0.00984144762198
H	7.12792799437674	-0.09879903108385	0.16309692304063
C	5.68098795072526	-1.53210591388554	-0.55204557828113
H	6.43081871492546	-2.28028741285071	-0.81689088636269
C	-3.21102806966002	-2.28749386620459	-2.58409236927216
H	-3.94240669341547	-2.80276363225915	-3.20863446544051
C	5.10392718963980	0.64027156562795	0.29375266345184
H	5.40365126522664	1.60556201004742	0.70583548342919
H	2.46509407784254	-1.07065686504520	2.18896687134322
H	-1.46964917667935	-2.49446095934745	1.53915703368641
H	-3.19750209397314	-2.84353935188475	1.28704470810473
H	-2.65461484920585	-1.19866006867213	1.67508132017198
H	-0.37793503442524	1.18393153203447	-2.53301575995028
H	-0.71790607051003	0.37398517914749	-4.09105191136969
H	0.62741643867978	-0.16606906251731	-3.06099337162996
H	4.87102908359110	-3.60152680232102	-1.86099346379373
H	3.18967099962195	-3.07101237311048	-2.13864381190844
H	3.62993718248786	-3.87706300577663	-0.62684837072024
H	3.31652434895812	2.36505236172196	0.83634364562937
H	2.07541717316665	1.16587449206050	1.25425078667521
H	2.15376256380226	1.80301404979661	-0.38686529098241
H	1.44553127102068	-4.38550084503091	3.13823917388779

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TS_**[CH₂ PPAuH]**

Au	0.08444303719677	0.02429831186824	-0.02908563357214
H	-0.27677493712296	-0.62818691699120	1.71047246062472
C	0.32960652152707	0.14545303355780	2.53437472550371
O	0.89689848023288	1.10902444065827	1.95335800686604
O	0.19761538312520	-0.25531720244273	3.66832869789327
P	0.03058022436706	0.00982416456758	-2.23265008031778
P	1.85222625877509	0.34442224237080	-3.42189069720288
H	1.40170338176501	-2.05658942624207	-2.54589689583716
H	0.43461138045314	-1.65877728977790	-4.04872236809554
C	-2.46786083618483	-0.62538360175692	-3.25967566216592
C	3.07582219955424	1.36241944117832	-1.09306791779223

C	-1.72673866698584	1.69838963911364	-3.63419330685230
C	0.92249584826859	-1.28378104760384	-3.14591932039079
C	-1.49465979149442	0.39637547677745	-3.13397498907879
C	3.03166144913015	0.27789335506601	-2.00331485255836
C	3.90741016758004	-0.82291128133726	-1.85090655484128
C	-2.27945774336822	-1.99073179934628	-2.65309485374548
C	2.24936145284232	2.60430554659417	-1.28371779319637
C	-0.74459888184245	2.81938316158505	-3.43747224525496
C	-2.92286645197639	1.93985935556541	-4.32004795913686
H	-3.11018485702030	2.93911162367413	-4.71695448272461
C	-3.65029294387478	-0.33182804412883	-3.94788264033614
H	-4.40943090172534	-1.10967641302705	-4.04817470691193
C	4.02038074703724	-1.93162477654302	-2.86906305965220
C	4.71212030645917	0.14955617842198	0.22887460705370
H	5.34478635785054	0.08460130439414	1.11478911882049
C	4.73223187395355	-0.86936380143789	-0.72027931515766
H	5.40413362785077	-1.72088773529405	-0.59280789358470
C	-3.87307517386464	0.93447489801451	-4.48526830139542
H	-4.80135041975526	1.14430524186385	-5.01849701422799
C	3.90690084553526	1.26740959895779	0.02763775402389
H	3.90493131294998	2.07990477866747	0.75509881123561
H	-1.55144405545402	-2.59383784396067	-3.21658513142672
H	-3.22936249289188	-2.53935481401750	-2.64186273060109
H	-1.90654138361131	-1.92516579131232	-1.61933524219361
H	-0.45479431093356	2.91760629458510	-2.38176713052660
H	-1.17782518956213	3.77338688676788	-3.76207224374520
H	0.18110650219790	2.64858976103411	-4.00726222181049
H	5.06531046663714	-2.26011037814069	-2.95068173295532
H	3.68724599565568	-1.61813898314956	-3.86769043866317
H	3.42906869168703	-2.81716288367070	-2.58680802608128
H	2.69614483198975	3.44831702850813	-0.74376749206976
H	1.23177044171669	2.46531280156221	-0.88389039093319
H	2.15659125133003	2.88165546482645	-2.34342285698530

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TS_**[NHCAuH]**

N	2.239610	-1.391056	-0.137381
C	3.594482	-1.093240	-0.112721
C	3.699377	0.252865	0.060205
N	2.406694	0.751140	0.131727
C	1.490108	-0.256858	0.012324
C	2.062851	2.150325	0.345328
Au	-0.460443	-0.101699	0.006110
C	1.684098	-2.725291	-0.319240
H	4.570449	0.891427	0.138482
H	4.356209	-1.855042	-0.222695
H	1.904848	-3.096868	-1.328705
H	2.103069	-3.410903	0.428273
H	0.598494	-2.659673	-0.186328
H	2.670563	2.784884	-0.311559
H	1.002183	2.279320	0.101697
H	2.230115	2.433567	1.393221
H	-2.121023	0.225476	-0.791228

C	-3.022865	0.085904	0.109306
O	-2.544063	-0.263380	1.219611
O	-4.115573	0.330149	-0.353238

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TS_**[O_NHCAuH]**

Au	-0.05366297650493	-0.02373010015277	1.92074539997914
H	-0.68747602896498	0.46808946790150	3.68684677151083
C	-0.06964895151947	-0.13055379268041	4.56543798363819
O	0.80502062265515	-0.92528035747213	4.12890631702232
O	-0.45534792037104	0.18865793670022	5.68553399744858
N	0.72913475010288	-0.78766471731047	-0.85728376419701
C	0.52552005512653	-0.49166980080326	-2.20703224221966
C	-0.39282661015153	0.57159893699495	-2.29741831622083
N	-0.68456739052849	0.84401994407782	-0.89214779407447
C	-0.00237655635927	0.01892522385581	-0.05171088554763
C	-1.60232310408101	1.88610989842836	-0.49957452725745
C	1.61349123383752	-1.82889693371262	-0.38585985036533
O	-0.91617687534089	1.21726916213104	-3.23083591250584
H	1.02889311630660	-1.04041314832409	-2.99219899475651
H	1.28835605213247	-2.81045090702484	-0.76535224107873
H	2.64361528402727	-1.64013438139086	-0.72684401877999
H	1.58538019208127	-1.83253935817945	0.71166538955468
H	-2.42961149626792	1.47844964594580	0.09855194362412
H	-1.09385507050777	2.66257022935661	0.09028688752732
H	-1.98635832567238	2.31776305165879	-1.43459614330172

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TS_**[Me₃B_NHCAuH]⁻**

H	0.35520152169191	-0.57829086868588	3.84378712977867
C	-0.08246985943964	0.22752783401202	4.67516731675230
O	-0.59119151085972	1.26101216749086	4.16407945226163
O	0.08826677411694	-0.17427264729071	5.81833556163074
Au	-0.01729723219077	0.03971825347516	2.05533611391095
N	-0.02245626786783	1.06612279589052	-0.74662525070270
C	0.00660763689223	0.64447336325336	-2.07230051562909
C	0.04876190182624	-0.72948678345856	-2.11139930682639
N	0.04488448050101	-1.09064245129426	-0.74965835231530
C	0.00081849997864	-0.01100220807639	0.08232040893302
C	0.05398723225447	-2.45998342253764	-0.25953576880054
C	-0.07543971206330	2.44819335131468	-0.31030412932828
B	0.11968137840425	-1.71807112350646	-3.40649056126667
H	-0.00071452858237	1.35548187750202	-2.88941436656999
H	-0.98054731986981	2.93576453600368	-0.70034044524180
H	0.80980171267208	2.99503049747156	-0.66593549757545
H	-0.09869972083737	2.46389918195149	0.78633717289222
H	-0.93122384826185	-2.92293568506914	-0.39997791117616
H	0.30196913677823	-2.43655097532038	0.80851461274053
H	0.79794511958280	-3.03940120770300	-0.81605498849367
C	-1.11609887148603	-2.81151700153352	-3.38958201723936
C	1.58233998541859	-2.48552725973093	-3.45020140722831
C	-0.02042570691991	-0.77074479005625	-4.74680202730005
H	0.79138745816043	-0.02444817960221	-4.84159130500694

H	0.02221997022810	-1.39133324866501	-5.65999794309411
H	-0.97695372659840	-0.21610825463911	-4.78903728265351
H	-1.05015731325018	-3.57137607874116	-2.59035340169655
H	-2.10825153825872	-2.33304554064769	-3.29417991350573
H	-1.12803753950292	-3.37299359174916	-4.34186104049006
H	1.76554902742917	-3.19101236208464	-2.61843303056610
H	1.66473594491892	-3.08310886590545	-4.37683603688747
H	2.42956691513479	-1.77585131206776	-3.45256526930574

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TS_ $[\text{H}_3\text{B_NHCAuH}]^-$

N	0.04110232062038	1.06894908183552	-2.83405406799811
C	0.03877639416723	0.69132007130367	-4.19071145383192
C	0.03777945107540	-0.68305373021197	-4.13597334771477
N	0.03258081986134	-1.08583904413425	-2.80097784230621
C	0.03669927010476	0.00289743363080	-1.98612592148299
C	0.03718512463937	-2.46037169461312	-2.34502321814912
C	0.03837704738244	2.45629102812656	-2.40714386531413
H	0.04296200271590	-1.40600245140256	-4.94305066914179
B	0.03783692883293	1.73312185537429	-5.40091720508697
H	-0.90263927544021	2.93613029241848	-2.70758684784342
H	0.86177106644204	2.98627993617245	-2.90235365074165
H	0.15345940758106	2.48785834096698	-1.31702259967934
H	-0.79925822827661	-3.01222615837046	-2.79812949502577
H	-0.07424253541984	-2.45712153697278	-1.25359956667548
H	0.98204403550433	-2.95628593979878	-2.61337191651240
H	-0.57555341624875	-0.55474845916028	1.72334073146915
C	0.05360442017631	0.03803392465850	2.61437836200939
O	0.81072500958211	0.94575638367570	2.18305687768350
O	-0.22216326394240	-0.40830707627924	3.72062795688821
Au	0.01191948309541	0.00733975027028	-0.01224084289699
H	0.03012744419469	1.11653237022029	-6.46425956617099
H	-0.95684580957008	2.46253725629803	-5.31305692141058
H	1.04294230292220	2.45051836599189	-5.32433493006754

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TS_ $[\text{F}_3\text{B_NHCAuH}]^-$

N	0.03923051835355	1.07966227647898	-2.81774328654435
C	0.04405979366553	0.68676538173231	-4.16087009645441
C	0.06426305417122	-0.67984785554903	-4.11504918505879
N	0.06345069548509	-1.07768756863787	-2.78019200508552
C	0.04937640064257	0.01664562451442	-1.96839258443529
C	0.10627259942665	-2.45101518598899	-2.31721610773810
C	-0.00141785430497	2.47186453199866	-2.39004162120780
H	0.08284227602746	-1.39729072420804	-4.92633276448944
B	0.02554649007588	1.71695444799475	-5.43370125274295
H	-1.00469772652807	2.88498624160446	-2.55495017176801
H	0.71617276583384	3.04354656982694	-2.98916692299134
H	0.25446413089457	2.51564822624416	-1.32481570636123
H	-0.68995938829274	-3.03519189422699	-2.79943557724768
H	-0.04684305711398	-2.45103863364434	-1.23120697541084
H	1.07990206457224	-2.90878114089807	-2.54571580537621
H	-0.79253837497163	-0.24362991385163	1.70727402616113

C	0.02899717142711	-0.01051520206807	2.61995121534898
O	1.13122609706198	0.43102591675234	2.20609762790014
O	-0.45129199426379	-0.27238334427436	3.71313565898974
Au	0.00401385164880	0.01940912069805	0.00244958942745
F	0.03445990666114	0.95223050867050	-6.62605201560932
F	-1.14415254115473	2.52561485880134	-5.37324615222782
F	1.17484312068229	2.55909775803049	-5.38020988707828

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TS_**[ox_NHCAuH]**

N	0.03790148526844	-1.09665604830446	2.78429877366905
C	-0.00969217167478	0.77532819883809	4.14753012544327
N	-0.11942972443464	1.09076367848124	2.78423431876439
C	-0.10262385112695	-0.00737660087452	1.96152021176549
Au	-0.07458458747926	-0.00590041817670	0.03750203504298
H	0.07759670416305	-2.04932139961261	2.43401237013034
C	0.10234633863117	-0.76869683639621	4.14744333784704
O	0.21089152567907	-1.52308131059194	5.08294872424633
O	-0.01226025042464	1.53745431275000	5.08302849942995
H	0.82416197786526	0.05209668292983	-1.50428401371105
C	-0.10615222838513	0.00203346911686	-2.50306698730676
O	-1.25271567649057	-0.08368269351058	-2.01422650549652
O	0.47658530990732	0.05647182266732	-3.54963021280896
H	-0.21934485149836	2.03910714268368	2.43419932298443

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TS_**[4H_NHCAuH]**

N	-0.06277699355726	-1.09375497056234	2.76553801710589
C	0.16353357526113	-0.75492438826370	4.17708903740360
C	-0.07726612939660	0.75979612472846	4.18226135262114
N	0.07938559692355	1.09767917431008	2.76122634311269
C	-0.00724243716816	0.00144958023628	1.97403612878092
C	-0.08661903504992	2.46136040620872	2.30385765076101
Au	0.00361156022005	-0.00107753616277	0.01795132683420
C	0.07798712465003	-2.45841977733050	2.30255646082459
H	1.10694543565693	-2.82675690531330	2.45248040890100
H	-0.61747293474494	-3.11203248601638	2.84810262856763
H	-0.15908606123514	-2.49132888090923	1.23291085625458
H	0.63481092900184	3.11727415627206	2.81175297657466
H	0.09562982685754	2.49180219128654	1.22328194246449
H	-1.10701849439150	2.82855104709385	2.50537707872118
H	0.82784891546431	-0.00197106536857	-1.64881113456793
C	-0.09713497162536	0.00322991542817	-2.54618644699921
O	-1.25031461980744	-0.01112199308387	-2.04584417138814
O	0.40172738267789	0.01987764319878	-3.64943988321391
H	-1.09618631056969	1.01839618059460	4.52163016220454
H	0.64351816075336	1.31108950005733	4.80108980777638
H	1.19798415444202	-1.01282638914393	4.46668967546167
H	-0.52604467436264	-1.30591152726029	4.83058978179895

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TS_**[H_H_NHCAuH]**

N	0.08537058180434	-1.06799679641638	2.77140681207278
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C	0.09249602929458	-0.68079074955251	4.10482076541531
C	-0.00104142595984	0.67620716191288	4.10819019248696
N	-0.06176538569681	1.06531297724369	2.77669981674657
C	-0.00929308158553	-0.00067952121508	1.92543852835154
H	-0.13870912426292	2.01890470521733	2.44379203991342
Au	-0.00526690364281	0.00480136090114	-0.02080164691890
H	0.14169226032957	-2.02131329194832	2.43367006707144
H	-0.02919770266300	1.38302026345605	4.92711854885137
H	0.16157970836170	-1.38880811067248	4.92027290999419
H	0.81743347962767	0.06000034985363	-1.69174279442913
C	-0.10932604351909	0.00721933069473	-2.58428015812646
O	-1.25853618629192	-0.05899301752313	-2.07699827217216
O	0.38093379420407	0.03601533804844	-3.69052680925698

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TS__[CN₂Me₄AuH]

N	-0.04785577274721	-1.14814266744695	2.77026154236438
N	0.02035438890478	1.16801286945608	2.77719430600409
C	-0.01761411328114	0.01212414566296	2.06445704402102
C	-0.38223278978070	-2.40416332670606	2.10329188088129
H	-0.96680725580753	-2.19761165267587	1.20084174335067
H	-0.98053383412962	-3.02557531581690	2.78543999474568
H	0.53002504408721	-2.95718698510696	1.82497664025417
C	0.63329039774958	-1.32042640921593	4.05522705933019
H	1.24103219146740	-0.43840538253577	4.27981180226927
H	1.30305870265955	-2.19030215028385	3.97802774574738
H	-0.06813365525566	-1.50072229546328	4.88409168602068
C	-0.61609022380337	1.31941741095740	4.08678148986210
H	-1.21510892272399	0.43323618191413	4.31834307325706
H	-1.28837555625798	2.18957803023328	4.04570407682904
H	0.11283686915086	1.48825633978547	4.89426151337215
C	0.32742669535188	2.43418490242549	2.11772184143254
H	0.87352174656180	2.23672379814522	1.18935806563821
H	0.95249065190477	3.04618020113759	2.78437516588900
H	-0.59556780943100	2.99013923487203	1.88495285982269
Au	0.01047864956093	0.00691725507878	0.09480483014189
C	-0.07867587682562	-0.04436887885607	-2.47291309896016
O	-1.19991306366429	-0.31384346357233	-1.97145102881817
O	0.40413429431692	0.06990382003278	-3.57810849686256
H	0.81684924199243	0.17216433797877	-1.57719173659272

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TS__{[NONAIAuH]⁻}

Au	-0.06439095566572	0.04948621855132	2.18452976428558
H	-0.53373132113759	0.27023788557247	4.04971333369426
C	0.15238960054560	-0.17151828662466	4.99178351804557
O	1.17022991033534	-0.78772855552688	4.62246333427097
O	-0.36381584689578	0.11943658642326	6.07262525341067
C	-0.14145288720512	3.12305797455914	-4.35317750744998
C	-0.94763027115348	2.24420207021832	-3.60275063447870
C	-0.38747784100344	1.75065940720369	-2.44297377485248
C	0.93865725145738	1.91913378393566	-1.99779457436176
C	1.70588130897200	2.83264742826587	-2.75868636675841

C	1.15237176825816	3.41604059581707	-3.90578000205373
O	-1.12106023438710	0.83913235628038	-1.65208670393511
C	-1.77064566231879	-0.13302869954324	-2.44423520870322
C	-2.40867764717332	0.25458813122314	-3.60403917022331
C	-2.35812479588586	1.74865004975917	-3.96688084683528
C	-3.00570430990038	-0.77754951166955	-4.35507102511002
C	-2.89788386844302	-2.10002088656534	-3.90839091055800
C	-2.17604357734007	-2.45407946007784	-2.76115018351100
C	-1.53439860483671	-1.44892644712431	-1.99967574615639
N	-0.70445438867680	-1.57275830933722	-0.91862355135521
C	-0.52120461354963	-2.89018299542416	-0.33847730856372
C	-2.66972697067556	1.97718453495827	-5.44824258558547
C	-3.39697333661850	2.51142475024685	-3.10590725879340
Al	0.00300179854773	0.01294220350382	-0.14079008866056
N	1.30439385135550	1.16363456687457	-0.91705025368978
C	2.61503670738875	1.38318601481422	-0.33401403046270
H	-2.07041906693635	-3.50200671091042	-2.48146135580806
H	-3.53149848654464	-0.55643672532408	-5.28280542250584
H	-0.51016006422788	3.55981041014095	-5.28019124134530
H	2.73726783976139	3.04550014138448	-2.47847869572206
H	-2.63679574708207	3.04938543251922	-5.68663240296850
H	-3.68069819142788	1.61797041845394	-5.68505312139780
H	-1.95264101095240	1.45356466789057	-6.09516746682231
H	-3.34690773437885	3.58912178248588	-3.32050075142151
H	-3.20633310758993	2.36384737916751	-2.03545988632215
H	-4.41161702011314	2.14978329080503	-3.32923591158522
H	0.03367176313520	-3.57200457846437	-1.01079199196025
H	0.04489274868912	-2.78704619793044	0.59821539630318
H	-1.48662619206878	-3.36946865610705	-0.09433293467539
H	2.68336957506541	0.81195071807858	0.60275645722076
H	3.43326483263261	1.05774197646298	-1.00432803159089
H	2.78309448405187	2.44773052536286	-0.08939371036830
H	-3.37432079669147	-2.89233821172785	-4.49013420478188
H	1.76605111068431	4.10806293139810	-4.48690219585707

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TS__{[Me₂NAuH]⁺}

N	-0.49458574545688	0.00675383654678	1.93629404485875
Au	-0.18727038820130	-0.02584821988825	-0.05976982618079
H	0.05186080141021	0.79568629756276	-1.83263378361410
C	0.05406303606210	-0.02203474080514	-2.72555249076580
O	-0.11081683252229	-1.21135350871829	-2.33682580047470
O	0.22096258063782	0.48263344245504	-3.83788653338587
C	-0.06651343506750	1.22797671852735	2.59249577553452
H	-0.49036777176464	2.10434429342144	2.08261727969471
H	1.04017853063842	1.36833907651470	2.64555485144426
H	-0.43377996534057	1.22892606638891	3.64443393279039
C	0.05395734036003	-1.14469408223189	2.63037405869337
H	-0.31392365842054	-1.15039615523664	3.68203235560501
H	1.16893406602206	-1.16993802929498	2.68751698312490
H	-0.27762855835691	-2.07536499524177	2.14891915267533

TS__{[CNAuH]⁻}

Au	-0.00048426299603	0.00553745378717	0.23678453162304
H	0.67478199928605	0.41209731227339	-1.50147657556458
C	-0.06848693716289	-0.03253058889479	-2.39008926107941
O	-1.07609493050783	-0.64655412836370	-1.95519207918802
O	0.36697597993356	0.23856297702145	-3.50298682198183
C	0.00005624825901	0.03009003556936	2.16623771021580
N	-0.05260809681187	0.10836693860714	3.33571249597500

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TS__[COAuH]

Au	-0.06545093283536	0.00007626886969	0.17098833393890
H	0.73078619913332	0.46727140985635	-1.39780276661685
C	-0.08475466344476	-0.04845449478560	-2.35411472956947
O	-1.04932532096805	-0.64821575980396	-1.81850507150971
O	0.36281401658847	0.22435555461680	-3.42956228915008
C	-0.07008474817687	0.02733296391330	2.03786076379520
O	0.02015544970325	0.09320405733343	3.18012575911204

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TS__{[ClAuH]⁻}

Au	-0.05766232784861	-0.02520745924296	0.10194687940725
H	0.47860559667756	0.61666886648483	-1.64057794148247
C	-0.06908847210743	-0.01755039255520	-2.53223663858297
O	-0.93960379835805	-0.83487197445124	-2.12119440522050
O	0.34698730102489	0.28112601557292	-3.64835682496655
Cl	0.03377170061164	-0.00528505580835	2.38105893084525

Products

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PC__[Me₃PAuH]

P	1.77005309078224	0.07879199777551	0.19328485768125
Au	-0.43629494956063	-0.14945323884420	0.22296023692940
H	-2.79470589551012	1.36040548461146	-0.69056942952750
C	-3.28124489527421	0.46214114701534	-0.23265096312480
O	-2.43922729543248	-0.42522717763204	0.28299186297098
O	-4.49032226681245	0.33320726554876	-0.22103775115003
C	2.42254482607013	0.76680048534005	-1.36865835444241
C	2.43212716651524	1.19141445017927	1.48318087623618
C	2.70026006538537	-1.47777024835707	0.42251023597724
H	2.42549151673409	-2.18369292143308	-0.37138191342255
H	2.42957967818943	-1.92311317781023	1.38816007216870
H	3.78389399758517	-1.29566162676026	0.39301738452346
H	1.97183377623628	1.75127762654563	-1.54717137287659
H	2.14506713123669	0.10567894274209	-2.19930583640076
H	3.51640633924729	0.86632593555101	-1.32699618390188
H	1.98187282091057	2.18560312363807	1.36901282738911
H	3.52587430873465	1.27285141979749	1.40983982224622
H	2.15869058496270	0.80181051209220	2.47191362872398

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PC__[Ph₃PAuH]

C	-1.24051282859003	1.60817007800876	-1.96429468680677
C	-0.58333262235359	1.57637720403031	-0.72560762131084
C	-0.34947884433641	2.76912516214831	-0.02589757192151
C	-0.75359835869502	3.98701909977317	-0.57244989080360
C	-1.40079421271397	4.01834711352736	-1.81089193005231
C	-1.64692338147408	2.82965169766828	-2.50333370062527
P	0.01406504374408	0.01487887082744	-0.00296001454700
C	1.65126774785143	-0.26900119221954	-0.74489261619066
C	2.09583911874225	0.45923595272990	-1.85617906866904
C	3.34582794334754	0.18181317028999	-2.41397829644244
C	4.15067234979002	-0.82059753207608	-1.86884046051380
C	3.70987356637385	-1.54521155696747	-0.75675530745511
C	2.46693071817535	-1.26813714586806	-0.19056845786553
H	4.34136832599028	-2.32092703096924	-0.32216215502021
H	5.12783367738951	-1.03276297125736	-2.30463078422764
H	3.69218576073558	0.75448703463369	-3.27526740330429
H	1.46895851447028	1.24484238090326	-2.27846245892606
H	-0.57400716528938	4.91195705927291	-0.02339045011337
H	-1.72480129102770	4.97091945407107	-2.23217561027424
H	-2.16283223712561	2.85218968247173	-3.46417993718700
H	0.13280563594584	2.73377536157230	0.95328767123802
H	-1.44088426941728	0.67906200507453	-2.49953313289703
H	2.12317345252032	-1.81456093524984	0.68978745627824
C	-1.06840110617077	-1.26386664912721	-0.71286836537056
C	-2.31882695303849	-1.48143074793970	-0.11427334234637
C	-3.19608181011609	-2.41911740846131	-0.65539750956308
C	-2.82732681963677	-3.15130493727549	-1.78864968863676
C	-1.57936916878059	-2.94356651819817	-2.37950028408760
C	-0.69814236488656	-2.00021735740404	-1.84577452679675
H	-4.16608509133580	-2.58693800990061	-0.18605918263413
H	-3.51181773240442	-3.89100827672801	-2.20581669826749
H	-1.28639658458835	-3.51935348936157	-3.25839907233336
H	0.27850842495827	-1.84169914824507	-2.30436987400406
H	-2.59457621409110	-0.92026631781354	0.78085865068016
H	0.31386532016833	-0.79475577466374	3.90822426222390
C	0.09640520847941	0.11867508124910	4.79026224701306
O	-0.19346916114915	1.22660332714318	4.27130976683123
O	0.23101849049475	-0.34017196666357	5.90224215655354
Au	0.07089891804408	-0.01609476900566	2.20952788837573

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PC__[F₃PAuH]

P	1.72098820767129	0.08476278809833	0.06823205558361
Au	-0.42771325630017	-0.12943406782870	-0.07828724412986
H	-2.84545158187610	1.57252405993093	0.20883746722692
C	-3.28535791867033	0.57681696414645	-0.03542677836187
O	-2.38822805244451	-0.40408559563284	-0.22491543303198
O	-4.47753863909859	0.39601300736637	-0.12269159925223
F	2.50731689313053	0.52289729401844	-1.21291043435198
F	2.56324026250904	-1.16599611436391	0.48852694186252
F	2.26173408507883	1.14013166426491	1.08932502445487

PC__{[Me₂PAuH]⁺}

P	1.40017737523459	0.65903246880959	-0.82544768918176
Au	-0.70649235341093	0.29627536741715	-0.02893219629207
H	-3.45619954748868	0.67267435925529	-1.07328881401662
C	-3.70933939266517	0.24611025316080	-0.06396140960830
O	-2.68183962119185	-0.03787384155174	0.68217336946530
O	-4.89202906588909	0.08567374338082	0.24829715268137
C	2.27035554080747	-0.99175789809680	-0.57528772142412
H	1.82043349747271	-1.73889399013311	-1.24424795711494
H	2.20003954526181	-1.36547546738680	0.45720252200872
H	3.33553695373265	-0.88871323148692	-0.84324914558013
C	2.26300412250829	1.58315171111900	0.57006632200567
H	1.80515356952348	2.57650131632297	0.67874952875882
H	3.32714455540091	1.72184208251924	0.31449559948813
H	2.19632482070382	1.06471312667052	1.53837043880993

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PC_1'

Au	5.49575836768895	6.58277301371126	17.42188387151684
P	3.29443479889038	6.69981308827378	16.93856396049949
P	2.86976315505222	5.17738501698283	15.34055846872937
O	7.55646458377977	6.59320608151184	17.85091092767314
N	5.21445048466828	3.52208566389540	15.85975546133996
N	3.35861562168247	2.80273942626061	16.74275395699328
C	3.87778743355494	3.77993412269377	15.94280677110569
C	4.37858036291532	7.91149946064259	14.17716087045700
C	4.18812979070314	4.77956550845680	19.56925197732777
C	5.53430507047516	2.43319139056965	16.64273827801409
C	3.68719597103651	5.47671328780275	13.71137062177931
O	7.62650225959314	4.31322061965665	17.76262393177525
C	2.24453376541744	5.75534804755130	18.15633687282461
C	4.28455937540747	6.69432517915247	13.30065923552671
C	4.37228108599940	1.97696586509470	17.19470042708090
C	2.73178221903838	4.98825946725106	19.25038819106928
C	0.83664033436741	5.90318869166901	17.98578670257150
C	6.19137555402251	4.27813784883311	15.08320387086789
H	6.03352977521257	4.10867040756998	14.01168827346936
H	7.18548667462418	3.95940744727694	15.40375674168203
H	6.07865121779591	5.34677740122911	15.31724334348474
C	8.12581330671967	5.43254564191167	17.94290782594226
H	9.20383889025390	5.52109316053185	18.21848546644277
C	3.59046018013878	4.39505531287682	12.79248382695970
C	0.43439558347035	4.48938306356296	19.92184747253833
H	-0.25992315060662	3.99749821758485	20.60505184475927
C	1.80836204873339	4.37444340631823	20.11321043358962
H	2.18927366735967	3.78997650532390	20.95346355192270
C	-0.04259579881840	5.25570319958666	18.86190033673916
H	-1.11782728805979	5.37521693038594	18.71351850120512
C	2.89777196998750	3.09736239763890	13.12825812643015
C	4.83010860875036	6.77502323468324	12.01208257654618
H	5.29993719815710	7.71156725584551	11.70595442869534
C	0.24560057620270	6.74681778547304	16.88625201683573
C	4.15521354049518	4.52424463111489	11.51771291101834

H	4.08235698535368	3.68518866020596	10.82269451482747
C	1.94150337419593	2.59517818625880	17.02984871859454
H	1.73168173540125	2.80283534069183	18.08570545628069
H	1.67654560413046	1.55941693065390	16.78208312378738
H	1.36210462953736	3.28969125424599	16.41266416376014
C	4.78576224412660	5.70136472521509	11.12748191283791
H	5.22252611579279	5.78940948038176	10.13180041546339
H	4.18282166762818	1.15907542824476	17.87757432173305
H	6.56213628289141	2.12483111935782	16.78033319781912
H	4.80196707468784	8.75398909071015	13.61588395418295
H	5.02545214667174	7.72900254490846	15.05203712784277
H	3.40038515305616	8.21566113847686	14.57247966125244
H	2.65961982967971	2.54613114393077	12.20927912442064
H	1.96257921116167	3.27200615567243	13.68242603284396
H	3.52250801722330	2.43898708755329	13.75277619289022
H	0.71747070696234	7.73921357555401	16.84938353537208
H	-0.83569369274065	6.86713995915881	17.03451184057425
H	0.40595988115708	6.29052177449480	15.89640710290104
H	4.77741325286608	4.44927409750159	18.70163593818248
H	4.29775594475866	4.03002071248509	20.36504824018055
H	4.66252660074841	5.70953381537283	19.91718334883682

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PC__[CH₂PPAuH]

Au	0.18777263032332	-0.13365124311616	2.15578140459073
O	0.17898161482809	-0.27707346120021	4.20658905358540
O	-1.49813251968080	-1.80208354279143	3.96686526310838
C	-0.72039810690135	-1.13074173858951	4.63798863771892
H	-0.71089891560916	-1.19302964970041	5.75027852742781
P	0.14249697861304	0.02411207608961	-0.04531928185666
P	1.85631947181489	0.38741131366064	-1.35956658874372
H	1.49226086160165	-2.02760763932026	-0.50539986734772
H	0.41083053098199	-1.61287751913001	-1.92681575648543
C	-2.43664245174745	-0.59634862256209	-0.81195341616339
C	3.31192012394588	1.34250837871492	0.86289433959123
C	-1.70050392489254	1.68643698693638	-1.39666172845156
C	0.96585940418805	-1.25019106220141	-1.05845160999717
C	-1.44132943630457	0.41314672321899	-0.84219541633540
C	3.18227569916741	0.29625762861478	-0.08258570415420
C	4.11476339021266	-0.76666391055318	-0.11055375879325
C	-2.21945064661667	-1.91584362606349	-0.12025271101526
C	2.40338170055253	2.54040429389206	0.85478399817936
C	-0.69728319550414	2.80656630203680	-1.34756963104975
C	-2.95008702260908	1.90794275742658	-1.98865396962848
H	-3.16002912219382	2.88494543528083	-2.42769256052861
C	-3.67066140194543	-0.32302448854459	-1.41264498312305
H	-4.44548099472201	-1.09157671373968	-1.39620655145888
C	4.11003143532487	-1.83148529860345	-1.17968220862699
C	5.19344541971675	0.16949724135018	1.85801537517952
H	5.96583267661261	0.11013238151142	2.62586790995760
C	5.10553615272245	-0.81554105195237	0.87783418885218
H	5.82422930278790	-1.63765904072045	0.86504804412867
C	-3.92332704612790	0.91143596455496	-2.00794903005671

H	-4.89184278386921	1.10472231551955	-2.47145948575857
C	4.31391429766447	1.24964353286268	1.83451962115918
H	4.40188288527247	2.04318177450304	2.57872568096599
H	-1.39459386233883	-2.48838320779483	-0.56967557903017
H	-3.12594349262860	-2.53112136793778	-0.17331241552469
H	-1.96630995295243	-1.77763030893831	0.94428422370997
H	-0.31196977781886	2.95444097464212	-0.32861175293612
H	-1.15575693577390	3.74706610931633	-1.67748821853260
H	0.17220689353451	2.60370807256576	-1.99080296982099
H	5.13475623336118	-2.17485324305190	-1.37417199786690
H	3.68957546214124	-1.46788756785099	-2.12758150608653
H	3.52535437846254	-2.71571903693828	-0.88133621522360
H	2.83144554883564	3.35532398886066	1.45180173168631
H	1.41997517545080	2.28918413769789	1.28636340950425
H	2.22683332211977	2.91559495204460	-0.16398649474909

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PC__[NHCAuH]

N	2.49256861566257	-0.86335859455531	-0.02401461957802
C	3.76053308673238	-0.30341176548719	-0.02531379711487
C	3.59275536972938	1.04806767616432	-0.01460708817700
N	2.22645390985552	1.28119657640409	-0.00546442545377
C	1.52851877595832	0.10598643579916	-0.01194914009696
C	1.60949580611771	2.60163038102621	-0.00574095651576
Au	-0.41784628970632	-0.13575313342662	-0.00734541609940
C	2.21551297919604	-2.29443689694925	-0.02731036810020
H	4.31812396276998	1.85217941055952	-0.01241263102063
H	4.66037288370487	-0.90595056502771	-0.03148519229067
H	2.65775041104146	-2.76272808896748	-0.91608711252589
H	2.62201812086907	-2.76163987768857	0.87909270425761
H	1.12782718165801	-2.42427760773584	-0.04840257937526
H	1.82877663798868	3.12462624930554	-0.94591932712803
H	0.52657565026610	2.46502503535446	0.09029755591663
H	1.98312530804345	3.19061566622581	0.84151009707105
H	-2.83645896461731	1.52535044155045	-0.08188670975405
C	-3.28263361351771	0.49798060767472	-0.04200006456998
O	-2.39941967640109	-0.48828336102555	0.00041680179395
O	-4.48891915535113	0.33530241079923	-0.03905873123878

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PC__[O₋NHCAuH]

N	2.50130061566298	-0.88382083361141	0.00475763424070
C	3.85945335475289	-0.34858335603264	0.05679584751792
C	3.62932503357974	1.03893257478684	0.04096475881958
N	2.24842860849288	1.25653507681676	-0.01445526947638
C	1.55327423202780	0.09376197505719	-0.03780316193737
Au	-0.40560417037833	-0.12995246240960	-0.11696765009710
C	2.25199906162166	-2.30526535843641	0.00229005700020
H	-2.82653170816252	1.53283283523239	0.10436709411938
C	-3.29175979242524	0.52638864978822	-0.07628454387343
O	-2.43861599101331	-0.45426470263040	-0.21741409831933
O	-4.51430702230077	0.41524803867522	-0.12761487716283
C	1.64388333922004	2.56672754592417	-0.04869940348251

O	4.87035667009126	-1.08455838550153	0.10076889412681
H	1.67366464762779	-2.61088399768558	0.88675403121797
H	3.24145494760969	-2.78435301640914	0.01994748853589
H	1.70116191667447	-2.61025993413747	-0.89930391661049
H	0.55428535749452	2.43935619856488	-0.09234927128859
H	1.98390966558768	3.12675074482870	-0.93486348949929
H	1.91037918522286	3.13994296683766	0.85410103316920
H	4.33464204861387	1.85908544034215	0.06919884299968

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PC_ $[\text{Me}_3\text{B_NHCuAuH}]^-$

N	-0.16855964547036	-1.17754797276183	2.73526893786670
C	-0.38114376071930	-0.71867207161058	4.05123914328604
C	-0.13019433512232	0.62895373488474	3.95626085454801
N	0.21218399603034	0.94034011076296	2.64280117485234
C	0.19103529042207	-0.18143460029244	1.87436564746011
C	0.53988598934327	2.26691883629760	2.16038860160506
Au	0.59017312827509	-0.29661189101761	-0.05456485907145
C	-0.27560526585416	-2.56796724010180	2.32218157673118
H	-0.17319501312060	1.39294359226967	4.72292582374319
B	-0.84569558728081	-1.58797595600128	5.35115776660032
H	0.55904556127142	-3.15172974893491	2.73066128958338
H	-1.21471834660192	-2.99073150389314	2.69526097554253
H	-0.25008280642169	-2.60497349472879	1.22630302014635
H	1.41906579968611	2.66143161415405	2.69082407646198
H	0.76293344997368	2.19643748991339	1.08879613476053
H	-0.30769661413599	2.95127677832881	2.31273486915497
H	0.85744278149862	1.54102325307841	-2.33241483358761
C	1.05268766316427	0.55932304348573	-2.84125083380687
O	0.99745347306707	-0.48759449698290	-2.05435896832615
O	1.29382804530408	0.52427920530378	-4.04299270036959
C	-2.37989451423443	-2.15920424795707	5.12826911346745
C	-0.84222963270028	-0.56666819615572	6.64386287159467
C	0.20113825967701	-2.83130607474659	5.64078408274278
H	-1.53612458058132	0.28716443366375	6.52417985939702
H	0.15702384788536	-0.14408105093122	6.86148736191491
H	-1.16214101783832	-1.10074538656505	7.55678453810525
H	0.16378773839247	-3.64379231421500	4.89305203422535
H	-0.03819099595542	-3.30221329916441	6.61208787509781
H	1.25440513928489	-2.50067269814415	5.70231790109130
H	-2.48662001947158	-2.89399638213767	4.30879915976936
H	-3.10537485690529	-1.35095209010631	4.92339900892076
H	-2.72626317086197	-2.67385137569440	6.04364849649221

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PC_ $[\text{H}_3\text{B_NHCuAuH}]^-$

N	-0.32841691056271	-1.09342380550331	2.81801597447921
C	-0.44245141347762	-0.64451987900479	4.14754455141361
C	-0.18617316843206	0.70288552219665	4.04725912855949
N	0.06394740729636	1.01886073841384	2.71219432447560
C	-0.02352748887519	-0.09732008781073	1.93836529573007
C	0.36975135613429	2.34410691604978	2.21442004138708
Au	0.23852888576130	-0.21157285441053	-0.01442815172373

C	-0.51808846450820	-2.48304263496859	2.44506928382188
H	-0.16367530826213	1.46115845409044	4.82103318706917
B	-0.80007797428915	-1.59844052643223	5.37775125077759
H	0.21361920930363	-3.10926870472016	2.97250981870040
H	-1.52162460171952	-2.81061056281890	2.74673877094361
H	-0.39124837967978	-2.57380737040190	1.35968389172608
H	1.29197320324416	2.72644976069992	2.67704670102060
H	0.50855082419968	2.27764882396332	1.12831834622622
H	-0.45534752498106	3.03781912566262	2.43485403580781
H	2.06281380848051	0.86298936460196	-2.06227010783607
C	1.36990133207321	0.25721712019566	-2.70500112167664
O	0.42634727390975	-0.37460845542049	-2.05107005055345
O	1.52811135208647	0.22202424248784	-3.92100515634410
H	-1.89712030366442	-2.13325705602456	5.17307909136112
H	-0.83198702019631	-0.93420220163760	6.41180113432862
H	0.04831390615879	-2.49492592920800	5.46476976030710

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PC_**[F₃B_NHCAuH]**

N	-0.30924957026152	-1.12846906899338	2.81607972963657
C	-0.45960906246698	-0.64195848329550	4.11846384028720
C	-0.18839321334320	0.69471380897864	4.01329185492938
N	0.11146439816977	0.97978514387620	2.68434678666573
C	0.03872882523432	-0.15416439374049	1.93006592696919
C	0.45909060279399	2.29070495115289	2.17061851921178
Au	0.37713898463383	-0.31022858317719	-0.00605786070216
C	-0.51003375021312	-2.52726147481262	2.46027566658571
H	-0.18450286005280	1.46016430007178	4.77978494784740
B	-0.86574112938199	-1.55840313834590	5.41259933720239
H	0.15243704611498	-3.15327830782037	3.06979246463057
H	-1.54761521670523	-2.81315891381197	2.67204393257823
H	-0.28696977610551	-2.64767172856130	1.39387554220596
H	1.38047032819590	2.65801430075340	2.64544216744400
H	0.61842018365055	2.20153352859676	1.08925535844704
H	-0.35472350846764	3.00475518615005	2.36237328598381
H	1.58276872655045	1.30373738617444	-2.14605424178225
C	1.28279156872844	0.38978860821164	-2.72495849305530
O	0.70030491962944	-0.54514189364318	-2.01275176276279
O	1.50506832599557	0.31982576855586	-3.92814732800846
F	-2.13933673385092	-2.15712961239422	5.19142497402354
F	-0.90662810198307	-0.72707700554713	6.55890610278760
F	0.10623901313472	-2.58692037837815	5.58600924887616

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PC_**[ox_NHCAuH]**

N	2.45914946170296	-0.90077550655134	-0.01754509691225
C	3.78062261395093	-0.42245241375776	-0.01380284437749
C	3.59788796369138	1.12020157666105	-0.01462808657073
N	2.20127930713951	1.27656114073643	-0.01882931262791
C	1.51572503751423	0.09167541664083	-0.02068292702466
Au	-0.39804674995325	-0.13416734916123	-0.02641070923344
H	2.21396926988347	-1.88736183325443	-0.01806129723045
H	-2.82494114783831	1.54132800432622	-0.03710018924789

C	-3.25661510365631	0.51098070961189	-0.03624501411648
O	-2.35250184717282	-0.47484125340696	-0.03221451469638
O	-4.45231329647686	0.31453138974723	-0.03888972111208
H	1.73171962453811	2.17813105431183	-0.02029128923573
O	4.43870486123009	1.98210604477838	-0.01224187814434
O	4.79977000544686	-1.06358698068213	-0.01058711947017

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PC_**[4H_NHCAuH]**

N	0.01626483668464	-0.99222350236352	2.72548944793119
C	0.14465237715089	-0.77096059944176	4.17241520170056
C	-0.15888659945039	0.72927539459316	4.29761942614038
N	-0.01450119938481	1.19003656386607	2.90979824529504
C	0.00382029360526	0.16527268588670	2.03185087785872
C	-0.22292917276665	2.58147254634255	2.56667867836448
Au	0.00186423225164	0.33021286100533	0.07647735917731
C	0.23386700221859	-2.30581413844873	2.15641025158532
H	1.25070474789122	-2.66913230646517	2.38079496872628
H	-0.49625570309084	-3.02075088566327	2.56324320207525
H	0.11002737490940	-2.23871028036055	1.06931473677539
H	0.49844176560365	3.21519890996443	3.10293854533173
H	-0.07724819360488	2.70022124363274	1.48680063791638
H	-1.24408770024593	2.90522292733833	2.82868932909012
H	0.10140825253337	-1.42312985144258	-2.27535178540646
C	0.03648723575123	-0.41537947183262	-2.76164032256225
O	-0.01569030979148	0.60447209150345	-1.91747679621404
O	0.01741975794606	-0.30030118460560	-3.97301064844737
H	-1.18677383309366	0.92126549759113	4.65152850704292
H	0.53810964910035	1.25701874199597	4.96290048085051
H	1.16865944522426	-1.02029848826792	4.50150175015507
H	-0.55953425944193	-1.40258875482808	4.73116790661338

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PC_**[H_H_NHCAuH]**

N	2.47454898784847	-0.85323648824782	-0.01955981359805
C	3.74943483628437	-0.30620111926290	-0.01604551248366
C	3.58202185906315	1.04481089715610	-0.01560675914509
N	2.21230201543920	1.26409264516731	-0.01873644189004
C	1.50085466423701	0.10132602872059	-0.02126414416614
H	1.75892481182971	2.17050188303914	-0.01963856775380
Au	-0.43570619484636	-0.13514116221625	-0.02548189902425
H	2.25672382978727	-1.84303432901698	-0.02054185654466
H	4.30597826906578	1.84916191971483	-0.01321554777474
H	4.64786753913411	-0.90951148662562	-0.01418373288599
H	-2.85739482712516	1.52896590528593	-0.04441098401929
C	-3.29971771448737	0.50007375462775	-0.03628423442464
O	-2.41230749637301	-0.48545495071093	-0.02653203948616
O	-4.50447257985715	0.33014450236886	-0.03667046680349

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PC_**[CN₂Me₄AuH]**

N	2.35902736418378	-0.95192020067337	-0.01146634654062
N	2.03477524257068	1.25081984351979	-0.64955894112901

C	1.50825404917820	0.09001954039753	-0.18356110815904
Au	-0.41926612127248	-0.07346546387385	0.23878880539011
H	-2.74515533066378	1.68164887262413	0.53527521433937
C	-3.20520817683351	0.68478716082354	0.76105847909730
O	-2.36676676799551	-0.33840130558765	0.69645227676581
O	-4.38616788181086	0.58493987097191	1.03997316902766
C	3.40213497209440	1.69521217674384	-0.37352640731979
H	4.03915434045083	1.70711412733325	-1.27106996915608
H	3.85950317602465	1.05666841387862	0.38839218511253
H	3.35269869616828	2.72066921408088	0.02172304411233
C	1.15687278706633	2.31396815266646	-1.13445107819756
H	0.16345213285003	1.90086048436843	-1.33805271078403
H	1.57260870167006	2.73452706634345	-2.06220965060582
H	1.06880297724666	3.11912902856978	-0.38720351691141
C	1.94215640757017	-2.12976684183174	0.74714419477732
H	1.72721430679249	-2.97147051755589	0.06961643958145
H	1.04320831047467	-1.89259144204347	1.32595726734750
H	2.74866076364938	-2.42416206525445	1.43517960630333
C	3.56837560210004	-1.16403630750361	-0.80874179653797
H	3.57993868050556	-0.48536676791635	-1.66726332699838
H	3.54865419288330	-2.19671087292358	-1.18712090769604
H	4.49357157509661	-1.03234216715766	-0.22715492181895

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PC__{[NONAlAuH]⁻}

Au	-0.20774529026168	0.08400369877321	2.24411970096904
H	1.09974521301393	1.55544853986508	4.51187119536372
C	0.45021863646542	0.86231423774354	5.11871165458086
O	-0.29010474724398	0.05713633712085	4.41910021501926
O	0.49594161638683	0.92472272626167	6.35047279267524
C	-0.15674545981186	3.12349365918023	-4.33786836390986
C	-0.97647034754882	2.24164863974800	-3.60557191114873
C	-0.44737418690084	1.75874534926566	-2.42674088093405
C	0.86519012490076	1.93839922959448	-1.94552024041442
C	1.64658781147448	2.85429294938946	-2.69037332972780
C	1.12163259813342	3.42838993484669	-3.85534849096738
O	-1.19754411390046	0.84505761419503	-1.65462723651051
C	-1.80175724300605	-0.14056621135078	-2.46492000763246
C	-2.40843262659312	0.23345856744453	-3.64598554114400
C	-2.36940618631189	1.72769440128617	-4.00972484214925
C	-2.95958828255988	-0.80966206027708	-4.41687696767082
C	-2.83863675400200	-2.13001425324880	-3.96734475197416
C	-2.14678429622005	-2.46980755994842	-2.79758313457469
C	-1.55098374166386	-1.45228073521865	-2.01421845356644
N	-0.75448562667612	-1.56019230414448	-0.90833855008244
C	-0.56195967987999	-2.87499980763529	-0.32787674888168
C	-2.64036789669514	1.94993399047667	-5.49994509078179
C	-3.44361812732601	2.47770099910018	-3.18172114579384
Al	-0.11242915743563	0.04117147031038	-0.08323079245876
N	1.20595572228500	1.19272517702850	-0.85168881261469
C	2.49719226763927	1.42844395110506	-0.23490877933639
H	-2.02663790527551	-3.51591645639646	-2.51660770678109
H	-3.45844825807386	-0.59858118656236	-5.36172242854780

H	-0.50240534421050	3.55213870510667	-5.27747728203091
H	2.66876673230970	3.07515552432227	-2.38355280985718
H	-2.61413272920203	3.02220932527289	-5.73912024502911
H	-3.63916460037313	1.57725066758784	-5.76615141939176
H	-1.89756141278883	1.43507778928298	-6.12451347231471
H	-3.40165107406584	3.55567418502565	-3.39691501453085
H	-3.28313643775446	2.33452597125629	-2.10575957210157
H	-4.44633154551509	2.10213073069317	-3.43444603556296
H	0.03632183240933	-3.54082110166950	-0.97952320195543
H	-0.03666073638339	-2.76190495428764	0.63145102112678
H	-1.52347605078155	-3.38123263536218	-0.12395962345344
H	2.53706596124446	0.87735832739270	0.71579616060614
H	3.33784942706769	1.09104302437798	-0.87153073076018
H	2.65687404853593	2.49827576569370	-0.00697844478811
H	-3.27892563173701	-2.93167762506271	-4.56478411385593
H	1.74659349833242	4.12225540241681	-4.42227656710579

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PC__{[Me₂NAuH]⁻}

N ⁻	1.36069340710183	0.41859099075255	-0.32747611404562
Au	-0.56521284570132	0.15935525536476	0.18061014061766
H	-3.12399629245316	0.78273156616923	-1.08320675757866
C	-3.49226385618426	0.30241275779717	-0.13769558856403
O	-2.55308013393986	-0.09913197703342	0.67351999599948
O	-4.70276244585491	0.19046060225351	0.06639148093941
C	2.13344752425805	-0.79570356764061	-0.47942265750324
H	1.59782778930267	-1.51431928514770	-1.11721764004443
H	2.38032953303966	-1.31857659132488	0.47987073091120
H	3.11017022762869	-0.56802765116022	-0.96670224324150
C	2.09351248394004	1.37427267231749	0.47541212340915
H	1.52631828152598	2.31234998498344	0.56742686324804
H	3.06955297200048	1.61084502349159	-0.00876496891782
H	2.33773335533611	1.02800021917706	1.51220463477037

7

PC__{[CNAuH]⁻}

Au	-0.29721563282408	-0.11034577170169	-0.05851227733292
H	-2.72558306581105	1.53965389598833	0.21608380426764
C	-3.17956531505999	0.54590824638171	-0.03871510319979
O	-2.31761198944696	-0.42171851116031	-0.22399044983590
O	-4.39933816664951	0.42845296521133	-0.12523744133372
C	1.61588700707978	0.10955339427718	0.06845326439628
N	2.77822716271181	0.24870578100345	0.14333820303840

7

PC__[COAuH]

Au	-0.29567956101812	-0.11863311935262	-0.06448432150034
H	-2.73885486568790	1.57655934939347	0.22293877268426
C	-3.15705734233679	0.57495338119470	-0.03025551103235
O	-2.23247543253055	-0.38803575477204	-0.21110814524209
O	-4.34180052144448	0.36749065992390	-0.13478489112537
C	1.55544932691241	0.08546700735565	0.05533390701213
O	2.68521839610542	0.24240847625695	0.14378018920374

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PC_₂[ClAuH]⁻

Au	-0.37560147394603	-0.31688946590869	0.27091034247515
H	0.84963990055137	0.81871572708091	-2.11118480400117
O	-0.63401314745967	-0.54869955324908	-1.74676035604939
C	0.10220969104918	0.13262810943760	-2.58728397118328
O	0.01476582352764	0.05704037459793	-3.81173251913844
Cl	-0.16399079372249	-0.12791519195868	2.52669130789714

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