Supporting Information
for
How Reduced are Nucleophilic Gold Complexes?
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Computational Details

All geometries were optimized in ORCA 5.0.2,1, 2 using with the low-cost composite DFT method B97-3c from Grimme and co-workers3 based on Becke’s 1997 local exchange correlation functional4 and uses the triple-zeta mTZVP basis set (based on the Ahlrichs basis set def2-TZVP)5 and the corresponding effective core potential,6, 7 to model relativistic effects by replacing the inner 60 electrons of gold. Dispersion effects are accounted for via the D3 model.8, 9 Analytical frequencies were computed, and all structures were found to be well defined minima i.e. all calculated frequencies were positive. An energetic convergence criterion of 10−8 au was request via the TightSCF keyword. The default integration grid (DefGrid2) was used. Solvent effects were included via the conductor-like polarization continuum model (CPCM),10 with toluene specified as the solvent.

Intrinsic bonding orbital analysis (IBO) was performed in IboView,11-13 via additional single point calculations which were performed at the (B97-3c) optimized geometries with the PBE0/def2-TZVPP5 level of theory. The RIJCOSX approximation15 was employed to speed up the integral evaluation, using Weigend’s universal fitting basis set (def2/J). An energetic
convergence criterion of $10^{-8}$ au was requested via the *TightSCF* keyword. The default integration grid (*DefGrid2*) was used. Solvent effects were included via the conductor-like polarisation continuum model (*CPCM*),\textsuperscript{10} with toluene specified as the solvent.

Structural depictions and orbital visualization of all species were produced with *IboView*\textsuperscript{11-13} (source code available at [http://www.iboview.org/]). Orbital were localized with *exp 2*.

*CASSCF*(4,4) calculations were performed by starting with a RHF/def2-SVP calculation at the optimized B97-3c geometries, with separate Pipek-Mezey (PM) orbital localization of the occupied and virtual spaces in ORCA 5.0.2. The CASSCF active space was chosen by identifying $\sigma$-bonding and $\sigma$-antibonding orbitals with large coefficients on the Al, Au and P centres (see Figure S1 for an example). Once the CASSCF(4,4) calculation was converged, further PM localization of the active space only was performed in ORCA, followed by a final CAS-CI calculation. The PM localized active spaces of 1a, 1b, 2a and 2b and shown in Figure 3 and Table S1, respectively.

**Examples inputs**

| Geometry optimization | ! B97-3c Opt Freq DefGrid2 TightSCF CPCM(Toluene) NoTrah SlowConv |
|-----------------------|---------------------------------------------------------------|
| Single point calculations | ! PBE0 def2-TZVPP def2/J RIJCOSX DefGrid2 TightSCF CPCM(Toluene) NoTrah SlowConv |
| CASSCF(4,4) calculations | ! def2-SVP def2/j def2-SVP/C RIJCOSX MoRead |
| %CASscf TratioStep RI Nel Norb Mult end | |

**Figure S1:** Localized PM orbitals of 1a calculated with RHF, used as the initial active space in the subsequent CASSCF(4,4) calculation. Shown is the Al-Au-P(Me$_3$) moiety with hydrogens and all other atoms hidden. Rendered in *IboView*.

**Table S1:** PM localized active spaces of 1b, 2a and 2b, calculated with CASSCF(4,4). The X-Au-L moieties are rendered in *IboView* with orbitals of arbitrary colours, all other atoms are hidden for clarity.
Energy Decomposition Analysis

To further probe the electronic structure, and in particular the Au configuration, Morokuma-Ziegler Energy Decomposition Analysis (EDA)\textsuperscript{16-18} was performed in the Amsterdam Density Functional (ADF) suite of the AMS2020 package.\textsuperscript{19} These calculations were performed at the B97-3c optimized geometry from ORCA, and employed the PBE0 functional\textsuperscript{14} in combination with the triple-$\zeta$ TZ2P basis set.\textsuperscript{20} No frozen core approximation was made. Scalar relativistic effects were modelled via a ZORA Hamiltonian.\textsuperscript{21-25} Numerical quality was defined with the Good keyword. For each EDA calculation only two fragments were defined: i) the metal centre, Au\textsuperscript{n+} and ii) the entire remaining ligand framework L\textsuperscript{n-}. The optimised coordinates were reoriented such that the Au-L bonds lay along the xy axes. The data in Table 2 are a summary of the results in Table S2.

Table S2: EDA of 1(a,b) and 2(a,b), calculated with PBE0-ZORA/TZVP//B97-3c. Along with the instantaneous interaction energy ($\Delta E_{\text{int}}$) the orbital interaction energy ($\Delta E_{\text{orb}}$), the quasiclassical Coulomb interaction ($\Delta E_{\text{elstat}}$) and repulsive Pauli exchange ($\Delta E_{\text{Pauli}}$) terms are also given. All energies are in kcal mol$^{-1}$. For each species, the most favourable configuration (with the smallest $\Delta E_{\text{orb}}$) is emphasized in bold.

| Species | Au configuration | $\Delta E_{\text{int}}$ | $\Delta E_{\text{orb}}$ | $\Delta E_{\text{elstat}}$ | $\Delta E_{\text{Pauli}}$ |
|---------|------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| 1a      | [Xe]4f$^{14}$5d$^{10}$6s$^0$ | -298.65 | -165.98 | -416.47 | 283.80 |
|         | [Xe]4f$^{14}$5d$^{10}$6s$^1$ | -105.97 | -123.34 | -286.88 | 304.25 |
|         | [Xe]4f$^{14}$5d$^{10}$6s$^2$ | -201.25 | -273.03 | -438.04 | 509.83 |
| 1b      | [Xe]4f$^{14}$5d$^{10}$6s$^0$ | -307.16 | -173.13 | -437.27 | 303.24 |
|         | [Xe]4f$^{14}$5d$^{10}$6s$^1$ | -110.43 | -137.38 | -299.10 | 326.04 |
|         | [Xe]4f$^{14}$5d$^{10}$6s$^2$ | -207.45 | -294.03 | -416.23 | 502.81 |
Au partial atomic charges

Partial atomic charges were calculated at the PBE0/def2-TZVPP level of theory, using various computational schemes. The Hirshfeld, Voronoi, Mulliken, Löwdin and Fuzzy partial atomic charges were calculated in MultiWFN 3.8.\textsuperscript{26,27} The IAO charges were calculated in IboView.\textsuperscript{12}

Note: these calculations used pseudopotentials to replace the inner 60 electrons of gold,\textsuperscript{6} and account for relativistic effects. When integrating electron density within an atomic basin (as in the fuzzy topological scheme), this causes a mismatch e.g. the integrated electron density is ~18 but the Au nuclear charge is set to 79, so the calculated net charge is ~61. To remedy this, the charge of Au in the ORCA molden file was manually changed to 19, as described in the MultiWFN manual. To verify the reliability of this procedure, an all-electron calculation was run for 1a, using a ZORA Hamiltonian, the ZORA-def2-TZVPP basis set for all atoms expect gold (for which the SARC-ZORA-TZVPP basis set was used). A comparison of entries 1a and 1a* in Table S3 shows that Hirshfeld, Voronoi and Fuzzy atomic partial charges are less sensitive to a change in the level of theory, as compared to Mulliken and Löwdin charges.

**Table S3:** Partial atomic charges of 1 and 2 calculated within various computational schemes at the PBE0/def2-TZVPP//B97-3c level of theory. The more negative (less positive) atomic charge is highlighted in each case.

| Au (X = Al, B) Partial Atomic Charge |
|--------------------------------------|
| Hirshfeld\textsuperscript{28} | Voronoi\textsuperscript{29} | Mulliken\textsuperscript{30} | Löwdin\textsuperscript{31} | IAO\textsuperscript{12} | Becke\textsuperscript{32} |
|-------------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 1a | -0.071 | -0.125 | -0.232 | -0.003 | 0.503 | -0.965 |
| (0.241) | (0.170) | (0.106) | (-0.291) | (0.084) | (-0.046) |
| 1a* | -0.075 | -0.129 | -0.403 | -0.620 | / | -0.968 |
| (0.241) | (0.169) | (0.342) | (0.249) | / | (-0.046) |
| 1b | -0.053 | -0.071 | -0.222 | 0.125 | 0.178 | -1.254 |
| (0.233) | (0.150) | (0.095) | (-0.299) | (0.472) | (-0.076) |
| 2a | 0.036 | 0.006 | -0.172 | 0.200 | 0.182 | -1.237 |
| (0.006) | (-0.077) | (-0.130) | (-0.614) | (-0.169) | (0.364) |
| 2b | 0.054 | 0.058 | -0.332 | 0.331 | 0.276 | -1.575 |
| (0.000) | (-0.093) | (-0.029) | (-0.620) | (-0.192) | (0.361) |

* Calculated with PBE0-ZORA/def2-TZVPP (for a comparison of the relativistic effects modelled with pseudopotentials vs. all electron with a ZORA Hamiltonian).

**IBOs of all species**

In addition to the IBO analysis of complex 1a (Figure 2) and the IAO partial charge distributions of all species (Table 1), the following plots of the key IBOs of 1a, 1b, 2a and 2b are included here for completeness.

**Table S4:** ($\sigma$-IBO)$^2$ of the X-Au and Au-L bonds in complexes 1 and 2, calculated with PBE0/def2-TZVPP//B97-3c. Orbital isosurfaces rendered in IboView\textsuperscript{11,12} using arbitrary colours to enclose 80% of their electron density.
Method dependency of IBOs

Given the large method dependencies exhibited by partial atomic charges calculated with various schemes (Table S3), we sought to test the method dependence of the IAO partial charge distributions. To this end, we reoptimized the geometry of 1a (starting from the B97-3c optimized geometry, vide supra) with a dispersion-corrected hybrid-GGA exchange-correlation functional paired with a split-valence basis set (B3LYP\textsuperscript{33-36}-D3\textsuperscript{8}(BJ)\textsuperscript{37}/def2-SVP)\textsuperscript{5};
a composite DFT method featuring geometrical counterpoise corrections,\textsuperscript{38} dispersion corrections\textsuperscript{8, 37} and an increased percentage of HF exchange (PBEh-3c),\textsuperscript{39} and a dispersion corrected\textsuperscript{40} tight-binding DFT method (GFN2-xTB).\textsuperscript{41} These methods performed well for gold complexes in our recent benchmark study.\textsuperscript{42}

As for the other calculations, these optimizations were also performed in ORCA 5.0.2. Increased convergence thresholds we requested with the \textit{TightOpt} keyword. The minima were verified \textit{via} frequency analysis. An analytical Hessian was calculated for B3LYP-D3(BJ)/def2-SVP using the \textit{Freq} keyword. Numerical Hessians were the requested for PBEh-3c and GFN2-xTB using the \textit{NumFreq} keyword. For B3LYP-D3(BJ)/def2-SVP and PBEh-3c, the cPCM solvation model was used, with toluene as the solvent. For the GFN2-xTB calculation, the \textit{xtb} executable (v6.4.1) was placed in the ORCA directory and was called using the \textit{xTB2} keyword. The ALPB solvation modelled was used, with toluene specified as the solvent. All of these calculations used effective core potentials to replace the inner 60 electrons of gold.\textsuperscript{6}

Additional single point calculations with PBE0/def2-TZVPP were performed at the optimized geometries to tease apart geometric and electronic effects in the method dependences. These calculations used the same settings as those performed at the optimized B97-3c geometry (\textit{vide supra}). The doubly occupied σ-IBOs of the Al-Au and Au-P bonds calculated with these methods, and with the PBE0 single point calculations, are shown in Table S5. The crucial Al-Au bond polarity varies by just 0.11e. The largest variation (0.22e) is seen for the Au-P bond, calculated with GFN2-xTB vs. PBE0-def2-TZVPP//GFN2-xTB. With all tested methods, the IAO partial charge distributions of the Al-Au and Au-P bonds leave their respective characterization as electron-sharing and dative covalent, and therefore all conclusions regarding oxidation states, unchanged.

Table S5: \((σ\text{-IBO})^2\) and interatomic distances \((d)\) of the Al-Au and Au-P bonds in complex 1a, calculated with SP//GEOM (where SP = PBE0/def2-TZVPP, B3LYP-D3/def2-SVP, PBEh-3c or GFN2-xTB and GEOM = B3LYP-D3/def2-SVP, PBEh-3c or GFN2-xTB). Orbital isosurfaces rendered in IboView using arbitrary colours to enclose 80% of their electron density.

| GEOM = (B3LYP-D3/def2-SVP, PBEh-3c, GFN2-xTB) | (σ\text{-IBO})^2 | d (pm) |
|--------------------------------------------|------------------|--------|
| Al-Au | Au-P | Al-Au | Au-P | Al-Au | Au-P |
| Au(0.85) Al(1.13) | Au(0.16) P(1.71) | Au(0.81) Al(1.18) | Au(0.18) P(1.70) | n/a | n/a |
| 242 | 249 | 242 | 247 | 237 | 258 |

SP=PBE0

| SP=PBE0 | |
|--------|--------|
| Au(0.82) Al(1.16) | Au(0.18) P(1.69) | Au(0.82) Al(1.17) | Au(0.19) P(1.69) | Au(0.89) Al(1.09) | Au(0.13) P(1.74) |
**Comparison to alkyl gold complexes**

To compare highly electron-sharing covalent nature of the Au-Al bond in 1 and 2, we applied the same PBE0/def2-TZVPP//B97-3c level of theory (*vide supra*) to calculate the IAO partial charges in the X-Au-L alkyl gold complexes, where X = Me and L= (P^tBu_3, Me-Au-IPr) i.e. the same L ligands as in 1 and 2. The gold-alkyl bonds are significantly less polarized than their gold-aluminy1 and gold-boryl analogues (Table S6). If we choose some arbitrary threshold for ‘ownership’ of the bonding pair, say 70%, we might say that the Au-Me bonds lie close to the boundary between the electron-sharing and dative bonding regimes. Similar IAO partial charge distributions are found in other coinage metal carbon bonds e.g., [Cu(CF_3)_4]^-.43

**Table S6**: (σ-IBO)^2 of the Me-Au and Au-L bonds in the X-Au-L alkyl gold complexes, where X = Me and L= (P^tBu_3, IPr). IPr = N,N'-bis(dipp)imidazole-2-ylidene, dipp = 2,6-Pr_2C_6H_3. Calculated with PBE0/def2-TZVPP//B97-3c. Orbital isosurfaces rendered in IboView using arbitrary colours to enclose 80% of their electron density.

| L             | Me-Au          | Au-L          |
|---------------|----------------|---------------|
| P^tBu_3       | ![Image](image1) | ![Image](image2) |
| Au(0.61)      | C(1.38)        | Au(0.31)      |
| C(1.61)       |                |               |
| Me-Au-IPr     | ![Image](image3) | ![Image](image4) |
| Au(0.57)      | C(1.41)        | Au(0.31)      |
| C(1.62)       |                |               |

**Valence bond calculations**

Valence bond SCF calculations44, 45 were performed with TURTLE,46, 47 as implemented in GAMESS-UK.48 For the Valence Bond calculations, the def2-SVP basis set5 was used. The model molecules (1a-VB and 2a-VB) were divided in two fragments, viz. the (PH_3)Au fragment and the Al(C_4N_2H_6O)/BH_2 fragment. Startup orbitals for the VB calculation were taken from a prior RHF calculation followed by a Pipek-Mezey49 localization. The Au-M localized bond was used to form the two orbitals, that are used to form the spin coupled Au-M bond. Three structures were included in the calculation: A Au-M, B Au' M', and C Au' M^+. The Gallup and Norbeck (GN)50 and Chirgwin and Coulson (CC)51 schemes are used to calculate the weights of the individual, non-orthogonal, VB structures. During the orbital optimization, the orbitals were kept localized on each fragment.

The final orbitals and their composition are depicted in Figure S2, and the weights of the individual structures are listed in Table S5.
**Figure S2:** VB orbitals of the small model complexes 1a-VB (top) and 2a-VB (bottom).

**Table S5:** GN weights (CC weights) for the three structures.

| Compound | Abbreviation | A Au-M | B Au⁺ M⁻ | C Au⁻ M⁺ |
|----------|--------------|--------|-----------|-----------|
| (PH₃)Au-Al(C₆H₆N₂H₆O) | 1a-VB | 0.620 (0.645) | 0.033 (0.006) | 0.374 (0.322) |
| (PH₃)Au-BH₂ | 2a-VB | 0.681 (0.644) | 0.242 (0.236) | 0.077 (0.120) |

The gold orbital in both compounds have a similar composition, and it has mainly s-character, with some p and d character. The orbital localized on Al is a sp hybrid, while the B orbital is more sp²-like hybridized. For both models, the covalent structure has the highest weight. For Au-Al, the bond is polarized towards the Au atom, indicating a nucleophilic Au species. For Al-B, the polarity is reversed, with the Au⁺ B⁻ structure more important than the Au⁻ B⁺ structure.
Cartesian Coordinates and Energies of Optimized Geometries

| 1a (X = [Al(NON)], L = P(Bu')) |
|----------------------------------|
| (energies in Hartree) |
| \(E_{\text{scf}}(\text{B97-3c})\) = -2419.486848402721 |
| \(E_{\text{SCF}}(\text{B97-3c})\) = -2418.451074492955 |
| \(E_{\text{CASSCF}(4,4)}\) = -2405.295056048773 |
| Thermal correction* (B97-3c) = 0.7132469 |
| **1 atm, 298.15 K, 1 M.** |

| Coordinates |
|-------------|
| \(E_{\text{scf}}(\text{B97-3c})\) = -2419.486848402721 |
| \(E_{\text{SCF}}(\text{B97-3c})\) = -2418.451074492955 |
| \(E_{\text{CASSCF}(4,4)}\) = -2405.295056048773 |
| Thermal correction* (B97-3c) = 0.7132469 |
| **1 atm, 298.15 K, 1 M.** |
| X (Å) | L = PBUS | E_{SCF} (PBEh-3c) |
|------|----------|-------------------|
| 3.25 | 1.067 | * -241.570256096932 |
| 3.23 | 1.081 | * -241.645141230496 |

*Thermal correction* (PBEh-3c) = 0.75101439

*1 at., 298.15 K, 1 M.*
1a (X = [Al(NON)]₄, L = P(Bu)₃)

| Energy in Hartree |
|-------------------|
| E_{SCF}(GFN2-xTB) = -126.091326242360 |
| E_{SCF}(PBE0/def2-TZVPP/GFN2-xTB) = -2418.420455195634 |

**Thermal correction** (GFN2-xTB) = 0.7006145

*1 atm, 298.15 K, 1 M.*

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**S12**
| X | (energies in Hartree) |
|---|----------------------|
| C | -2.41161769825403 | 0.1497345867895 |
| C | -1.17037444829262 | -0.4922497868723 |
| C | 0.40594432125256 | 0.00015200517417 | -0.87705807459499 |
| C | 0.193652456856888 | -0.6335201557190 |
| C | -0.43887187440997 | 0.22007773850492 | 0.09159236029695 |
| C | 0.35641192682819 | -0.65192036243088 |
| N | 0.10589950713017 | 0.30841750232499 |
| C | 0.88538868067111 | 0.95428546731256 |
| C | 0.17118497277121 | 0.6203583831124 |
| N | 1.62524057378733 | 0.345493205743 |
| C | 0.57939427989828 | 0.54422584614400 |
| Au | 0.11600644956764 | -0.00175299759789 |
| Al | -0.53129167510671 | 0.0613989227327 |
| N | 0.46121389353201 | 0.06487195152655 |
| N | 0.81704672999778 | 0.25135200532325 |
| N | 0.16748857368241 | 0.21534030168466 |
| N | 0.21246795607275 | 0.4293409210848 |
| N | 0.12303673262068 | 0.14101753493293 |
| N | 0.57516076666486 | 0.495321906219 |
| N | 0.85715630381684 | 0.36376751031342 |
| N | 0.43208869368733 | 0.8673738262257 |
| N | 0.91354026420120 | 0.49928938960919 |
| N | 0.25976653302200 | 0.39627087562466 |
| N | 0.258762427746340 | 0.537126652149311 |
| N | 0.4042022010772 | 0.33298725373499 |
| N | 0.52475616014114 | 0.5442938389524 |
| N | 0.31767856515608 | 0.56350720757519 |
| N | 0.71168314124601 | 0.43941444526192 |
| N | -0.23330540843733 | -0.28522507058167 |
| N | -0.33731919506299 | -0.23217705432999 |
| N | -0.39159632965994 | -0.17933761479671 |
| N | -0.51204138239739 | -0.8400429314817 |
| N | -0.56211496086889 | -1.966735035517 |

$1b$ ($X = [\text{Al}(\text{NON})], \text{L} = \text{IPr}$)
### 2a

**Equations and Energy Values**

\[ E_{SCF}(B97-3c) = -1517.2278441329 \]

\[ E_{SCF}(PBE0/def2-TZVP//B97-3c) = -1516.438379805822 \]

**Thermal Correction**

**B97-3c**

\[ T = 0.54316597 \]

*1 atm, 298.15 K, 1 M.*

### 2b

**Equations and Energy Values**

\[ E_{SCF}(B97-3c) = -1862.134268302139 \]

\[ E_{SCF}(PBE0/def2-TZVP//B97-3c) = -1861.164407763792 \]

*Additional Information*
E_{\text{CASSCF}(4,4)} = -1848.863824963147

Thermal correction* (B97-3c) = 0.7276547

*1 atm, 298.15 K, 1M.
### 1a-VB (X = [Al(C₅H₇O₃)], L=PH₃)

| Bond | (energies in Hartree) |
|------|----------------------|
| C    | 4.756302971518      |
| O    | 2.52187957403738     |
| H    | 2.42799271355529      |
| C    | 2.70786325752984     |
| H    | 2.08805440852669      |
| C    | 2.72379425158691     |
| H    | 0.75662869572635      |
| C    | 1.45097332273148     |
| H    | 0.37802419192766      |
| C    | 2.7574195193066      |

### 2a-VB (X = [BH₃], L=PH₃)

| Bond | (energies in Hartree) |
|------|----------------------|
| B    | 2.25975224304806      |
| H    | 0.000000629171614     |
| C    | 0.00445631154604      |
| B    | 0.20319645586456     |
| H    | 0.00359714318173      |
| C    | 0.09869820430473     |
| B    | 0.47997925605556      |
| H    | 0.1044338967845      |
| C    | 0.07968876355593      |
| B    | 0.23044166749723      |
| H    | 0.1127071007500      |
| C    | 0.49626888988881     |

### Me–Au–P'B₃

| Bond | (energies in Hartree) |
|------|----------------------|
| Au  | 0.3791519420158      |
| P    | 1.0754142974555     |
| C    | 0.79117457180441     |
| H    | 0.24002637030266     |
| C    | 0.11532489296867     |
| H    | 0.6842153226256      |
| C    | 0.64901735268877     |
| H    | 0.2052264929632601   |
| C    | 0.8086942092601      |
| H    | 0.37802149197766     |
| C    | 0.84900402305455     |
| H    | 0.207037103483211    |
| C    | 0.75662869572635     |
| H    | 0.8086942092601      |
| C    | 0.84900402305455     |
| H    | 0.207037103483211    |

*1 atm, 298.15 K, 1M.
| atom   | x         | y         | z         | energy (Hartree) |
|--------|-----------|-----------|-----------|-----------------|
| H      | 1.17145796399253 | 3.7668940212594 | -0.35677924345036 |                      |
| H      | 3.40106689555853 | 2.04842859189298 | -0.49013215706087 |                      |
| H      | 4.13839394601151 | 0.45342812153741 | 0.0675686316866 |                      |
| H      | 3.07497099253966 | 1.98520359052530 | -1.1217729587394 |                      |
| H      | 3.63066878004251 | 3.65083598880304 | -0.10420343729755 |                      |
| H      | 0.78914780941029 | 2.99407292898513 | -0.1915703738453 |                      |
| H      | 1.5487230553522 | 4.5856067774801 | -0.9716616845997 |                      |
| H      | 0.34322189570578 | 4.14919668251651 | 0.2248736377170 |                      |
| H      | 4.3378183105778 | 1.4530097839262 | 2.6676118405290 |                      |
| H      | 0.4133596802286 | 2.0639122861913 | 3.50702910695481 |                      |
| H      | 5.0975507047967 | 0.76566558977510 | 0.30373249460336 |                      |
| H      | 4.82399108027593 | 2.10840558577553 | 1.94796826370294 |                      |
| H      | -0.34256919249964 | 3.31296236379328 | 2.50080248130934 |                      |
| H      | 0.1275633221282 | 4.26076999725952 | 2.27410409482111 |                      |
| H      | -0.9158204338383 | 2.98550312525914 | 0.6833565705702 |                      |
| H      | -1.14807118908789 | 3.48877452501900 | 1.3662190179598 |                      |
| H      | 2.9177972809604 | 4.38281221857604 | 1.37355336703638 |                      |
| H      | 2.01235512636032 | 4.80727843756870 | 1.99729954058669 |                      |
| H      | 3.6804159267665 | 0.43219753851333 | 0.20374532996467 |                      |
| H      | 3.26476879571645 | 5.14786675010399 | 0.7347223985681 |                      |

**E_{SCF} (B97-3c)**

\[-1335.500171218346\]

**E_{SCF} (BPEO/de2-TZVPP/B97-3c)**

\[-1334.743071377256\]

**Thermal correction**

\[B97-3c\]

\[0.53908188\]

*1 atm, 298.15 K, 1M.*
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