Supporting Information for:

A Heterodinuclear, Formal $Au^{+I}Pt^{0}$ Complex with Weakly Bound Alkene Ligands

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1 Experimental Methods and Characterization Techniques

1.1 General Considerations

Unless otherwise stated, reactions were performed in an inert atmosphere by using standard vacuum and Schlenk techniques employing an argon Schlenk line or a nitrogen glove box (atmosphere kept below 1 ppm O_2/H_2O). All solvents were dried over CaH_2 under a continuous flow of argon and distilled on freshly activated 3 Å molecular sieves for storage. For the preparation of $[(Ph_3P)AuPt(nbe)_3][BAr_4^F]$ (**3**$[BAr_4^F]$), special H- or double-Schlenk flasks sealed with teflon or glass valves (Gebr. Rettberg GmbH) were employed, which enable filtration from one side into the other through a G4 frit at low temperature. For this purpose, the entire apparatus is cooled in a large cooling bath. NMR tubes with a PTFE valve were used to exclude air and moisture. The glassware was stored overnight in an oven set to 140 °C and heated under vacuum prior to use. All this diligence has been exercised particularly as a precaution and in order to avoid water to condense while working at low temperatures. However, all starting compounds are air stable and also the crystalline product in its solvent-free form appears to be stable in air for at least one week. All commercially available reagents were used as received. $H_2[PtCl_6] \cdot 6\ H_2O$ and $H[AuCl_4] \cdot 3\ H_2O$ were synthesized by dissolving elemental Pt and Au, respectively, in *aqua regia*, followed by the destruction of nitric acid by repeated additions of hydrochloric acid and finally careful evaporation of all volatiles. $[(Ph_3P)AuCl]$,[1] $[Pt(nbe)_3]$ (**4**),[2] and $Na[BAr_4^F]$[3] were synthesized following known procedures.

1.2 NMR Spectroscopy

NMR spectra were recorded using a Bruker Avance II$^+$ 400 MHz WB NMR spectrometer with a 5mm ATM-BBFO probe head and a variable-temperature device. The data were processed with the Topspin 3.6 software. ^1H and ^{13}C chemical shifts are reported relative to TMS. The (residual) solvent signals were used for calibration.[4] For the other nuclei, chemical shifts are given with respect to: 15 % $BF_3 \cdot OEt_2$ in $CDCl_3$ (^{11}B), neat $CFCl_3$ (^{19}F), 85 % H_3PO_4 (^{31}P), and 1.2 M Na_2PtCl_6 in D_2O (^{195}Pt). Chemical shifts are reported in ppm, and coupling constants (*J*) are reported in Hz. NMR assignments were assisted by 2D experiments as required.

1.3 Raman Spectroscopy

Raman spectra were recorded at –78 °C on a Vertex 70 IR-spectrometer with a RAM II Raman module (1064 nm exciting line of a Nd:YAG laser) by using a highly sensitive liquid-N_2 cooled Ge detector with a resolution of 4 cm^{-1}. The data were processed with the software package OPUS 7.5. For all spectra, the signal intensity was normalized to 1 and the relative band

intensities are described as follows: ≥ 0.8 very very strong (vvs), ≥ 0.7 very strong (vs), ≥ 0.6 strong (s), ≥ 0.5 medium strong (ms), ≥ 0.4 medium (m), ≥ 0.3 medium weak (mw), ≥ 0.2 weak (w), ≥ 0.1 very weak (vw), < 0.1 very very weak (vvw).

1.4 Single-Crystal X-Ray Diffraction

Single-crystal X-ray data were collected on a Bruker APEX2 QUAZAR three-circle diffractometer and a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer both with a microfocus sealed X-ray tube using Incoatec mirror optics as a monochromator. Both diffractometers are equipped with an Oxford Cryostream 800 low-temperature device, and MoK_α radiation (λ = 0.71073 Å) was used for all measurements. Single crystals of solvated [(Ph$_3$P)AuPt(nbe)$_3$][BAr$_4^F$] (**3**[BAr$_4^F$] · 3 CH$_2$Cl$_2$) and [Pt(nbe)$_3$] (**4**) were mounted at –50 °C in perfluoroether oil under an N$_2$ stream employing a custom-built low-temperature mounting-device and were shock-cooled to 100.0 K on the diffractometer. Solvent-free crystals of [(Ph$_3$P)AuPt(nbe)$_3$][BAr$_4^F$] (**3**[BAr$_4^F$]) were mounted at room temperature and measured at 100.0 K. All data were integrated with SAINT,[5] and a multi-scan absorption-correction using SADABS-2016/2 was applied.[6] The structures were solved by direct methods using SHELXT 2014/5[7] and refined by full-matrix least-squares methods against F2 by SHELXL-2018/3[8] employing shelXle (Revision 940).[9] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond-length restraints and displacement-parameter restraints. Some parts of the disorder model were introduced by the program DSR.[10] This was particularly important for the treatment of the disorder found for [Pt(nbe)$_3$] (**4**). Crystallographic data (including structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. CCDC 1966140, 1966141, and 1966142 contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

1.5 Mass Spectrometry

The mass-spectrometric experiments were performed with a Thermo-Fischer LTQ XL linear ion-trap mass-spectrometer equipped with an electrospray-ionization (ESI) source. Mass spectra of [(PPh$_3$)AuPt(nbe)$_3$][BAr$_4^F$] (**3**[BAr$_4^F$]) were obtained by electrospray ionization from a millimolar solution in dichloromethane cooled to −60 °C. In order to avoid decomposition,

we employed the so-called "pressurized sample infusion" technique described by McIndoe and co-workers.[11] However, we employed a very thin and short silica capillary instead of the described PEEK tubing. We adjusted the Capillary Temperature to 75 °C in order to avoid fragmentation of the ions on their way to the analyzer. Nitrogen was used as a Sheath, Sweep, and Auxiliary Gas at flow rates to 5, 0, and 0, respectively (given in arbitrary units). The Source Voltage was set to 3.5 kV, the Tube Lens Voltage was adjusted to 95 V, and the Capillary Voltage was set to 20 V. Given *m/z* values are based on the isotopologues, which contain only ^{1}H, ^{13}C, ^{31}P, ^{194}Pt, and ^{197}Au. Note, that this signal is not necessarily the highest signal of the corresponding isotope pattern. The identity of the ions was confirmed by comparison of the relative signal intensities with simulated isotope patterns, complemented by collision-induced dissociation (CID). In the CID experiments, helium served as collision gas. The supplied collision energy was adjusted by varying the Normalized Collision Energy (NCE) between 0 and 40. Note that this value is given in arbitrary units, and a conversion to an E_{lab} scale is difficult. Therefore, we refrain from a more detailed discussion of absolute collision energies.

1.6 Quantum Chemical Calculations

The majority of the DFT calculations has been performed using the program package TURBOMOLE V7.2.[12] Geometry optimizations were performed with the generalized-gradient approximation (GGA) density functional BP86[13] together with the split-valence basis set def2-SVP and the corresponding ECPs.[14,15] The RI approximation was used.[16,17] For the energies, single-point calculations were added employing the non-empirical global hybrid GGA PBE0[18] (with 25% exact exchange) together with a valence triple-zeta basis set with two sets of polarization functions, def2-TZVPP.[15,19] For the calculations of the molecular orbitals, [Pt(nbe)$_3$] (**4**) and [Pt(PPh$_3$)$_3$] (**5**) were optimized on the higher level of theory. The accuracy of the DFT method was improved by adding the empirical dispersion correction DFTD3[20] (V3.1) using Becke-Johnson damping (BJ-damping).[21] The m4 grid was used for both the geometry optimizations and the single-point calculations. The discussion of the computational findings is confined to the singlet state of the various complexes because the NMR data do not indicate any paramagnetic components to be involved in the experiments. All electronic energies (given in kJ mol^{-1}) are corrected for zero-point vibrational energy contributions;[22] for the single-point energies on the higher level of theory, the zero-point correction from the lower level has been added. The frequency calculations also aid in confirming the optimized geometries to be minimum structures on the potential-energy surfaces.

1.7 Calculations of Raman Spectra

The Raman spectra were calculated with the program Gaussian 16.[23] Both the geometry optimizations and the Raman-frequency calculations were performed with the B3LYP[24] functional employing the split-valence basis set with polarization functions def2-TZVP (together with the corresponding ECPs) for all atoms.[15,17] It was crucial to employ this flexible basis set in order to identify the relevant vibrational modes unequivocally. The employment of smaller basis sets caused some vibrational modes to be "contaminated" with contributions present in other modes. The employment of the B3LYP functional reproduced the measured spectra best.

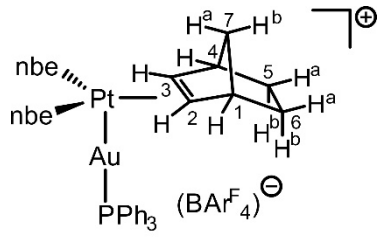
1.8 Population Analyses

MULLIKEN[25] and NPA[26] calculations were performed as single-points on the PBE0/def2-TZVPP//BP86/def2-SVP level of theory with TURBOMOLE, employing the $pop keyword in the control file. For the QTAIM calculations (QTAIM = Quantum Theory of Atoms In Molecules),[27] wfn files were generated by the $wfn keyword. The multifunctional wavefunction analyzer Multiwfn was employed to analyze the wfn files.[28] A basin analysis (options 17 + 1) was performed on the electron density (option 1) employing a high quality grid (spacing = 0.06 Bohr, option 3). The electron density was integrated with atomic-center + uniform grids and with exact refinement of the basin boundaries (options 7 + 2 + 1). As a result, the atomic charges after normalization are given.

2 Synthesis and Characterization of 3[BAr$_4^F$]

2.1 Synthesis of 3[BAr$_4^F$]

[Pt(nbe)$_3$] (**4**) (130.9 mg, 0.274 mmol, 1.0 eq.), [(Ph$_3$P)AuCl] (135.7 mg, 0.274 mmol, 1.0 eq.), and Na[BAr$_4^F$] (243.1 mg, 0.274 mmol, 1.0 eq.) were weighed into one arm of a double-Schlenk flask equipped with a G4 frit. While cooling the whole apparatus to –78 °C in an ethanol/dry-ice bath, dry methylene chloride (29 ml) was filled into the other arm of the flask, and after two freeze-pump-thaw cycles, the solvent was condensed onto the solids. The reaction mixture was stirred at –50 °C until all components were completely dissolved. A slight turbidity indicates the formation of sodium chloride as a by-product. The mixture was cooled to –78 °C and filtered at this temperature (it is necessary that the frit and the whole flask is cooled to –78 °C in order to prevent decomposition). After another set of two freeze-pump-thaw cycles, the solution was allowed to warm up to −50 °C, and the volatile components were removed. Partial removal of the solvent by gas-phase transfer into the other leg of the double-Schlenk flask and storage of the resulting solution at −78 °C gave rise to crystals of [(Ph$_3$P)AuPt(nbe)$_3$][BAr$_4^F$] (**3**[BAr$_4^F$] · 3 CH_2Cl_2). Complete removal of the solvent resulted in 423 mg (0.232 mmol, 85 %) of the crude product as a beige powder, which was pure enough for our experiments. After several washings with methylene chloride (4 x 1 ml; the CH_2Cl_2 was condensed onto the solid from the other side of the flask) at –78°C, the title compound was obtained as a pale yellow powder.



3(BAr$^F_4$)

^{1}H-NMR (400.17 MHz, CD_2Cl_2, 223 K) **3**$^+$: δ = –0.58 (d, $^2J_{7a7b}$ = 10.0 Hz, 3H, 7-H^a), 0.36 (d, $^2J_{7b7a}$ = 10.0 Hz, 3H, 7-H^b), 1.29 (d, $^2J_{5b5a}$/$^2J_{6b6a}$ = 7.8 Hz, 6H, 5-H^b, 6-H^b), 1.72 (d, $^2J_{5a5b}$/$^2J_{6a6b}$ = 7.8 Hz, 6H, 5-H^a, 6-H^a), 3.17 (s, 6H, 1-H, 4-H), 4.45 (s, 6H, 2-H, 3-H), 7.14 (m, 6H, *o*-H), 7.43 (m, 6H, *m*-H), 7.53 (s, 3H, *p*-H) ppm. [BAr$_4^F$]$^-$: δ = 7.53 (s, 4H, *p*-H), 7.71 (s, 8H, *o*-H) ppm.

^{13}C{^{1}H}-NMR (100.62 MHz, CD_2Cl_2, 223 K) **3**$^+$: δ = 27.2 (s, 5-C, 6-C), 40.8 (s, 7-C), 42.6 (s, 1-C, 4-C), 74.7 (s, 2-C, 3-C), 132.4 (s, *p*-C), 126.3 (d, $^1J_{CP}$ = 62.4 Hz, *ipso*-C), 129.4 (d, $^3J_{CP}$ = 12.2 Hz, *m*-C), 133.2 (d, $^2J_{CP}$ = 13.4 Hz, *o*-C) ppm. [BAr$_4^F$]$^-$: δ = 124.2 (q, $^1J_{CF}$ = 272.5 Hz, CF_3), 128.4 (qq, $^2J_{CF}$ = 31.6 Hz, $^3J_{CB}$ = 2.9 Hz, *m*-C), 117.3 (s, *p*-C), 134.4 (s, *o*-C), 161.5 (q, $^1J_{CB}$ = 49.5 Hz, 8H, *ipso*-C) ppm.

$^{31}P\{^{1}H\}$-NMR (161.99 MHz, CD_2Cl_2, 223 K) δ = –1.84 ppm (s with ^{195}Pt satellites, $^{2}J_{PPt}$ = 770 Hz).

^{195}Pt-NMR (86.02 MHz, CD_2Cl_2, 223 K) δ = –4364 (d, $^{2}J_{PtP}$ = 770 Hz) ppm.

^{19}F-NMR (376.54 MHz, CD_2Cl_2, 223 K) δ = –62.57 (s, Ar-CF_3) ppm.

^{11}B-NMR (128.39 MHz, CD_2Cl_2, 223 K) δ = –6.65 (s) ppm.

FT Raman (38 x 100 scans, 70 mW, 200 K, 4 cm^{-1}): $\tilde{\nu}$/cm^{-1} (intensity) = 3066 (w), 3025 (vw), 2993 (vw), 2961 (vw), 2928 (vw), 2878 (vw), 1611 (vw), 1589 (m), 1450 (vw), 1406 (vw), 1366 (vw), 1276 (vw), 1209 (vw), 1174 (vw), 1101 (w), 1081 (vw), 1030 (vw), 1001 (vs), 964 (vw), 934 (vw), 874 (vw), 857 (vw), 803 (vw), 745 (vw), 705 (w), 674 (vw), 646 (vw), 618 (vw), 565 (vw), 542 (vw), 476 (vw), 456 (vw), 408 (vw), 286 (vw), 264 (w), 229 (w), 209 (vw), 184 (vw), 174 (vw), 163 (vw), 129 (vw), 75 (vs).

An elemental analysis could not be performed due to the high sensitivity of the compound towards elevated temperatures. The amount of the solvent-free crystals, obtained as "survivors" by controlled decomposition at room temperature, was not high enough for elemental analysis.

2.2 Choice of CH_2Cl_2 as a Solvent

Numerous experiments have shown that **3**[BAr_4^F] decomposes in solution at elevated temperatures. A solution in CH_2Cl_2 starts to decompose above −40 °C, and the color changes from light yellow to black. The time until complete decomposition occurs amounts to few hours at −20 °C according to NMR-experiments at different temperatures. As a consequence, all manipulations were performed at temperatures below −50 °C and in special "double-Schlenk flasks", in which two volumes are separated by a frit. This setup allows filtration at low temperatures. Further, the choice of the anion is crucial to stabilize $[(Ph_3P)AuPt(nbe)_3]^+$ (**3**). Previous experiments showed that $[BF_4]^-$ is unsuitable for the generation of this cation and particularly for its crystallization. We are aware that dichloromethane is not an ideal solvent for AuPt chemistry since solutions of $[(Ph_3P)AuPt(PPh_3)_3][BF_4]$ (**1**[BF_4]) in dichloromethane decompose at ambient temperature.[29] However, at low temperature, $[(Ph_3P)AuPt(nbe)_3][BAr_4^F]$ (**3**[BAr_4^F]) is stable in dichloromethane, and this solvent combines good dissolving power and a high vapor pressure, the latter of which is crucial for the evaporation at low temperatures. The temperature lability is also observed in other solvents (see below).

2.3 Solubility and Stability of 3[BAr_4^F] in Different Solvents

To a small amount of **3**[BAr_4^F] (≈ 5 mg), toluene, 2,2,2-trifluoroethanol, acetonitrile, diethyl ether, and *ortho*-difluorobenzene were added at −50 °C. The mixtures were then allowed to

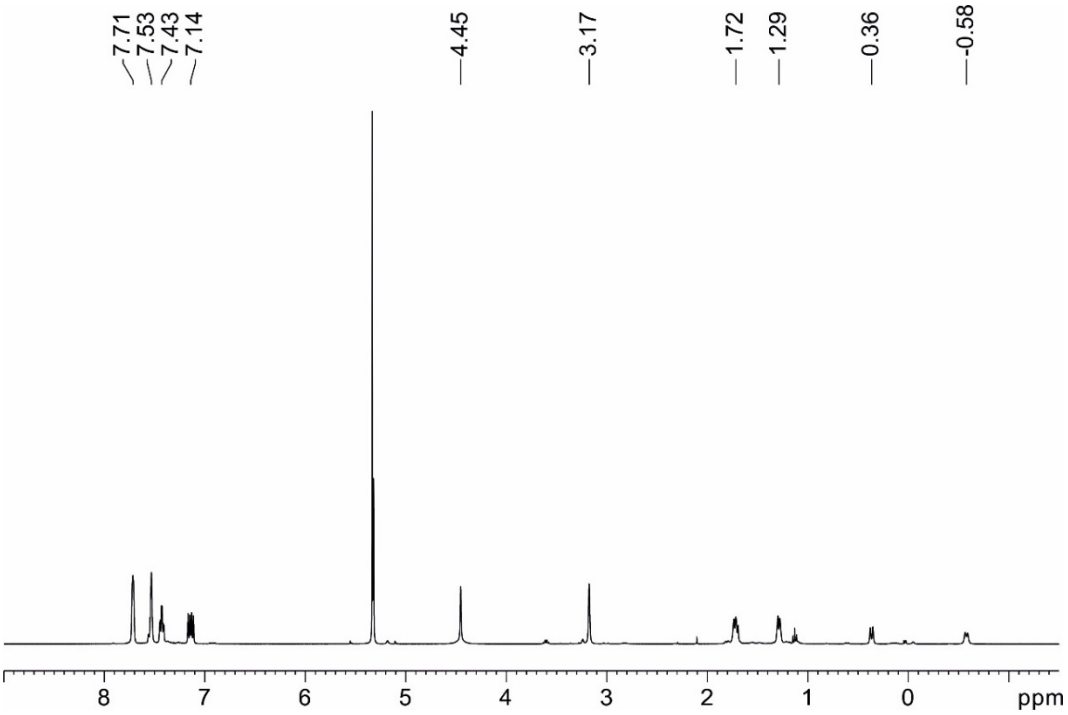
warm to room temperature. At low temperature, **3**[BAr_4^F] is completely insoluble in toluene and 2,2,2-trifluoroethanol; at room temperature, the solid turns deep brown. In acetonitrile, diethyl ether, and *ortho*-difluorobenzene, **3**[BAr_4^F] is soluble at –50 °C. When the colourless solutions are warmed to room temperature, they turn deep orange. ESI-MS spectra of the three solutions at room temperature did not show any sign of the presence of **3**.

2.4 Stability of Crystals of 3[BAr_4^F] · 3 CH_2Cl_2 and 3[BAr_4^F]

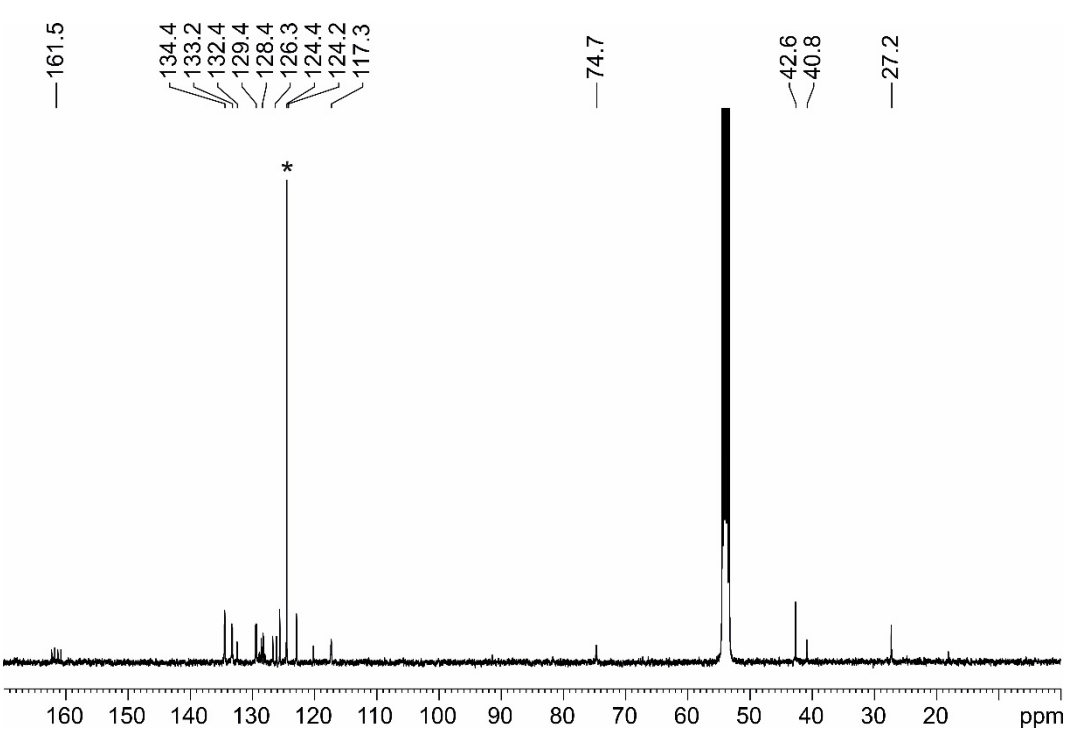
3[BAr_4^F] is generated from a mixture of [(Ph_3P)AuCl], [Pt(nbe)$_3$] (**4**), and Na[BAr_4^F] in dichloromethane at −50 °C. A saturated solution of **3**[BAr_4^F] is obtained by partial evaporation of the solvent and filtration at −50 °C. From this solution, crystals of **3**[BAr_4^F] · 3 CH_2Cl_2 suitable for single-crystal X-ray diffraction (SC-XRD) were obtained by cooling to −78 °C. The reflections of a crystal of **3**[BAr_4^F] · 3 CH_2Cl_2, monitored in a temperature-dependent SC-XRD experiment, are observed even after hours when the crystal is kept below 273 K. At room temperature, while kept under a stream of nitrogen on the diffractometer, the reflections of this crystal disappear after minutes. When the crystalline bulk material (covered with perfluoroether oil) is allowed to reach room temperature, a continuous color change from colorless to brown occurs within minutes. Upon microscopic inspection of the amorphous bulk material after one day, however, a small amount of crystalline, solvent-free **3**[BAr_4^F] is found. These solvent-free crystals are stable at room temperature in air for at least one week. Thus, decomposition of **3**[BAr_4^F] at room temperature occurs only in the presence of solvent molecules, while the crystalline compound did not react with the surrounding oil or traces of solvent possibly dissolved in the oil.

We have evidence that the solvent-free crystals were not generated by the desolvation of **3**[BAr_4^F] · 3 CH_2Cl_2 but that both **3**[BAr_4^F] and **3**[BAr_4^F] · 3 CH_2Cl_2 crystallized together. We conclude this from experiments, in which we applied vacuum to a crystalline sample of **3**[BAr_4^F] · 3 CH_2Cl_2 in a Schlenk-flask, which was cooled to −40°C. We allowed the material to warm to room temperature over several hours, while being kept under vacuum. The resulting material did not differ from the material obtained before in the drop of oil as judged by microscopic inspection. We conclude from this experiment that the solvent-free (and thus room-temperature stable) form of **3**(BAr_4^F) was present already before warming. While the structural parameters of **3** in **3**[BAr_4^F] and **3**[BAr_4^F] · 3 CH_2Cl_2 differ slightly (SI 32), we interpret these differences in terms of packing effects and as a consequence of the different cell parameters (SI 29).

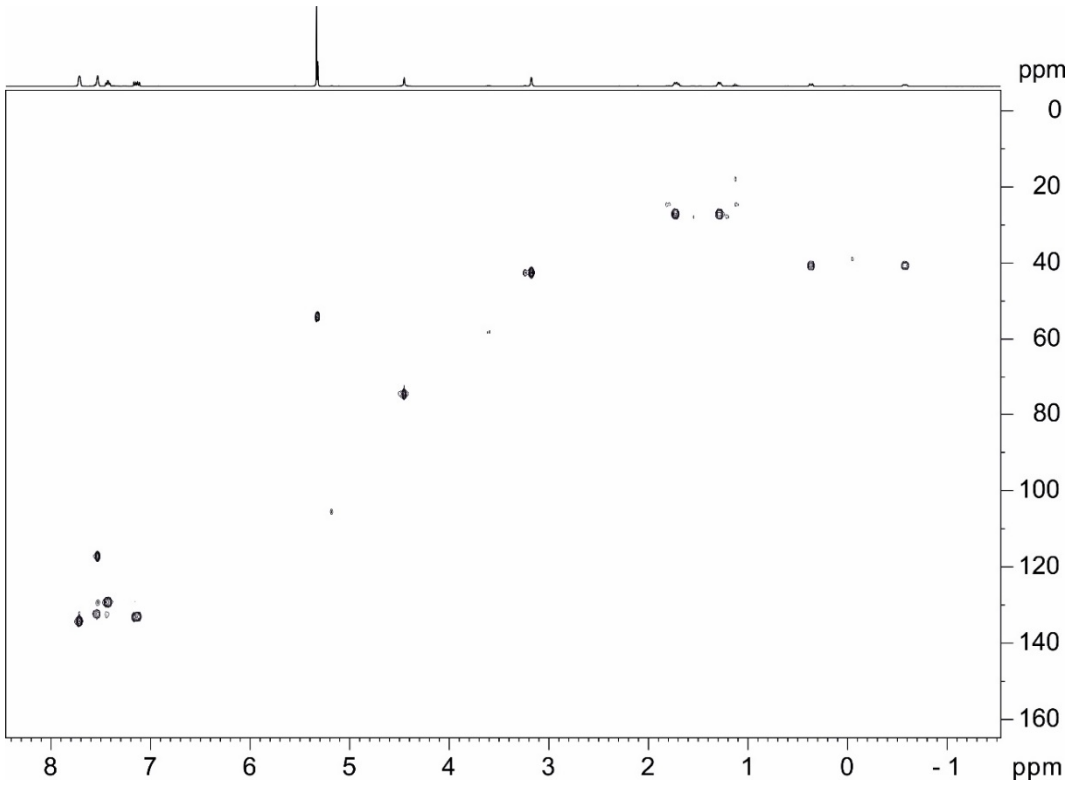
2.5 NMR Spectra of 3[BAr_4^F] at 223 K



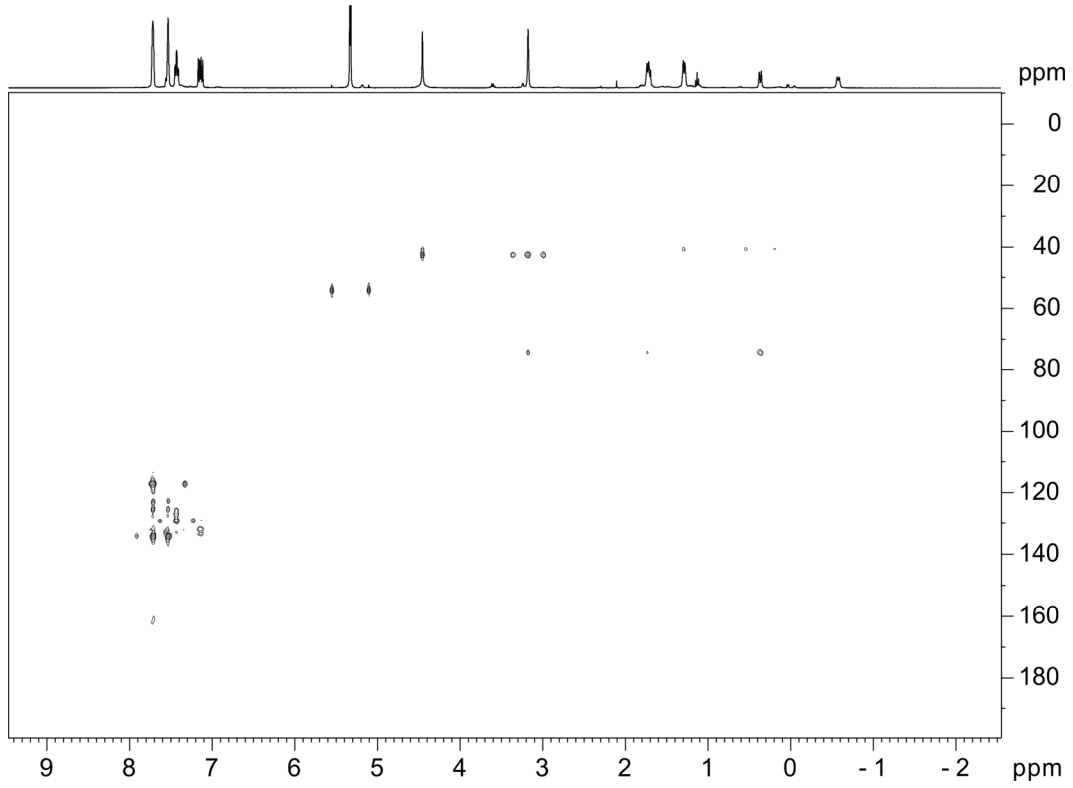
SI 1: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F].



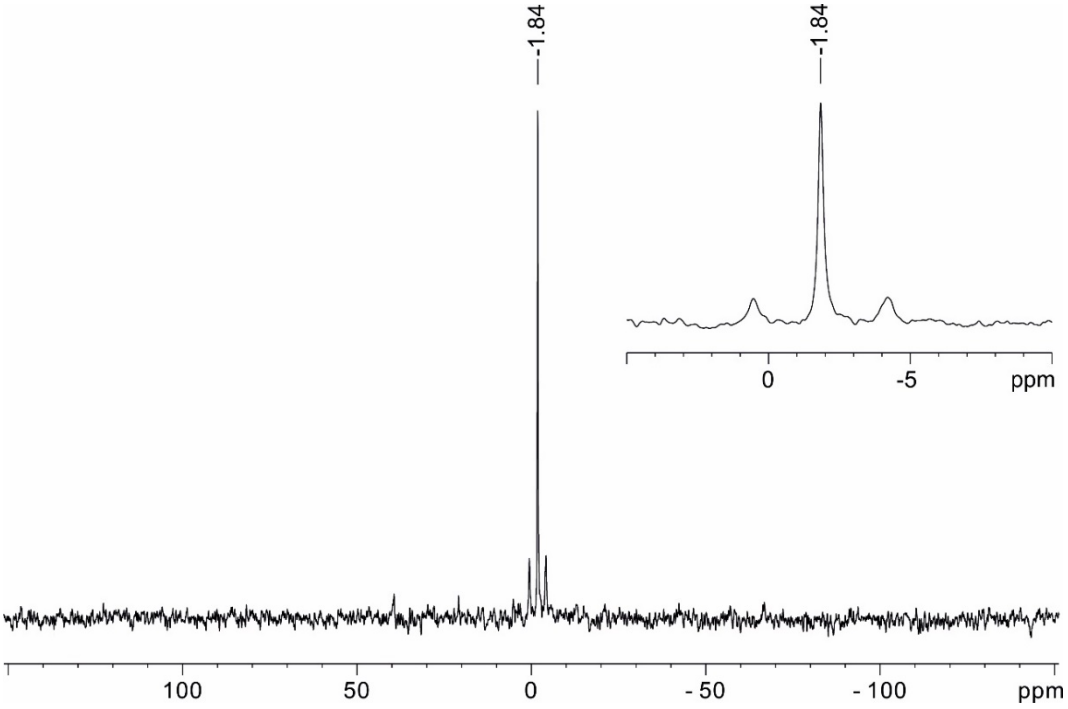
SI 2: $^{13}C\{^1H\}$-NMR spectrum (100.62 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F]. The signal indicated with an asterisk corresponds to CO_2, which must have leaked into the NMR tube during storage in dry ice overnight before the VT-NMR experiments.



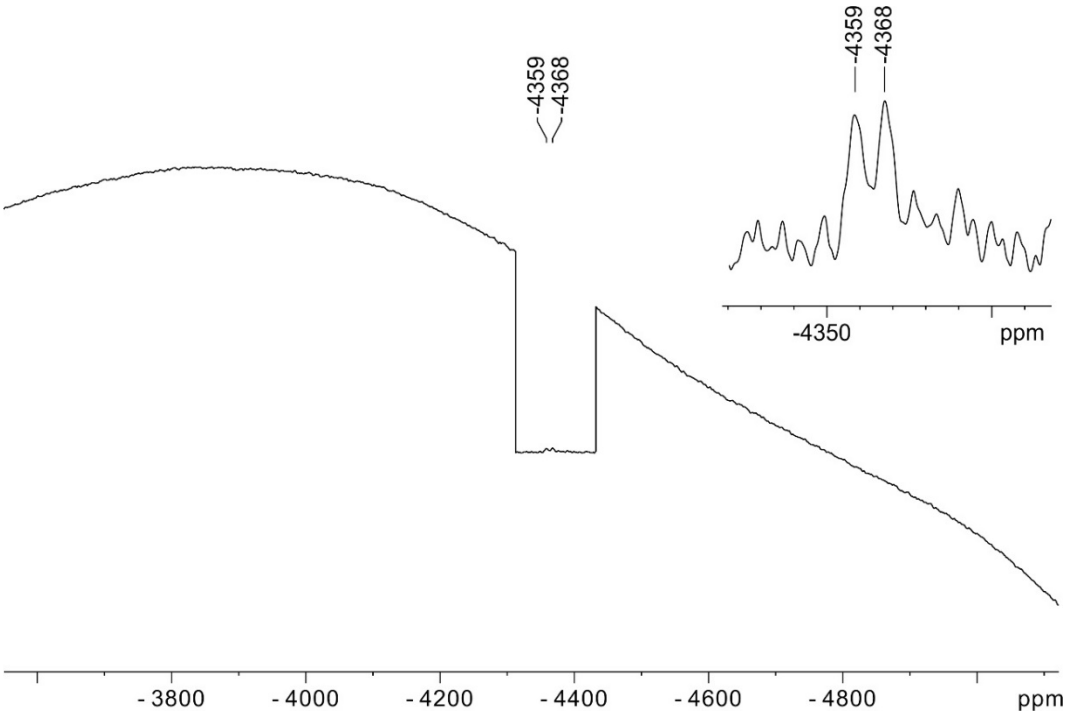
SI 3: $^{1}H,^{13}C$-HSQC spectrum (400.17 MHz, 100.62 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F].



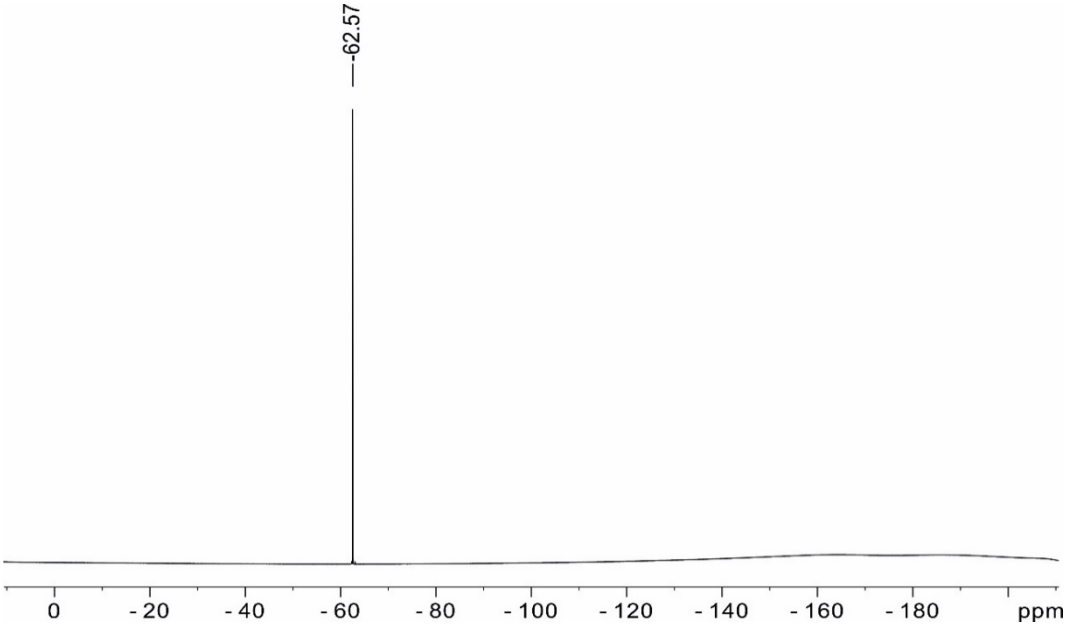
SI 4: $^{1}H,^{13}C$-HMBC spectrum (400.17 MHz, 100.62 MHz, CD_2Cl_2, 223 K, optimized for coupling constants of 8 Hz) of isolated crystals of **3**[BAr_4^F].



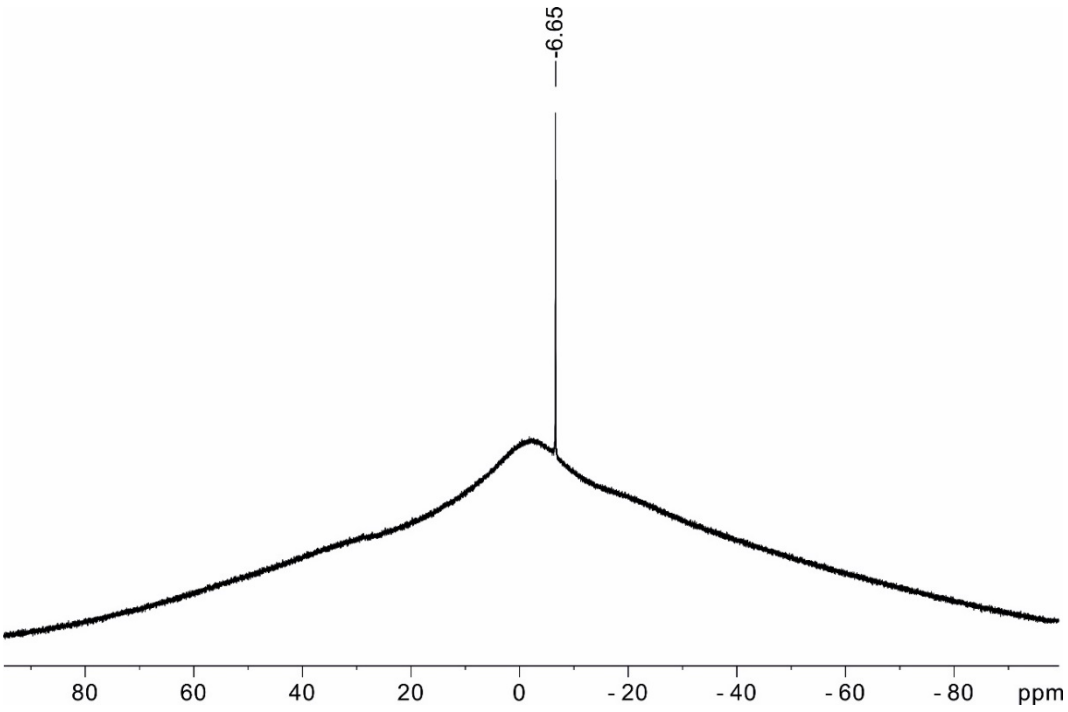
SI 5: $^{31}P\{^{1}H\}$-NMR spectrum (161.99 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F]. The inset shows the characteristic singlet with ^{195}Pt-satellites ($^2J_{PPt}$ = 770 Hz) in more detail.



SI 6: Partially baseline-corrected ^{195}Pt-NMR spectrum (86.02 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F]. The inset shows the characteristic doublet ($^2J_{PPt}$ = 770 Hz) in more detail.



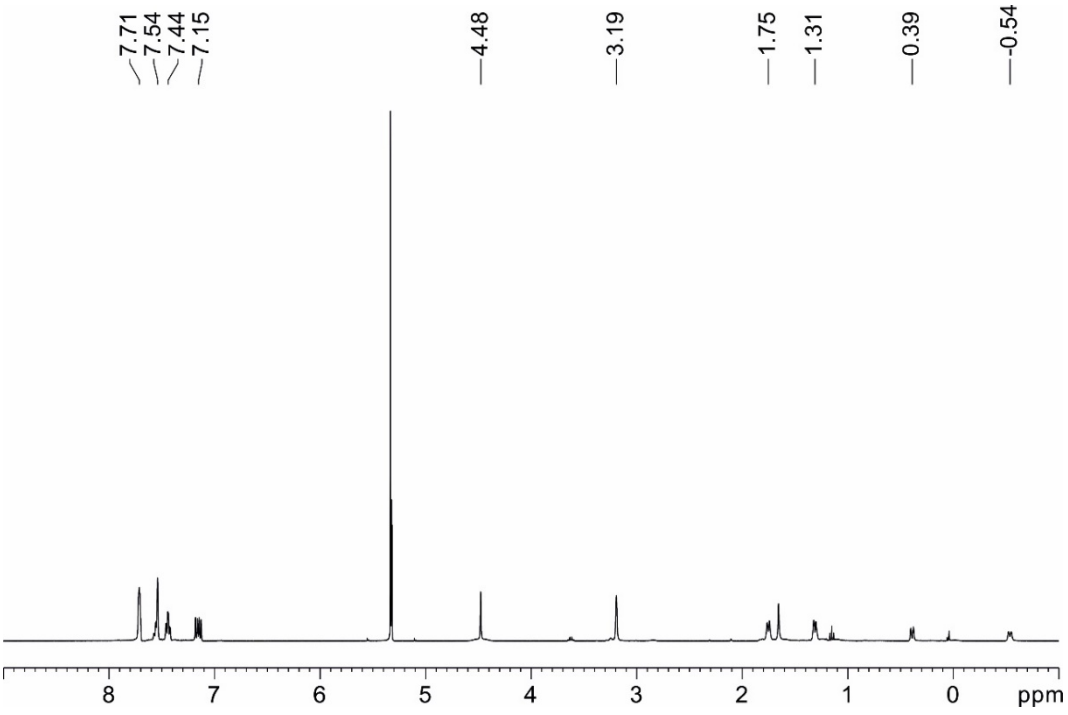
SI 7: ^{19}F-NMR spectrum (376.54 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F].



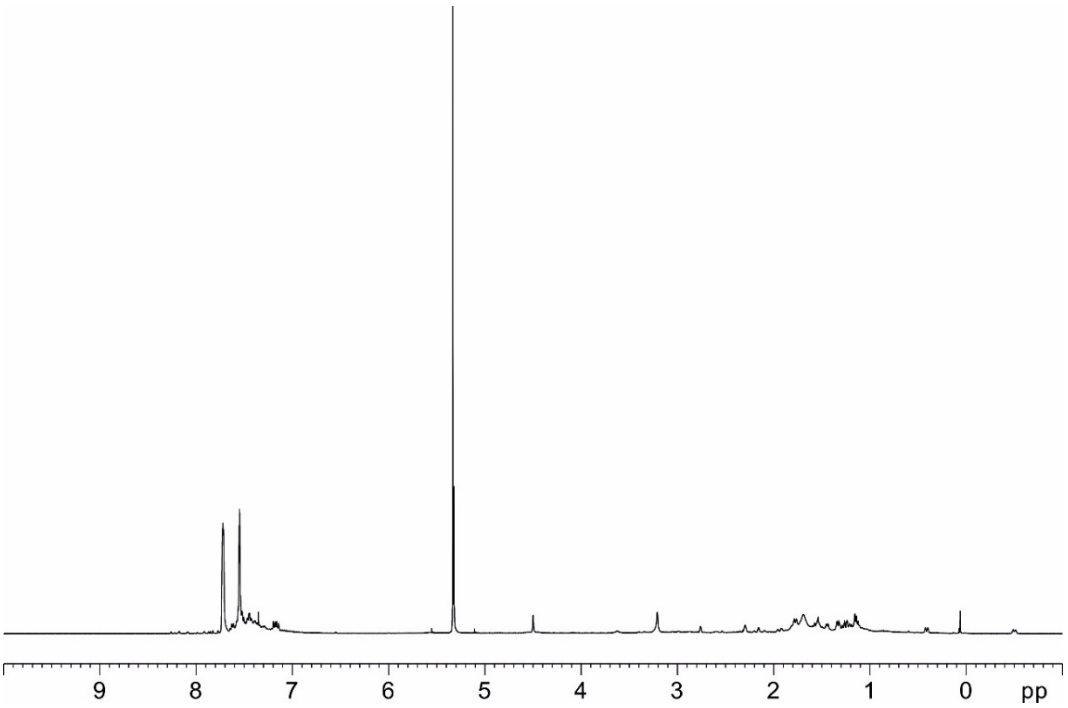
SI 8: ^{11}B-NMR spectrum (128.39 MHz, CD_2Cl_2, 223 K) of isolated crystals of **3**[BAr_4^F].

2.6 NMR Spectra of 3[BAr_4^F] at Temperatures above 223 K

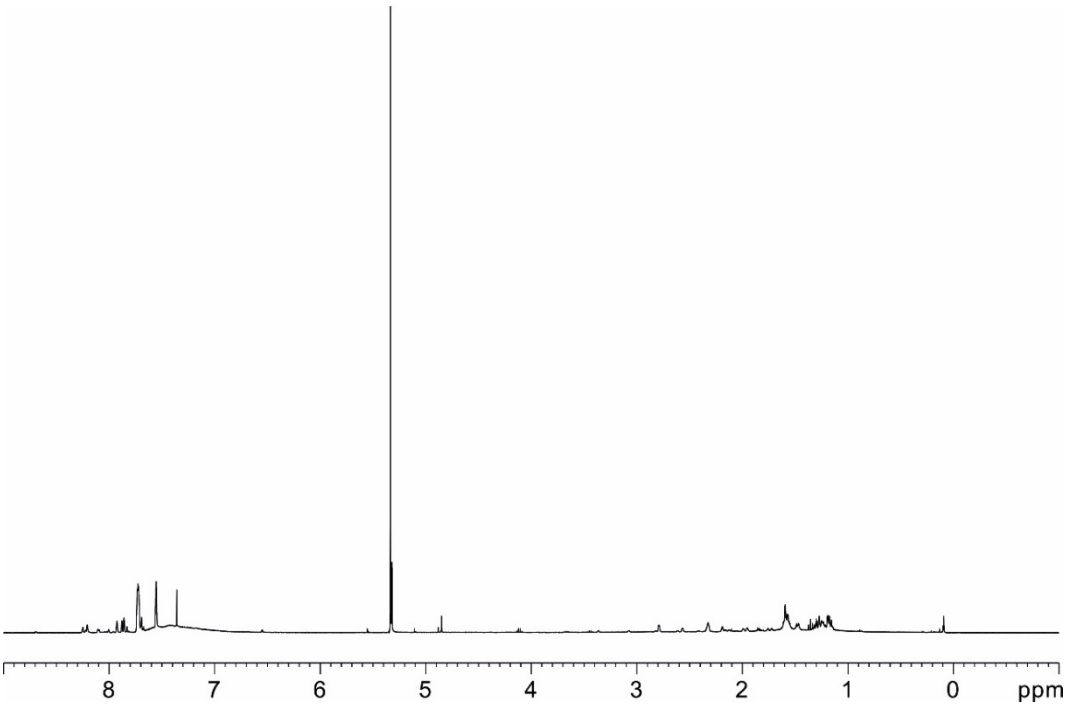
The following NMR spectra demonstrate the decomposition of **3**[BAr_4^F] in CD_2Cl_2 at temperatures of 253 K and above.



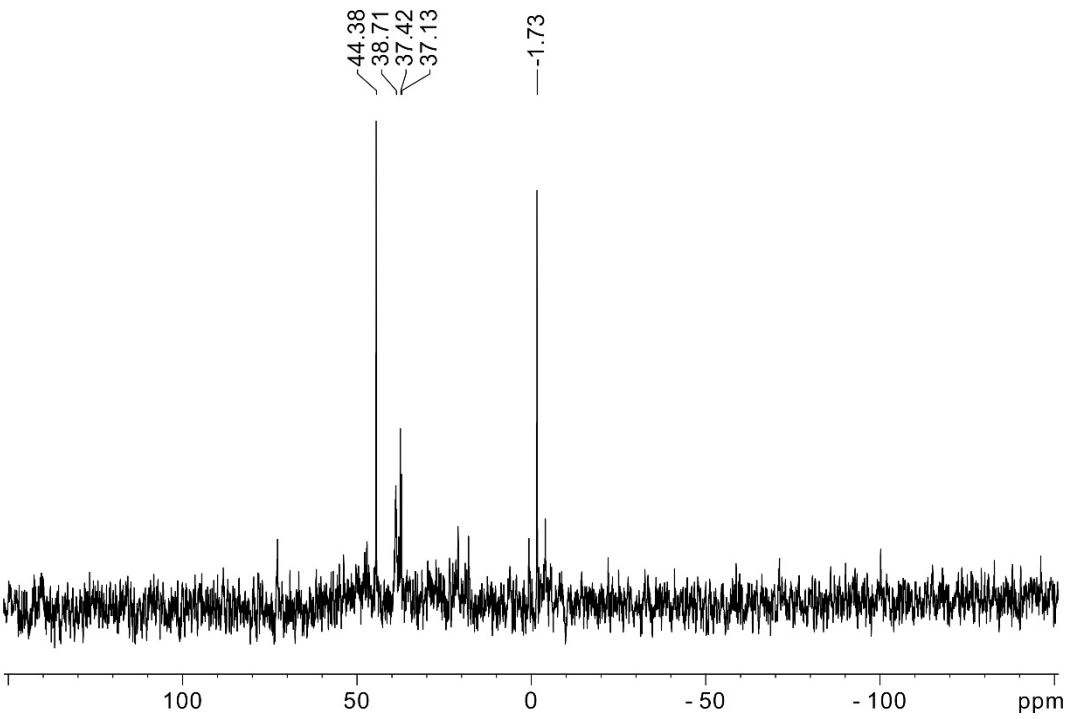
SI 9: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 243 K) of isolated crystals of **3**[BAr_4^F].



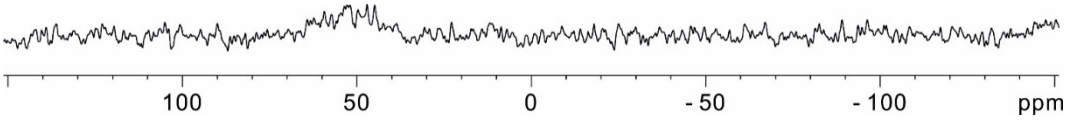
SI 10: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 253 K) of isolated crystals of **3**[BAr_4^F].



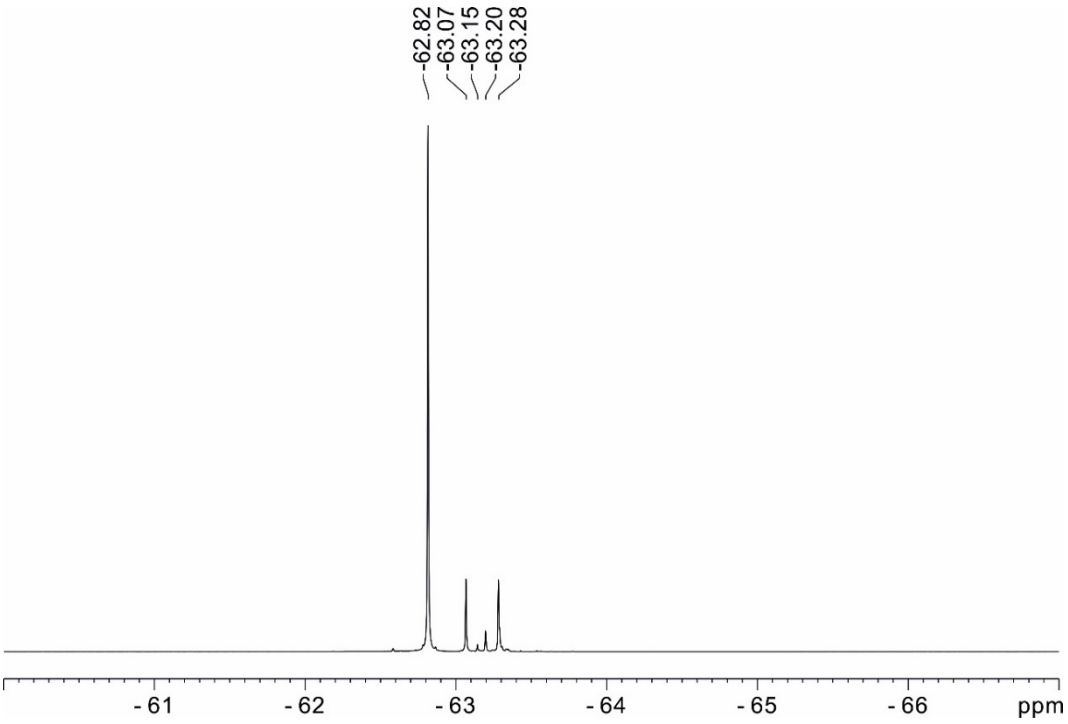
SI 11: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 273 K) of isolated crystals of **3**[BAr_4^F].



SI 12: ^{31}P{^{1}H}-NMR (161.99 MHz, CD_2Cl_2, 253 K) of isolated crystals of **3**[BAr_4^F] after more than 6 h at this temperature.

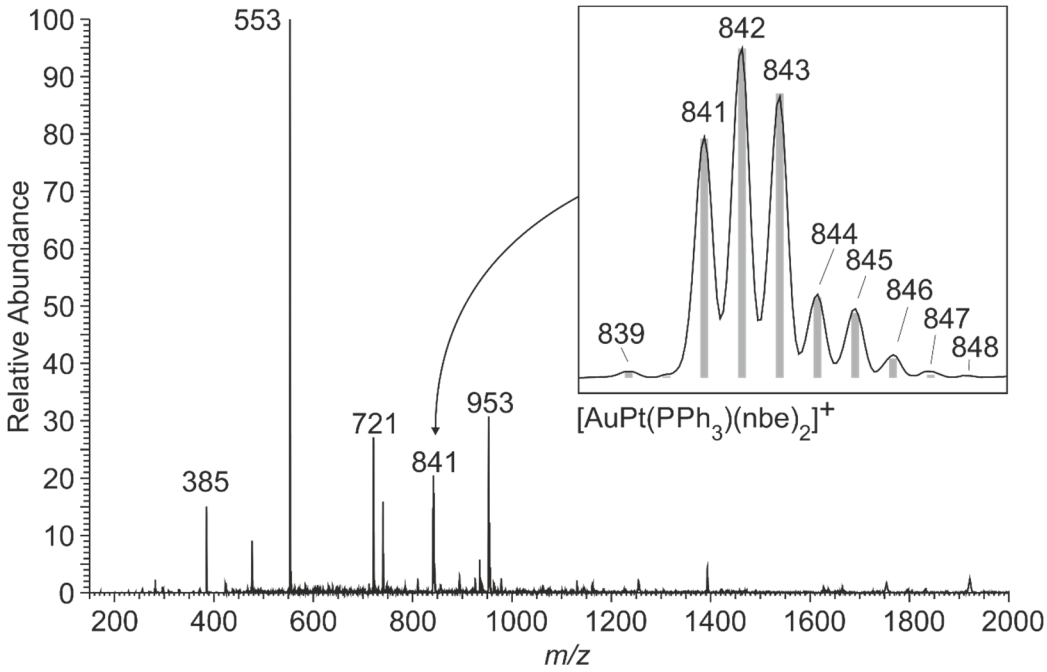


SI 13: $^{31}P\{^{1}H\}$-NMR spectrum (161.99 MHz, CD_2Cl_2, 298 K) of isolated crystals of **3**[BAr_4^F].

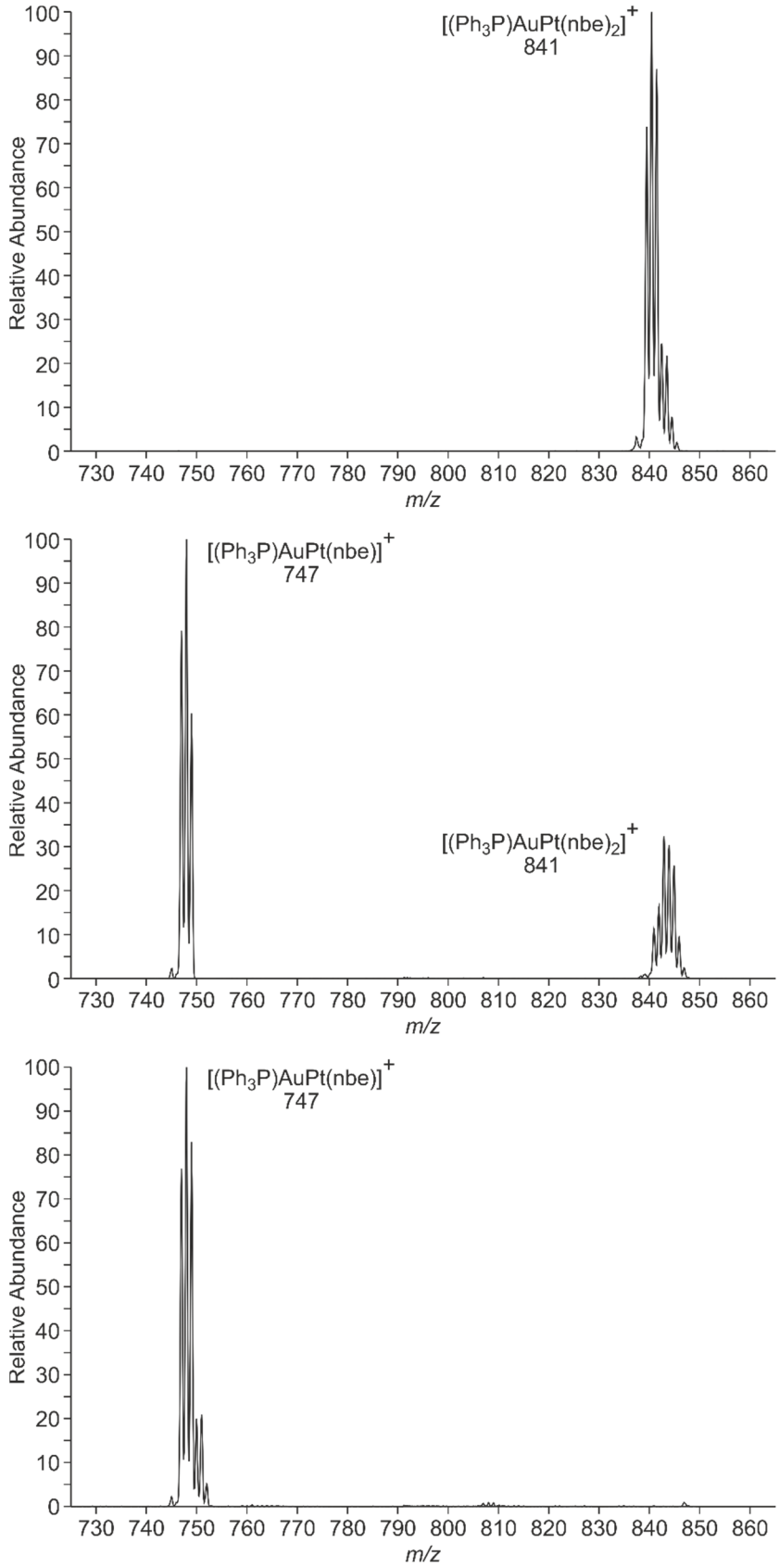


SI 14: ^{19}F-NMR spectrum (376.54 MHz, CD_2Cl_2, 273 K) of isolated crystals of **3**[BAr_4^F].

2.7 Mass Spectra of 3[BAr_4^F]

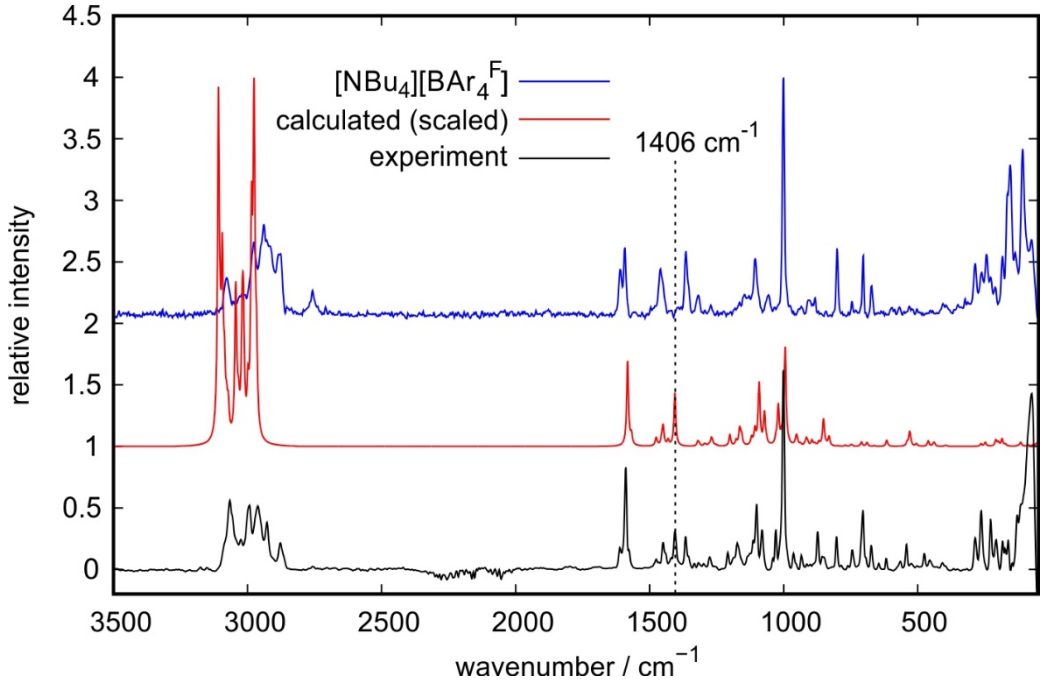


SI 15: ESI mass spectrum of [(Ph_3P)AuPt(nbe)$_3$][BAr_4^F] (**3**[BAr_4^F]) dissolved in dichloromethane at −60 °C. The enlarged isotope pattern of [(Ph_3P)AuPt(nbe)$_2$]$^+$ at *m/z* 841 is shown in the inset together with the expected isotope pattern for comparison. The signals at *m/z* 953, 721, 553, and 385 can be assigned to [$Au_2(PPh_3)_2Cl$]$^+$, [$Au(PPh_3)_2$]$^+$, [$Au(PPh_3)(nbe)$]$^+$, and [$Au(nbe)_2$]$^+$, respectively.



SI 16: CID spectra of $[(Ph_3P)AuPt(nbe)_2]^+$ (*m/z* 841) at Normalized Collision Energies of 0 (top), 10 (center), and 25 (bottom).

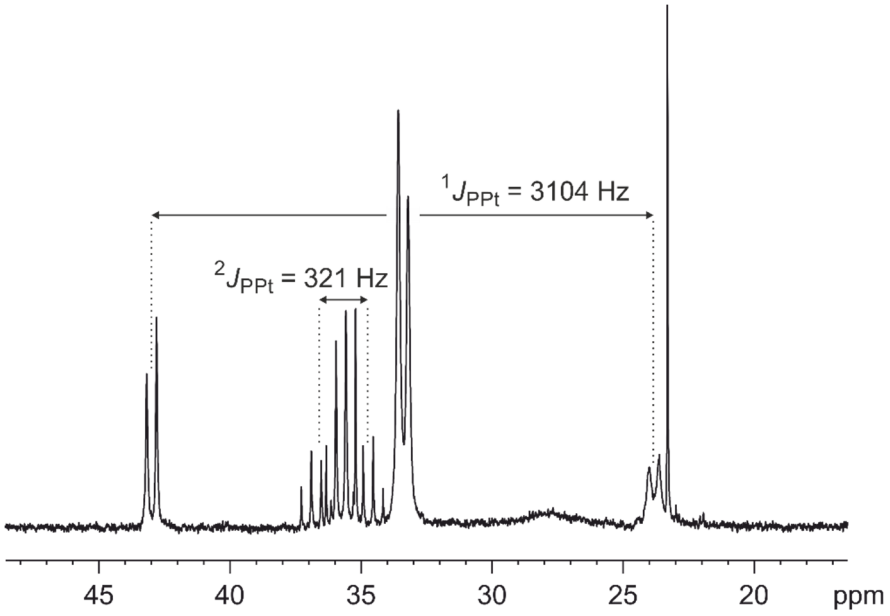
2.8 Raman Spectrum of 3[BAr_4^F]



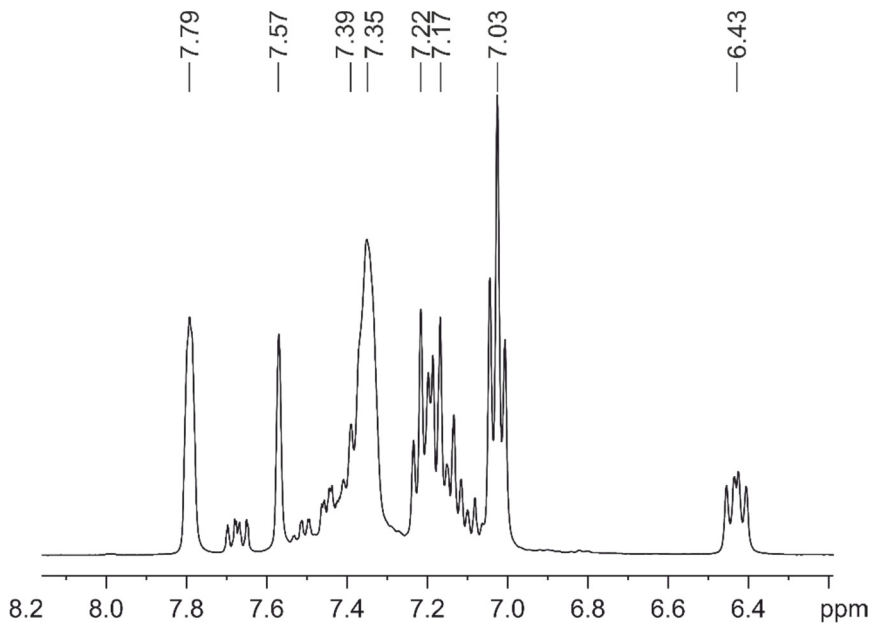
SI 17: Experimental Raman spectrum of crystalline **3**[BAr_4^F] (70 mW, 38 x 100 scans, 200 K, 4 cm^{-1}) and [NBu_4][BAr_4^F] (measured at room temperature) together with a calculated spectrum of **3**[BAr_4^F] (B3LYP/def2-TZVP, scaled by a factor of 0.9694). The band at 1406 cm^{-1} is composed of three normal modes involving the C=C stretching modes of **3**.

3 Ligand Exchange in 3[BAr$_4^F$]

To a mixture of solid **3**[BAr$_4^F$] · 3 CH_2Cl_2 (11.8 mg, 0.0057 mmol) and PPh_3 (5.2 mg, 0.0198 mmol, 3.5 eq.) cooled to −78 °C, toluene (2 ml) was slowly added, allowing the solvent to cool down at the walls of the reaction vessel. The thermosensitive AuPt complex was weighed at room temperature as quickly as possible and transferred to the Schlenk tube immediately. The colorless reaction mixture was stirred and allowed to warm to room temperature, resulting in a pale yellow solution. After stirring for another hour at ambient temperature, the volatile components were removed under reduced pressure. The solid residue was dissolved in THF-d_8 for NMR characterization. The obtained spectra clearly prove the formation of [(Ph_3P)AuPt(PPh_3)$_3$][BAr$_4^F$] (**1**[BAr$_4^F$]).



SI 18: $^{31}P\{^1H\}$-NMR spectrum (161.99 MHz, 298 K, THF-d_8) of the solid residue obtained by the reaction of **3**[BAr$_4^F$] · 3 CH_2Cl_2 (11.8 mg, 0.0057 mmol) and PPh_3 (5.2 mg, 0.0198 mmol, 3.5 eq.) in toluene after evaporation of all volatiles at room temperature. The spectrum is essentially identical to that obtained for an authentic sample of [(Ph_3P)AuPt(PPh_3)$_3$][BAr$_4^F$] (**1**[BAr$_4^F$]).[30] The broad signal located at 27.8 ppm is due to chemical exchange of the PPh_3 ligands between complexes such as [Au(PPh_3)$_2$]$^+$ and [Pt(PPh_3)$_3$] as generated in the reaction of **1**[BAr$_4^F$] with the slight excess of PPh_3. The signal at 23.1 ppm is due to an impurity of triphenylphosphine oxide.

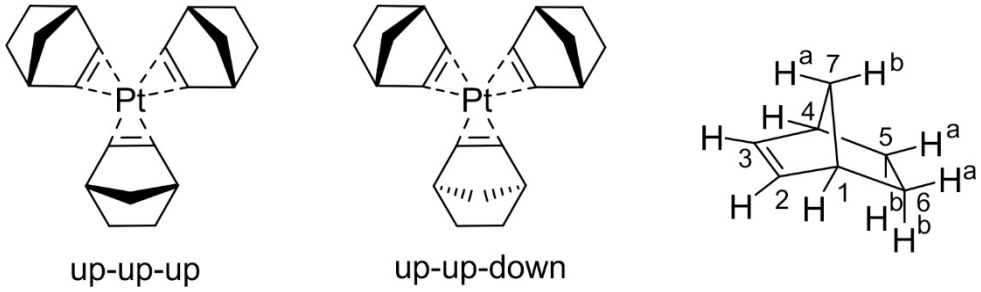


SI 19: ^{1}H-NMR spectrum (400.17 MHz, 298 K, THF-d_8) of the solid residue obtained by the reaction of **4**[BAr_4^F] · 3 CH_2Cl_2 (11.8 mg, 0.0057 mmol) and PPh_3 (5.2 mg, 0.0198 mmol, 3.5 eq.) in toluene after evaporation of all volatiles at room temperature. Apart from the impurities and solvent signals between 0 and 4 ppm, the spectrum is identical to that obtained for an authentic sample of [$(Ph_3P)AuPt(PPh_3)_3$][BAr_4^F] (**1**[BAr_4^F]).[30]

4 VT-NMR and Raman Spectra of [Pt(nbe)$_3$] (4)

4.1 Chemical Exchange of [Pt(nbe)$_3$] (4)

The ^{195}Pt chemical shift of [Pt(nbe)$_3$] (**4**) at room temperature amounts to −4368 ppm (in C_6D_6). At this temperature, this complex also exhibits well-resolved ^{1}H- and ^{13}C-NMR resonances, which suggest the presence of a single compound with chemically equivalent nbe ligands. However, the observed resonances are averages of the signals of different isomers ("up-up-up" and "up-up-down", see below), which cannot be distinguished on the NMR time scale at room temperature due to chemical exchange. The spectroscopic data of **3**[BAr$_4^F$] were mainly collected at 223 K. Therefore, we also recorded NMR spectra of [Pt(nbe)$_3$] (**4**) at 223 K in order to determine the $^{2}J_{HPt}$ coupling constant as well as the ^{13}C and ^{195}Pt-NMR chemical shifts at that temperature. However, at 223 K, the chemical exchange of the isomers of [Pt(nbe)$_3$] (**4**) has slowed down close to the coalescence point, and the crucial signals are thus significantly broadened. Particularly, the olefinic resonances in the ^{1}H- and the ^{13}C{^{1}H}-NMR spectra are broadened so that the ^{195}Pt satellites cannot be identified. At temperatures below 203 K, at least three closely neighbored signals of olefinic protons can be distinguished in the ^{1}H-NMR spectrum, and it is just visible that there is also more than one resonance of the bridgehead atoms. The fact that a ^{195}Pt signal cannot be measured at low temperature is due to enhanced relaxation of the ^{195}Pt nuclear spin.



SI 20: Illustration of the two types of isomers of [Pt(nbe)$_3$] (**4**) together with the numbering scheme of the nbe ligand.

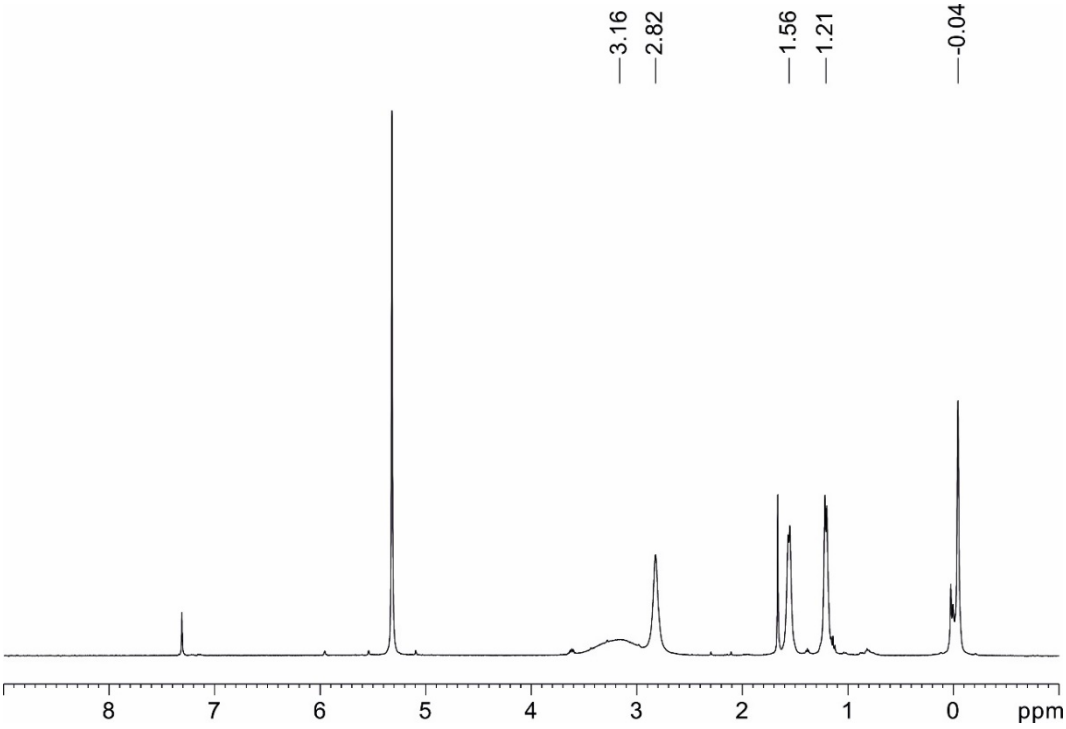
^{1}H-NMR (400.17 MHz, CD_2Cl_2, 223 K) δ = –0.04 (s, 2H, 7-H^a, 7-H^b), 1.21 (d, $^{2}J_{5b5a}/^{2}J_{6b6a}$ = 7.2 Hz, 5-H^b, 6-H^b), 1.56 (d, $^{2}J_{5a5b}/^{2}J_{6a6b}$ = 7.2 Hz, 5-H^a, 6-H^a), 2.82 (s, 2H, 1-H, 4-H), 3.16 (s, 2H, 2-H, 3-H) ppm.

^{13}C{^{1}H}-NMR (100.62 MHz, CD_2Cl_2, 223 K) δ = 28.0 (5-C, 6-C), 39.0 (7-C), 42.3 (1-C, 4-C), 66.5 (2-C, 3-C) ppm.

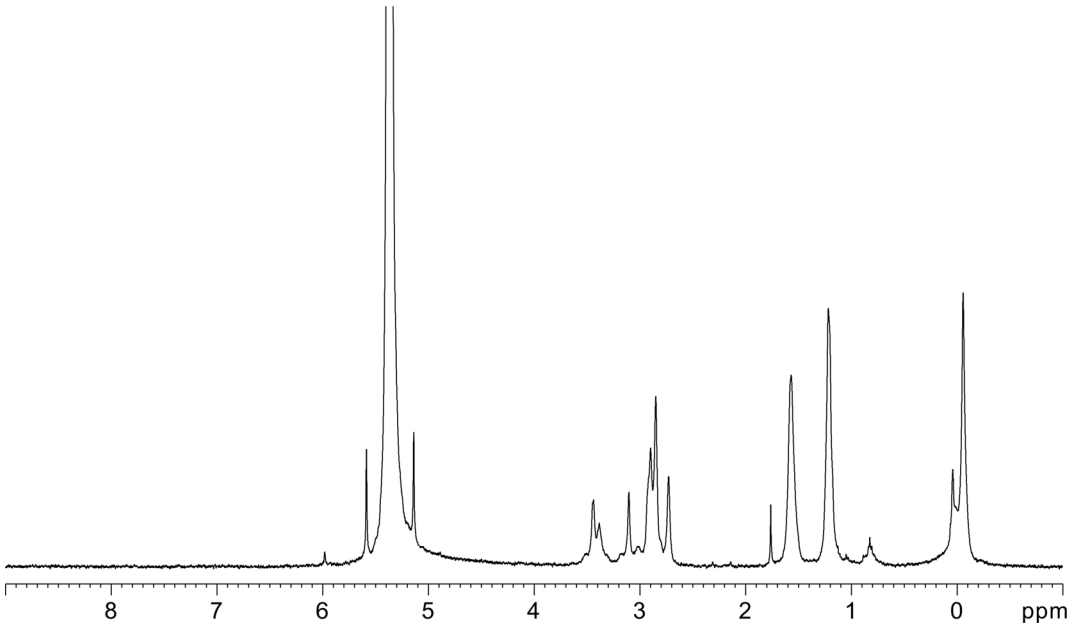
^{195}Pt-NMR (86.02 MHz, C_6D_6, 298 K) δ = –4368.0 ppm.

FT Raman (100 x 100 scans, 70 mW, 200 K, 4 cm^{-1}): $\tilde{\nu}/cm^{-1}$ (intensity) = 3021 (w), 3005 (vw), 2960 (vs), 2911 (vw), 2865 (vw), 1472 (vw), 1443 (vw), 1393 (w), 1314 (vw), 1293 (vw), 1271 (vw), 1251 (vw), 1207 (vw), 1168 (vw), 1122 (vw), 1076 (m), 1040 (vw), 1012 (vw), 958 (vw), 935 (w), 911 (vw), 879 (vw), 869 (vw), 846 (vw), 761 (vw), 685 (vw), 571 (vw), 551 (vw), 477 (vw), 242 (w), 220 (vw), 173 (w), 79 (m).

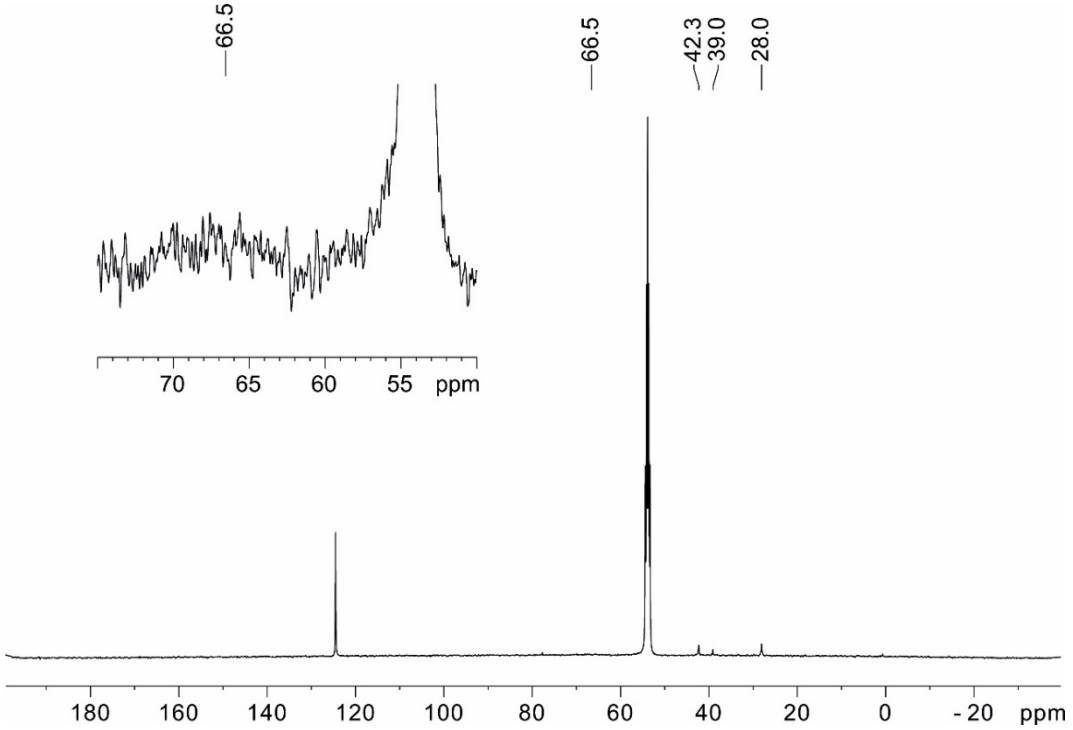
4.2 NMR Spectra of [Pt(nbe)$_3$] (4)



SI 21: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 223 K) of [Pt(nbe)$_3$] (**4**). The olefinic proton resonance at 3.16 ppm is broadened due to chemical exchange (FWHM approx. 150 Hz).

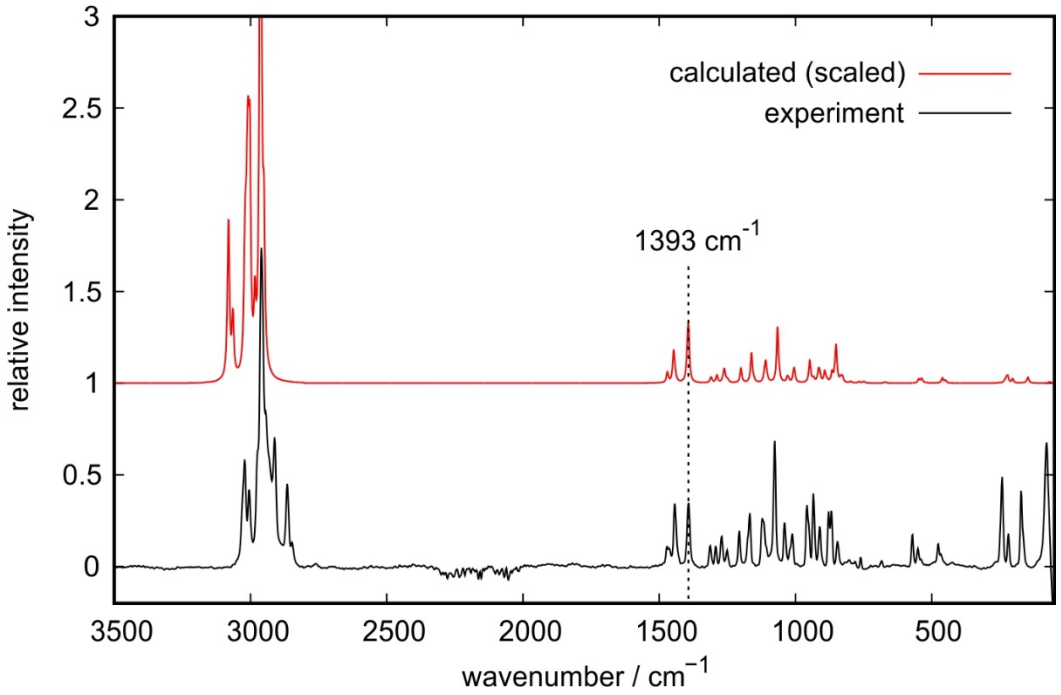


SI 22: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 193 K) of [Pt(nbe)$_3$] (**4**).



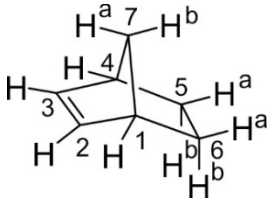
SI 23: ^{13}C{^{1}H}-NMR spectrum (100.62 MHz, CD_2Cl_2, 223 K) of [Pt(nbe)$_3$] (**4**). The inset shows the olefinic carbon resonance at 66.5 ppm in more detail, which is broadened due to coalescence. At room temperature in C_6D_6, the olefinic ^{13}C-NMR resonance of [Pt(nbe)$_3$] (**4**) is located at 68.0 ppm.[31]

4.3 Raman Spectrum of [Pt(nbe)$_3$] (4)



SI 24: Experimental Raman spectrum of [Pt(nbe)$_3$] (**4**) (70 mW, 100 x 100 scans, 200 K, 4 cm^{-1}) together with a calculated spectrum of **4** (B3LYP/def2-TZVP, scaled by a factor of 0.9694). The band at 1393 cm^{-1} is composed of three normal modes involving the C=C stretching modes.

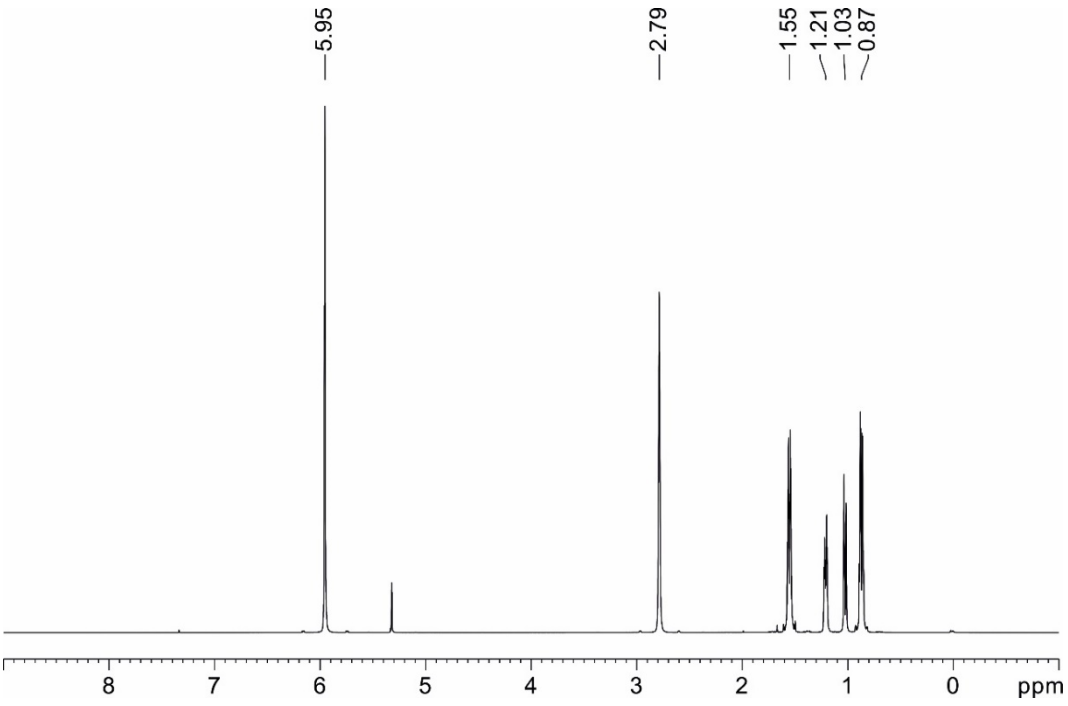
5 Low-Temperature NMR and Raman Spectra of nbe



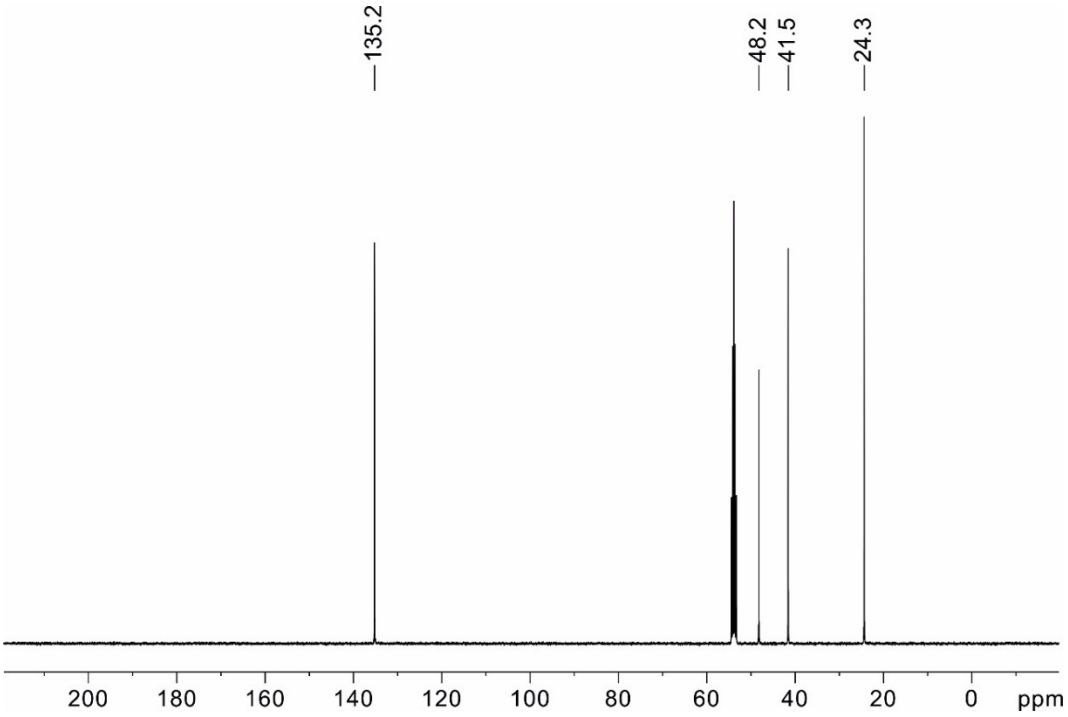
^{1}H-NMR (400.17 MHz, CD_2Cl_2, 223 K) δ = 0.81-0.93 (m, 2H, 5-H^{b}, 6-H^{b}), 1.03 (d, $^{2}J_{7a7b}$ = 8.0 Hz, 1H, 7-H^{a}), 1.19-1.23 (m, 1H, 7-H^{b}), 1.50-1.61 (m, 2H, 5-H^{a}, 6-H^{a}), 2.79 (s, 2H, 1-H, 4-H), 5.95 (s, 2H, 2-H, 3-H) ppm.

^{13}C{^{1}H}-NMR (100.62 MHz, CD_2Cl_2, 223 K) δ = 24.6 (2C, 5-C, 6-C), 41.8 (2C, 1-C, 4-C), 48.5 (1C, 7-C), 135.5 (2C, 2-C, 3-C) ppm.

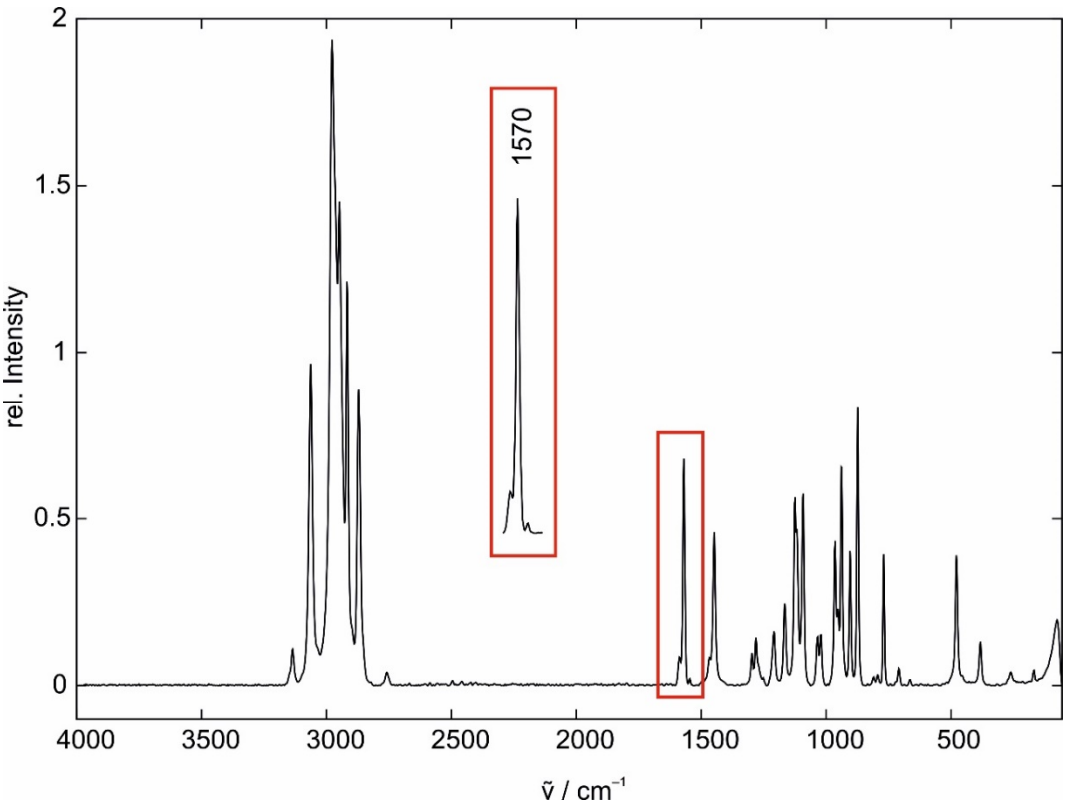
FT Raman (20 x 100 scans, 70 mW, 200 K, 4 cm^{-1}): $\tilde{\nu}$/cm^{-1} (intensity) = 3136 (vw), 3063 (m), 2977 (vs), 2948 (vw), 2917 (w), 2871 (w), 2758 (vw), 1570 (w), 1447 (w), 1296 (vw), 1280 (vw), 1208 (vw), 1165 (vw), 1124 (w), 1092 (w), 1034 (vw), 1020 (vw), 964 (vw), 952 (vw), 938 (w), 903 (vw), 873 (m), 793 (vw), 769 (w), 709 (vw), 477 (w), 382 (vw), 261 (vw), 168 (vw), 75 (vw).



SI 25: ^{1}H-NMR spectrum (400.17 MHz, CD_2Cl_2, 223 K) of nbe.



SI 26: $^{13}C\{^{1}H\}$-NMR spectrum (100.62 MHz, CD_2Cl_2, 223 K) of nbe.

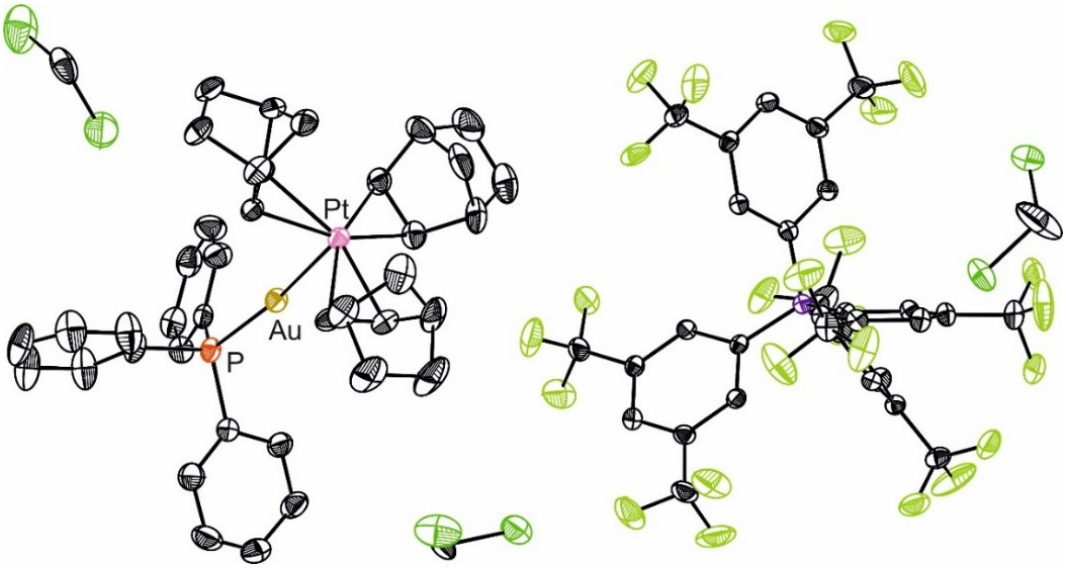


SI 27: Raman spectrum of nbe (70 mw, 20 x 1000 scans, 200 K, 4 cm^{-1}). The inset highlights the C=C stretching mode of nbe in more detail. The assignment is based on DFT-calculated Raman spectra.

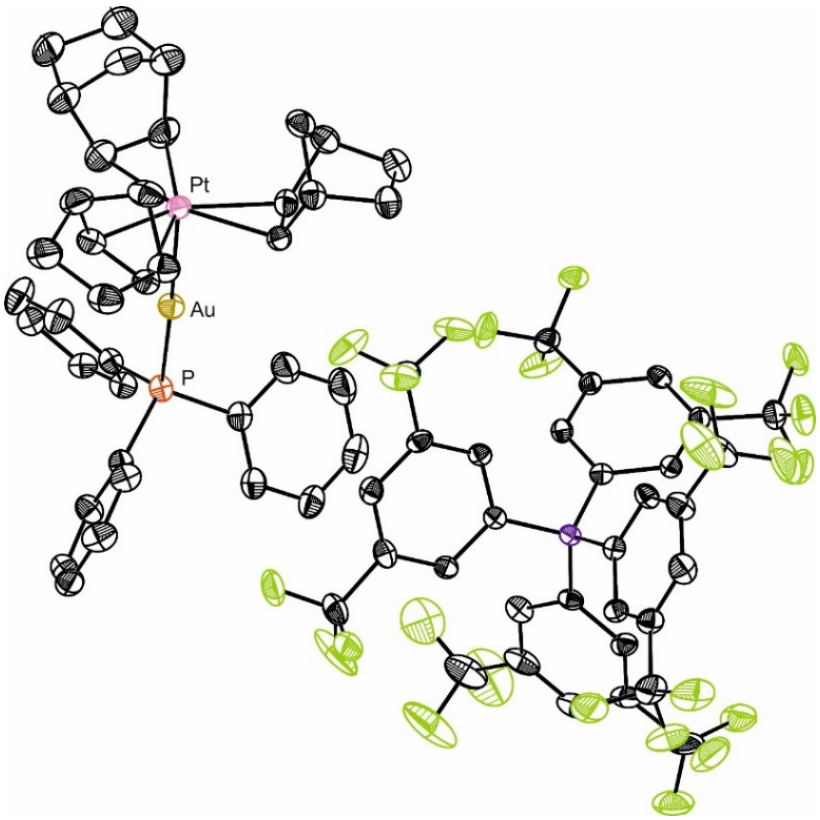
6 X-Ray Structural Data

SI 28: Crystal data and summary of the data collection and refinement for complexes **3**[BAr_4^F] · 3 CH_2Cl_2, **3**[BAr_4^F], and [Pt(nbe)$_3$] (**4**).

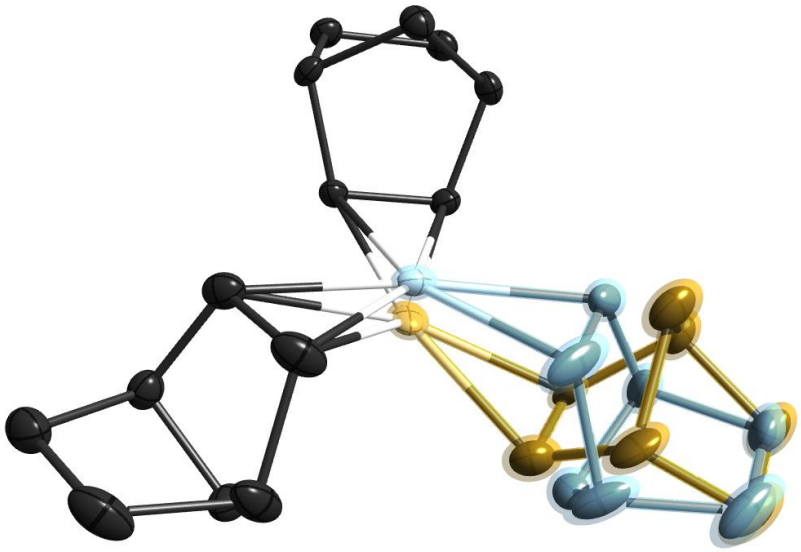
Complex	**3**[BAr_4^F] · 3 CH_2Cl_2	**3**[BAr_4^F]	[Pt(nbe)$_3$] (**4**)
CCDC number	1966141	1966142	1966140
Empirical formula	$C_{74}H_{63}AuBCl_6F_{24}PPt$	$C_{71}H_{57}AuBF_{24}PPt$	$C_{21}H_{30}Pt$
Formula weight	2054.78	1800	477.54
Temperature [K]	100	100	100
Crystal system	triclinic	triclinic	orthorhombic
Space group (number)	*P*1 (1)	*P*-1 (2)	$P2_12_12_1$ (19)
a [Å]	12.7747(6)	12.3657(11)	5.5867(4)
b [Å]	12.7853(6)	15.5627(14)	10.710(3)
c [Å]	13.1193(6)	19.1346(18)	28.421(8)
α [Å]	82.1010(10)	95.961(3)	90
β [Å]	88.7640(10)	108.064(3)	90
γ [Å]	64.2590(10)	101.326(3)	90
Volume [Å^3]	1910.06(15)	3378.6(5)	1700.5(8)
Z	1	2	4
ρ_{calc} [g/cm^3]	1.786	1.769	1.865
μ [mm^{-1}]	4.079	4.369	8.247
F(000)	1002	1752	936
Crystal size [mm^3]	0.050×0.050×0.020	0.040×0.040×0.040	0.100×0.060×0.050
Crystal colour	colourless	colourless	colourless
Crystal shape	block	block	needle
Radiation	MoK_α (λ=0.71073)	MoK_α (λ=0.71073)	MoK_α (λ=0.71073)
2Θ range [°]	3.78 to 61.18	3.84 to 61.22	4.06 to 75.69
Index ranges	-18 ≤ h ≤ 18	-17 ≤ h ≤ 17	-9 ≤ h ≤ 9
	-18 ≤ k ≤ 18	-22 ≤ k ≤ 22	-18 ≤ k ≤ 18
	-18 ≤ l ≤ 18	-27 ≤ l ≤ 27	-49 ≤ l ≤ 48
Reflections collected	289821	311174	142301
Independent reflections	23248	20666	9167
	R_{int} = 0.0613	R_{int} = 0.1122	R_{int} = 0.1048
	R_{sigma} = 0.0245	R_{sigma} = 0.0516	R_{sigma} = 0.0317
Completeness to θ=25.242°	100 %	100 %	99.9 %
Data / Restraints /	23248/872/1171	20666/371/974	9167/962/272
Goodness-of-fit on F^2	1.045	1.04	0.938
Final *R* indexes	R_1 = 0.0230	R_1 = 0.0386	R_1 = 0.0183
[$I \geq 2\sigma(I)$]	wR_2 = 0.0560	wR_2 = 0.0858	wR_2 = 0.0372
Final *R* indexes	R_1 = 0.0250	R_1 = 0.0591	R_1 = 0.0207
[all data]	wR_2 = 0.0568	wR_2 = 0.0930	wR_2 = 0.0376
Largest peak/hole [eÅ^3]	1.80/-0.89	1.74/-1.92	1.71/-1.40
Flack X parameter	-0.0146(10)		0.012(3)



SI 29: Molecular structure of $[(Ph_3P)AuPt(nbe)_3][BAr_4^F]$ (**3**$[BAr_4^F]$) with three molecules CH_2Cl_2 per unit cell. Ellipsoids are drawn at 50 % probability level. Hydrogen atoms are omitted for clarity.



SI 30: Molecular structure of $[(Ph_3P)AuPt(nbe)_3][BAr_4^F]$ (**3**$[BAr_4^F] \cdot 3\ CH_2Cl_2$) without co-crystallized CH_2Cl_2. Ellipsoids are drawn at 50 % probability level. Hydrogen atoms are omitted for clarity.



SI 31. Illustration of the molecular structure and of the disorder model for [Pt(nbe)$_3$] (**4**). Ellipsoids are drawn at 50 % probability level. Hydrogen atoms are omitted for clarity. The disordered parts highlighted in blue and yellow have an occupation of 93.4 % and 6.6 %, respectively.

SI 32. Summary of selected bond lengths and angles the molecular structures of **3**[BAr$_4^F$] · 3 CH_2Cl_2, **3**[BAr$_4^F$], and [Pt(nbe)$_3$] (**4**).

	3[BAr$_4^F$] · 3 CH_2Cl_2	**3**[BAr$_4^F$]	[Pt(nbe)$_3$] (**4**)
Au1–P1	**2.2370(11)**	**2.2445(10)**	
Au1–Pt1	**2.57868(18)**	**2.5911(3)**	
P1–Au1–Pt1	**171.75(3)**	**177.05(3)**	
Pt1–C2_1	2.231(4)	2.193(4)	2.164(3)
Pt1–C3_1	2.220(4)	2.226(4)	2.171(3)
Pt1–C2_2	2.217(4)	2.221(4)	2.189(2)
Pt1–C3_2	2.195(5)	2.230(4)	2.191(2)
Pt1–C2_3	2.211(4)	2.192(4)	2.171(3)
Pt1–C3_3	2.213(5)	2.216(5)	2.175(3)
average Pt–C	**2.215(4)**	**2.213(4)**	**2.177(3)**
C2_1–C3_1	1.413(6)	1.400(5)	1.408(4)
C2_2–C3_2	1.404(7)	1.395(6)	1.416(3)
C2_3–C3_3	1.409(7)	1.394(7)	1.408(5)
average C–C	**1.409(7)**	**1.396(6)**	**1.411(4)**

7 DFT Calculations

7.1 Energetic Differences Between Square Planar and Trigonal Pyramidal Geometries

For the series of complexes $[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**), $[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**), $[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**), and $[(Ph_3P)AuPt(nbe)_3]^+$ (**3**) as well as for $[(Ph_3P)AuPt(CO)_3]^+$ (**8**) and $[(Ph_3P)AuPt(PF_3)_3]^+$ (**9**), we performed geometry optimizations of different isomers. This treatment allowed us to determine the preference for a square planar or a trigonal pyramidal geometry. For the square planar structures of **6** and **7**, two isomers have to be distinguished (see SI 33).

SI 33. Results of the geometry optimizations of different cationic complexes at the PBE0/def2-TZVPP//BP86/def2-SVP level of theory. Zero-point-corrected electronic energies are given in kJ mol^{-1}. For each complex, the energetically lowest geometry is set to 0 kJ mol^{-1} and highlighted in bold.

compound	square planar form	trigonal pyramidal form
$[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**)	**0**	48
$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**)	**0**[a], 46[b]	27
$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**)	4[c], 24[d]	**0**
$[(Ph_3P)AuPt(nbe)_3]^+$ (**3**)	65	**0**
$[(Ph_3P)AuPt(CO)_3]^+$ (**8**)	**0**	58[e]
$[(Ph_3P)AuPt(PF_3)_3]^+$ (**9**)	**0**	50

[a] The nbe ligand is bound in the position *trans* to the Au atom.

[b] The nbe ligand is bound in the position *cis* to the Au atom.

[c] The PPh_3 ligand is bound in the position *cis* to the Au atom.

[d] The PPh_3 ligand is bound in the position *trans* to the Au atom.

[e] Note that this structure has an imaginary frequency of −8.4 cm^{-1}, which could not be eliminated even after several attempts.

For $[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**), the most favorable geometry is the square planar form, which is 48 kJ mol^{-1} more stable than the trigonal pyramidal form. This result is in agreement with the crystal structure.[29,30] Cation $[(Ph_3P)AuPt(nbe)_3]^+$ (**3**), however, is more stable in the trigonal pyramidal form (by 65 kJmol^{-1}) as found experimentally (see Figure 1 in the main text). The homologous cations $[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**) and $[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**) mark the border between these two extremes: While the energetically most favorable geometry of **6** is square planar, the more favorable form of **7** is trigonal bipyramidal.

Initially, we tried to understand the trigonal pyramidal coordination in **3** as a consequence of a *trans* effect of the nbe ligands, thus forcing them into a wheel-like geometry and thus to avoid a *trans* situation between the carbon-based ligands. Alternatively, we were wondering if the wheel-like geometry might be a consequence of strong metal-to-ligand π-back-bonding, which is stronger for olefins when compared with phosphines. The latter interpretation, however, could be excluded through DFT calculations on the homologous complexes $[(Ph_3P)AuPt(CO)_3]^+$ (**8**) and $[(Ph_3P)AuPt(PF_3)_3]^+$ (**9**), which contain CO and PF_3 as prototypical π-back-bonding ligands. Also for these two complexes, the square planar coordination around the platinum atom is favored.

One might argue that the preference for the "planar" geometry in **1** with respect to the "pyramidal" structure in **3** could also be related to steric factors caused by the "bulkiness" of the nbe ligands. In the square planar form of **3**, however, the two nbe ligands in *cis* position to the gold atom act as bridging ligands for the two metal atoms, thus releasing possible strain in a thermodynamically favorable fashion. Nevertheless, the trigonal pyramidal form is energetically favored, and we interpret this mainly in terms of the favorable orbital interactions.

7.2 Population Analyses

We performed population analyses for complexes **1** – **7** as well as for $AuPt^+$ (**10**), $[(Ph_3P)Au]^+$ (**11**), $[(Cy_3P)Au]^+$ (**12**), and $[Pt(PCy_3)_2]$ (**13**). Our goal was to analyze the changes associated with the coordination of the formal Au^{+I} fragment to the corresponding formal Pt^0 complexes to generate complexes **1** – **3** as well as **6** and **7**. We employed the methods MULLIKEN,[25] QTAIM,[27] and NPA.[26] The results are summarized in Tables SI 34, SI 35, and SI 36.

The first six columns summarize the charges of the ligands at the gold and the platinum atom ($q(L_{Au})$, $q(L_{Pt}^1)$, $q(L_{Pt}^2)$, $q(L_{Pt}^3)$) as well as of the metal atoms (q(Au), q(Pt)) within the various complexes. Based on these values, we calculated:

$$\boldsymbol{q([(L)Au])} = q(L_{Au}) + q(Au) \quad (1)$$

$$\boldsymbol{q([Pt(L)_3])} = q(Pt) + q(L_{Pt}^1) + q(L_{Pt}^2) + q(L_{Pt}^3) \quad (2)$$

$$\boldsymbol{q(L^1{+}L^2{+}L^3)} = q(L_{Pt}^1) + q(L_{Pt}^2) + q(L_{Pt}^3) \quad (3)$$

$$\boldsymbol{q(Au{+}Pt)} = q(Au) + q(Pt) \quad (4)$$

$$\boldsymbol{q(Au{-}Pt)} = q(Au) - q(Pt) \quad (5)$$

Due to the neutral charge of $[Pt(L)_3]$, $q([Pt(L)_3])$ is a direct measure for the charge shifted towards $[(L)Au]^+$ upon formation of the Au–Pt bond. These values are depicted in Figure 4 in the main text. While q(Au+Pt) denotes the charge accumulated at the AuPt core, q(Au−Pt) is a measure for the polarity within the AuPt core.

SI 34. Results of the population analyses for complexes **1** – **7** as well as $AuPt^+$ (**10**), $[(Ph_3P)Au]^+$ (**11**), $[(Cy_3P)Au]^+$ (**12**), and $[Pt(PCy_3)_2]$ (**13**) employing the MULLIKEN method.[25] To facilitate reading, values associated with nbe and PPh_3 are colored green and red, respectively. Values printed in bold have been employed for the construction of Figure 4 in the main article.

MULLIKEN	$q(L_{Au})$	q(Au)	q(Pt)	$q(L_{Pt}^1)$	$q(L_{Pt}^2)$	$q(L_{Pt}^3)$	q([(Ph$_3$P)Au])	q([Pt(L)$_{2/3}$])	$q(L^1+L^2+L^3)$	q(Au+Pt)	q(Au−Pt)
$[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**)	0.56	−0.44	−0.38	0.47	0.41	0.38[a]	0.13	**0.87**	1.25	−0.82	−0.05
$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**)	0.56	−0.20	−0.35	0.46	0.42	0.11[a]	0.36	**0.64**	0.99	−0.55	0.16
$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**)	0.54	−0.05	−0.34	0.32	0.25	0.27	0.49	**0.51**	0.85	−0.38	0.29
$[(Ph_3P)AuPt(nbe)_3]^+$ (**3**)	0.56	−0.09	−0.39	0.30	0.31	0.30	0.47	**0.53**	0.91	−0.47	0.30
$[(Cy_3P)AuPt(PCy_3)_2]^+$ (**2**)	0.53	−0.27	−0.33	0.52	0.54	-	0.27	**0.73**	1.06	−0.59	0.06
$AuPt^+$ (**10**)	-	0.60	0.40	-	-	-	-	-	-	1.00	0.20
$[(Ph_3P)Au]^+$ (**11**)	0.62	0.38	-	-	-	-	-	-	-	-	-
$[(Cy_3P)Au]^+$ (**12**)	0.62	0.38	-	-	-	-	-	-	-	-	-
$[Pt(nbe)_3]$ (**4**)[b]	-	-	−0.05	0.02	0.02	0.02	-	-	0.05	-	-
$[Pt(PPh_3)_3]$ (**5**)	-	-	−0.67	0.24	0.27	0.16	-	-	0.67	-	-
$[Pt(PCy_3)_2]$ (**13**)	-	-	−0.59	0.30	0.30	-	-	-	0.59	-	-

[a] Ligand in position *trans* to Au

[b] "up-up-up" isomer

SI 35. Results of the population analyses for complexes **1** – **7** as well as $AuPt^+$ (**10**), $[(Ph_3P)Au]^+$ (**11**), $[(Cy_3P)Au]^+$ (**12**), and $[Pt(PCy_3)_2]$ (**13**) employing the NPA method.[26] To facilitate reading, values associated with nbe and PPh_3 are colored green and red, respectively. Values printed in bold have been employed for the construction of Figure 4 in the main article.

NPA	$q(L_{Au})$	q(Au)	q(Pt)	$q(L_{Pt}^1)$	$q(L_{Pt}^2)$	$q(L_{Pt}^3)$	$q([(Ph_3P)Au])$	$q([Pt(L)_{2/3}])$	$q(L^1+L^2+L^3)$	q(Au+Pt)	q(Au−Pt)
$[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**)	0.25	0.23	−0.10	0.21	0.20	0.21[a]	0.48	**0.52**	0.62	0.13	0.32
$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**)	0.28	0.31	0.11	0.23	0.22	−0.15[a]	0.58	**0.42**	0.31	0.41	0.20
$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**)	0.39	0.34	0.39	0.27	−0.21	−0.18	0.73	**0.27**	−0.12	0.72	−0.05
$[(Ph_3P)AuPt(nbe)_3]^+$ (**3**)	0.43	0.31	0.51	−0.08	−0.08	−0.08	0.74	**0.26**	−0.25	0.82	−0.20
$[(Cy_3P)AuPt(PCy_3)_2]^+$ (**2**)	0.35	0.25	−0.28	0.34	0.34	-	0.60	**0.40**	0.68	−0.03	0.53
$AuPt^+$ (**10**)	-	0.48	0.52	-	-	-	-	-	-	1.00	−0.04
$[(Ph_3P)Au]^+$ (**11**)	0.71	0.29	-	-	-	-	-	-	-	-	-
$[(Cy_3P)Au]^+$ (**12**)	0.70	0.30	-	-	-	-	-	-	-	-	-
$[Pt(nbe)_3]$ (**4**)[b]	-	-	0.54	−0.18	−0.18	−0.18	-	-	−0.54	-	-
$[Pt(PPh_3)_3]$ (**5**)	-	-	−0.11	0.03	0.04	0.04	-	-	0.11	-	-
$[Pt(PCy_3)_2]$ (**13**)	-	-	−0.47	0.23	0.23	-	-	-	0.47	-	-

[a] Ligand in position *trans* to Au

[b] "up-up-up" isomer

SI 36. Results of the population analyses for complexes **1** – **7** as well as $AuPt^+$ (**10**), $[(Ph_3P)Au]^+$ (**11**), $[(Cy_3P)Au]^+$ (**12**), and $[Pt(PCy_3)_2]$ (**13**) employing QTAIM.[27] To facilitate reading, values associated with nbe and PPh_3 are colored green and red, respectively. Values printed in bold have been employed for the construction of Figure 4 in the main article.

QTAIM	$q(L_{Au})$	q(Au)	q(Pt)	$q(L_{Pt}^1)$	$q(L_{Pt}^2)$	$q(L_{Pt}^3)$	$q([(Ph_3P)Au])$	$q([Pt(L)_{2/3}])$	$q(L^1+L^2+L^3)$	q(Au+Pt)	q(Au−Pt)
$[(Ph_3P)AuPt(PPh_3)_3]^+$ (**1**)	0.42	−0.18	−0.27	0.35	0.35	0.32[a]	0.24	**0.76**	1.03	−0.45	0.09
$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (**6**)	0.48	−0.11	−0.18	0.39	0.39	0.03[a]	0.36	**0.64**	0.82	−0.30	0.07
$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (**7**)	0.61	−0.06	0.04	0.41	−0.01	0.01	0.56	**0.44**	0.41	−0.02	−0.10
$[(Ph_3P)AuPt(nbe)_3]^+$ (**3**)	0.64	−0.04	0.16	0.08	0.08	0.08	0.60	**0.40**	0.24	0.11	−0.20
$[(Cy_3P)AuPt(PCy_3)_2]^+$ (**2**)	0.58	−0.12	−0.33	0.44	0.43	-	0.46	**0.54**	0.87	−0.45	0.21
$AuPt^+$ (**10**)	-	0.42	0.58	-	-	-	-	-	-	1.00	−0.16
$[(Ph_3P)Au]^+$ (**11**)	0.98	0.02	-	-	-	-	-	-	-	-	-
$[(Cy_3P)Au]^+$ (**12**)	0.99	0.01	-	-	-	-	-	-	-	-	-
$[Pt(nbe)_3]$ (**4**)[b]	-	-	0.14	-0.05	-0.05	-0.04	-	-	-0.14	-	-
$[Pt(PPh_3)_3]$ (**5**)	-	-	−0.52	0.17	0.17	0.18	-	-	0.52	-	-
$[Pt(PCy_3)_2]$ (**13**)	-	-	−0.53	0.27	0.27		-	-	0.53	-	-

[a] Ligand in position *trans* to Au

[b] "up-up-up" isomer

There is some general observations:

- **Upon coordination of $[(Ph_3P)Au]^+$ (11) to $[Pt(nbe)_3]$ (4)**, the charge at the platinum atom, q(Pt), barely changes (with NPA and QTAIM) or becomes even more negative (with MULLIKEN). The generally increased positive charge at the $[Pt(nbe)_3]$ fragment (see $q([Pt(L)_3])$) is mostly the consequence of an increase of the positive charge at the nbe ligands ($q(L^1+L^2+L^3)$).
- **Upon coordination of $[(Ph_3P)Au]^+$ (11) to $[Pt(PPh_3)_3]$ (5)**, the charge at the platinum atom, q(Pt), becomes less negative (with QTAIM and MULLIKEN) or barely changes (with NPA). The generally increased positive charge at the $[Pt(PPh_3)_3]$ fragment (see $q([Pt(L)_3])$), which is higher than for **4** (see Figure 4 in the main text), is associated with an increase of the positive charge of the PPh_3 ligands ($q(L^1+L^2+L^3)$).
- **Upon coordination of $[(Cy_3P)Au]^+$ (12) to $[Pt(PCy_3)_2]$ (13)**, the charge of both the platinum atom (q(Pt)) and the PCy_3 ligands ($q(L^1+L^2)$) becomes more positive.
- **In the series 1 → 6 → 7 → 3**, the charge of the AuPt core (q(Au+Pt)) becomes continuously more positive (with one anomaly with the MULLIKEN method). The polarity within the AuPt core (q(Au−Pt)) is inverted within the series (particularly with NPA and QTAIM). The corresponding values of q(Au) and q(Pt) do not indicate any commonality with possible formal oxidation-state assignments such as $Au^{+I}Pt^0$ or $Au^{-I}Pt^{+II}$. This is due to the fact that the major amount of positive charge is accumulated at the ligands rather than at the AuPt core.
- **$[(Ph_3P)AuPt(nbe)_3]^+$ (3)** exhibits the most positive charge at the AuPt core when compared with the other complexes. Depending on the method, absolute charges q(Au+Pt) between −0.47 (MULLIKEN) and +0.82 (NPA) are calculated. However, independently of the method, the AuPt core in **3** is more positively charged when compared with complexes **1** and **2**. In terms of the charge of the AuPt core, **3** is thus located between those two complexes and bare $AuPt^+$ (**10**).

8 Cartesian Coordinates and Energies for the DFT Calculations

$[(Ph_3P)AuPt(PPh_3)_3]^+$ (1) (square planar form)

ZPE(BP86/def2-SVP) = 1.0755444 Hartree (optimized geometry)
E(BP86/def2-SVP) = −4398.9997244 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −4397.77201121538 Hartree (single point)

Cartesian coordinates in Å:

Au	0.33302	0.06429	0.04067
Pt	-1.71709	1.53075	-0.73512
P	2.11014	-1.24234	0.74126
P	-1.49636	2.17930	1.46571
P	-3.42254	2.84591	-1.67376
P	-0.82764	0.64532	-2.69444
C	3.17553	-1.80681	-0.62890
C	3.61483	-3.14146	-0.72693
H	3.34660	-3.86763	0.05445
C	4.38071	-3.54310	-1.83318
H	4.71803	-4.58744	-1.91220
C	4.71611	-2.61668	-2.83523
H	5.31529	-2.93643	-3.70090
C	4.28402	-1.28240	-2.73289
H	4.53677	-0.55227	-3.51536
C	3.50633	-0.87750	-1.63896
H	3.13413	0.15653	-1.58000
C	1.50994	-2.74285	1.58948
C	0.34189	-3.34611	1.07740
H	-0.15970	-2.90586	0.20255
C	-0.18035	-4.49334	1.68996
H	-1.08947	-4.96224	1.28458
C	0.44810	-5.03176	2.82730
H	0.03086	-5.92453	3.31673
C	1.60887	-4.42830	3.34078
H	2.10244	-4.84990	4.22915
C	2.14707	-3.28860	2.72113
H	3.05579	-2.81757	3.12402
C	3.18414	-0.37039	1.93287
C	4.48466	0.05644	1.60222
H	4.92661	-0.22096	0.63394
C	5.21477	0.83761	2.51398
H	6.23197	1.16720	2.25436
C	4.65470	1.19157	3.75275
H	5.23048	1.80335	4.46305
C	3.35852	0.75774	4.08544
H	2.91205	1.02955	5.05348
C	2.62125	-0.01534	3.17948
H	1.60282	-0.34083	3.43765
C	-0.61367	-1.18294	-2.59480
C	0.55900	-1.84646	-3.00189
H	1.41001	-1.27784	-3.39764
C	0.66378	-3.23996	-2.86211

H	1.59832	-3.74036	-3.15444
C	-0.41102	-3.98349	-2.35066
H	-0.32772	-5.07547	-2.24774
C	-1.59072	-3.32556	-1.95545
H	-2.43538	-3.90186	-1.54864
C	-1.68728	-1.93100	-2.05939
H	-2.58975	-1.40564	-1.71188
C	0.82900	1.36620	-3.05489
C	1.46435	2.19646	-2.10631
H	0.95785	2.42128	-1.15427
C	2.73685	2.72637	-2.36810
H	3.21378	3.37056	-1.61549
C	3.38694	2.43117	-3.57846
H	4.38667	2.84302	-3.78305
C	2.75178	1.61961	-4.53470
H	3.25039	1.39793	-5.49023
C	1.47376	1.09707	-4.28060
H	0.97077	0.48473	-5.04368
C	-1.68121	0.86061	-4.31787
C	-2.46781	-0.16731	-4.87449
H	-2.57155	-1.12967	-4.35499
C	-3.11309	0.02811	-6.10493
H	-3.72038	-0.78371	-6.53153
C	-2.98499	1.24762	-6.78842
H	-3.48957	1.39464	-7.75503
C	-2.20900	2.27807	-6.23311
H	-2.09955	3.23798	-6.75939
C	-1.55786	2.08657	-5.00653
H	-0.93849	2.89290	-4.59326
C	-1.12720	0.97483	2.81408
C	-0.68552	1.44172	4.06946
H	-0.56742	2.52136	4.24596
C	-0.38751	0.52917	5.09299
H	-0.03264	0.89828	6.06695
C	-0.54195	-0.85217	4.87503
H	-0.29941	-1.56660	5.67562
C	-1.01060	-1.31975	3.63636
H	-1.13281	-2.39814	3.46046
C	-1.30732	-0.40840	2.60970
H	-1.67272	-0.76634	1.63391
C	-0.03227	3.28139	1.34985
C	1.24531	2.83465	1.74178
H	1.35657	1.88544	2.28090
C	2.38549	3.59047	1.42950
H	3.37390	3.22128	1.74126
C	2.25812	4.79788	0.72104
H	3.15144	5.39174	0.47545
C	0.98466	5.25047	0.33141
H	0.87664	6.19364	-0.22449
C	-0.15687	4.49632	0.64201
H	-1.14809	4.84189	0.31430
C	-2.81533	3.15887	2.28125
C	-2.56059	4.33848	3.00653
H	-1.54978	4.77269	3.01917
C	-3.60086	4.95598	3.72048
H	-3.40149	5.87860	4.28614

C	-4.88708	4.39413	3.72037
H	-5.69824	4.87752	4.28483
C	-5.14385	3.22116	2.98916
H	-6.15509	2.79029	2.97323
C	-4.11480	2.61078	2.26276
H	-4.31182	1.70085	1.67431
C	-4.69979	3.74881	-0.70522
C	-4.32569	4.94456	-0.05372
H	-3.29288	5.31463	-0.13643
C	-5.26947	5.67696	0.67512
H	-4.96795	6.60876	1.17510
C	-6.59616	5.22088	0.76878
H	-7.33844	5.79948	1.33837
C	-6.96931	4.02530	0.13651
H	-8.00693	3.66513	0.20408
C	-6.02651	3.28811	-0.59920
H	-6.33108	2.36215	-1.10787
C	-4.43616	1.78572	-2.77747
C	-4.73996	0.50102	-2.27398
H	-4.32012	0.19745	-1.30026
C	-5.56276	-0.36990	-3.00249
H	-5.80016	-1.36611	-2.59990
C	-6.07791	0.03138	-4.24646
H	-6.72066	-0.65038	-4.82309
C	-5.75942	1.29931	-4.75867
H	-6.14361	1.60863	-5.74179
C	-4.94447	2.17809	-4.02818
H	-4.68816	3.15945	-4.44885
C	-2.70746	4.22968	-2.64884
C	-1.30910	4.40123	-2.64531
H	-0.68768	3.69461	-2.07678
C	-0.71734	5.45660	-3.35547
H	0.37689	5.57220	-3.34441
C	-1.52387	6.35176	-4.07705
H	-1.06515	7.17778	-4.64106
C	-2.92302	6.20442	-4.06170
H	-3.55757	6.91905	-4.60703
C	-3.51611	5.15875	-3.33843
H	-4.61231	5.07919	-3.29042

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	-0.43580	3.11594	6.64437	9.66105	0.01421	0.00023
2pt	-0.38204	2.85469	6.68876	8.81159	0.02625	0.00075
3p	0.43385	5.57575	8.50355	0.44500	0.04184	
4p	0.25297	5.52068	8.70027	0.48344	0.04264	
5p	0.32019	5.54195	8.65257	0.44525	0.04004	
6p	0.21987	5.54743	8.70485	0.48648	0.04137	
7c	0.08629	3.24909	2.52297	0.13378	0.00788	
8c	-0.12547	3.17311	2.83400	0.11104	0.00733	
9h	0.13872	0.81950	0.03988	0.00189		
10c	-0.16522	3.20093	2.84653	0.11058	0.00718	
11h	0.14069	0.82276	0.03477	0.00178		

12c	-0.10079	3.16306	2.82021	0.11038	0.00713
13h	0.14105	0.82242	0.03476	0.00176	
14c	-0.12437	3.16990	2.83710	0.11021	0.00717
15h	0.13650	0.82667	0.03507	0.00176	
16c	-0.22041	3.29701	2.80134	0.11462	0.00744
17h	0.13472	0.82148	0.04198	0.00182	
18c	-0.03020	3.25822	2.63009	0.13399	0.00790
19c	-0.04082	3.21094	2.70970	0.11273	0.00745
20h	0.12386	0.82911	0.04512	0.00191	
21c	-0.19210	3.21597	2.85864	0.11034	0.00716
22h	0.13047	0.83303	0.03471	0.00178	
23c	-0.08976	3.15541	2.81691	0.11029	0.00714
24h	0.14202	0.82153	0.03469	0.00176	
25c	-0.14942	3.18957	2.84232	0.11036	0.00717
26h	0.14086	0.82245	0.03491	0.00178	
27c	-0.10154	3.15459	2.82720	0.11248	0.00728
28h	0.14250	0.81626	0.03936	0.00189	
29c	0.02745	3.25668	2.57341	0.13467	0.00779
30c	-0.15296	3.17797	2.85673	0.11093	0.00732
31h	0.14226	0.81543	0.04043	0.00188	
32c	-0.14374	3.18512	2.84066	0.11077	0.00719
33h	0.13971	0.82376	0.03475	0.00178	
34c	-0.12955	3.18103	2.83185	0.10955	0.00713
35h	0.14030	0.82319	0.03475	0.00176	
36c	-0.11484	3.17649	2.82067	0.11050	0.00718
37h	0.13410	0.82952	0.03461	0.00178	
38c	-0.10732	3.18713	2.79602	0.11672	0.00745
39h	0.07611	0.87903	0.04305	0.00182	
40c	0.01491	3.21702	2.62474	0.13534	0.00799
41c	-0.03234	3.15905	2.75340	0.11257	0.00732
42h	0.10379	0.84961	0.04461	0.00199	
43c	-0.13199	3.20182	2.81256	0.11043	0.00718
44h	0.12666	0.83537	0.03616	0.00181	
45c	-0.11904	3.18076	2.82137	0.10979	0.00712
46h	0.13271	0.83058	0.03493	0.00178	
47c	-0.15739	3.18109	2.85782	0.11133	0.00715
48h	0.13255	0.83097	0.03469	0.00178	
49c	-0.11561	3.20738	2.78717	0.11366	0.00740
50h	0.09997	0.85822	0.03994	0.00187	
51c	0.04863	3.26509	2.54887	0.12961	0.00779
52c	-0.04395	3.23636	2.67985	0.12027	0.00747
53h	0.12209	0.82698	0.04885	0.00207	
54c	-0.19425	3.21522	2.85943	0.11244	0.00716
55h	0.12983	0.83217	0.03622	0.00179	
56c	-0.07881	3.15022	2.81165	0.10983	0.00711
57h	0.14184	0.82191	0.03449	0.00177	
58c	-0.23019	3.24823	2.86378	0.11100	0.00718
59h	0.14404	0.81999	0.03420	0.00176	
60c	-0.10170	3.13297	2.84516	0.11624	0.00733
61h	0.16020	0.79923	0.03868	0.00188	
62c	0.09675	3.25697	2.50359	0.13490	0.00780
63c	-0.09625	3.16519	2.81145	0.11219	0.00741
64h	0.12517	0.83036	0.04253	0.00194	
65c	-0.16569	3.20890	2.83730	0.11215	0.00732
66h	0.12651	0.83699	0.03471	0.00179	
67c	-0.09933	3.16324	2.81822	0.11069	0.00718

68h	0.13347	0.83025	0.03452	0.00176	
69c	-0.18440	3.21384	2.85171	0.11163	0.00722
70h	0.13172	0.83196	0.03454	0.00178	
71c	-0.15720	3.20610	2.82960	0.11410	0.00740
72h	0.12903	0.82441	0.04460	0.00196	
73c	0.09418	3.21616	2.55203	0.12982	0.00781
74c	-0.14521	3.19196	2.83090	0.11499	0.00736
75h	0.12502	0.83451	0.03860	0.00188	
76c	-0.19823	3.22199	2.85850	0.11062	0.00712
77h	0.13619	0.82700	0.03502	0.00179	
78c	-0.07866	3.14448	2.81611	0.11095	0.00711
79h	0.13464	0.82887	0.03472	0.00178	
80c	-0.11623	3.19289	2.80421	0.11196	0.00717
81h	0.12514	0.83550	0.03753	0.00183	
82c	-0.14157	3.17560	2.84313	0.11538	0.00747
83h	0.16814	0.78889	0.04099	0.00198	
84c	0.04136	3.24007	2.57853	0.13228	0.00777
85c	0.08355	3.13475	2.65760	0.11663	0.00747
86h	0.08296	0.86821	0.04684	0.00199	
87c	-0.24988	3.28822	2.84285	0.11163	0.00718
88h	0.12271	0.83952	0.03600	0.00178	
89c	-0.09476	3.14443	2.83153	0.11167	0.00712
90h	0.14442	0.81980	0.03403	0.00174	
91c	-0.19312	3.22226	2.85257	0.11113	0.00715
92h	0.13202	0.83107	0.03511	0.00179	
93c	-0.07752	3.17781	2.77536	0.11691	0.00745
94h	0.10782	0.85162	0.03871	0.00185	
95c	0.05032	3.26355	2.54484	0.13339	0.00790
96c	-0.16892	3.18027	2.86890	0.11244	0.00731
97h	0.13939	0.81872	0.04000	0.00189	
98c	-0.15699	3.18815	2.84980	0.11181	0.00723
99h	0.13620	0.82761	0.03442	0.00177	
100c	-0.12337	3.18432	2.82068	0.11112	0.00724
101h	0.13175	0.83209	0.03439	0.00176	
102c	-0.11632	3.18319	2.81452	0.11133	0.00728
103h	0.12797	0.83514	0.03508	0.00181	
104c	-0.11521	3.16445	2.82875	0.11444	0.00756
105h	0.10709	0.85222	0.03881	0.00187	
106c	-0.00174	3.28727	2.57123	0.13538	0.00786
107c	-0.12624	3.16772	2.83661	0.11438	0.00752
108h	0.13029	0.82737	0.04040	0.00193	
109c	-0.14468	3.19565	2.82983	0.11190	0.00729
110h	0.12676	0.83650	0.03494	0.00180	
111c	-0.11042	3.17322	2.81944	0.11055	0.00721
112h	0.13238	0.83136	0.03449	0.00177	
113c	-0.17405	3.20450	2.85147	0.11085	0.00723
114h	0.13528	0.82850	0.03444	0.00178	
115c	-0.11676	3.17013	2.82912	0.11017	0.00734
116h	0.13282	0.82424	0.04105	0.00190	
117c	0.02837	3.22635	2.60396	0.13334	0.00797
118c	-0.13469	3.18165	2.83428	0.11134	0.00742
119h	0.12697	0.83039	0.04070	0.00193	
120c	-0.17261	3.20604	2.84933	0.11005	0.00720
121h	0.12941	0.83392	0.03489	0.00179	
122c	-0.09454	3.16048	2.81718	0.10969	0.00719
123h	0.13575	0.82781	0.03468	0.00176	

124c	-0.15963	3.20933	2.83046	0.11252	0.00731
125h	0.12928	0.83443	0.03451	0.00179	
126c	-0.08434	3.15781	2.80532	0.11387	0.00735
127h	0.11534	0.84034	0.04236	0.00196	
128c	0.03179	3.28723	2.54061	0.13254	0.00784
129c	-0.06711	3.20372	2.73514	0.12075	0.00749
130h	0.12614	0.82653	0.04535	0.00198	
131c	-0.20603	3.22746	2.86082	0.11062	0.00713
132h	0.13525	0.82832	0.03467	0.00176	
133c	-0.08513	3.15404	2.81394	0.10999	0.00716
134h	0.13989	0.82364	0.03471	0.00176	
135c	-0.17041	3.20087	2.85130	0.11106	0.00718
136h	0.13968	0.82367	0.03488	0.00178	
137c	-0.14704	3.15631	2.86717	0.11627	0.00730
138h	0.15528	0.80441	0.03846	0.00186	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.22712	2.96721	6.00615	9.79800	0.00146	0.00006
2 pt	-0.09782	2.66910	6.00651	9.41926	0.00274	0.00021
3 p	0.94261	5.20602	8.81183	0.03813	0.00141	0.00000
4 p	0.98756	5.18811	8.78370	0.03927	0.00135	0.00000
5 p	0.93771	5.22784	8.79746	0.03586	0.00113	0.00000
6 p	0.98733	5.19043	8.78234	0.03863	0.00127	0.00000
7 c	-0.36616	3.00889	3.34745	0.00735	0.00248	0.00000
8 c	-0.19433	2.98343	3.20356	0.00528	0.00207	0.00000
9 h	0.23589	0.76330	0.00073	0.00008	0.00000	0.00000
10 c	-0.21198	2.99186	3.21307	0.00508	0.00198	0.00000
11 h	0.22996	0.76934	0.00062	0.00008	0.00000	0.00000
12 c	-0.19831	2.99571	3.19552	0.00511	0.00197	0.00000
13 h	0.22897	0.77036	0.00060	0.00008	0.00000	0.00000
14 c	-0.21744	2.99042	3.21996	0.00514	0.00193	0.00000
15 h	0.23066	0.76858	0.00068	0.00008	0.00000	0.00000
16 c	-0.20604	2.98251	3.21609	0.00542	0.00202	0.00000
17 h	0.24282	0.75628	0.00082	0.00008	0.00000	0.00000
18 c	-0.36783	3.00880	3.34920	0.00734	0.00249	0.00000
19 c	-0.19824	2.98334	3.20743	0.00541	0.00205	0.00000
20 h	0.24449	0.75463	0.00081	0.00008	0.00000	0.00000
21 c	-0.22042	2.99026	3.22310	0.00511	0.00196	0.00000
22 h	0.22687	0.77243	0.00062	0.00008	0.00000	0.00000
23 c	-0.19687	2.99631	3.19344	0.00514	0.00198	0.00000
24 h	0.22982	0.76950	0.00060	0.00008	0.00000	0.00000
25 c	-0.21141	2.99194	3.21242	0.00506	0.00199	0.00000
26 h	0.23046	0.76886	0.00061	0.00008	0.00000	0.00000
27 c	-0.19929	2.98391	3.20795	0.00536	0.00207	0.00000
28 h	0.23697	0.76223	0.00072	0.00008	0.00000	0.00000
29 c	-0.36536	3.01033	3.34514	0.00743	0.00246	0.00000
30 c	-0.20316	2.98277	3.21311	0.00521	0.00207	0.00000
31 h	0.23646	0.76275	0.00071	0.00008	0.00000	0.00000
32 c	-0.21091	2.99180	3.21207	0.00506	0.00197	0.00000
33 h	0.22926	0.77004	0.00062	0.00008	0.00000	0.00000
34 c	-0.20307	2.99551	3.20046	0.00513	0.00198	0.00000
35 h	0.22956	0.76976	0.00060	0.00008	0.00000	0.00000
36 c	-0.20947	2.98937	3.21309	0.00508	0.00193	0.00000
37 h	0.22872	0.77057	0.00063	0.00008	0.00000	0.00000

38 c	-0.22111	2.98235	3.23127	0.00547	0.00202	0.00000
39 h	0.24717	0.75183	0.00092	0.00009	0.00000	0.00000
40 c	-0.35602	3.01267	3.33337	0.00754	0.00244	0.00000
41 c	-0.21454	2.98087	3.22615	0.00546	0.00205	0.00000
42 h	0.24046	0.75861	0.00085	0.00008	0.00000	0.00000
43 c	-0.20401	2.98958	3.20737	0.00518	0.00189	0.00000
44 h	0.23302	0.76624	0.00067	0.00007	0.00000	0.00000
45 c	-0.20776	2.99340	3.20722	0.00518	0.00195	0.00000
46 h	0.22827	0.77103	0.00062	0.00008	0.00000	0.00000
47 c	-0.22700	2.98874	3.23126	0.00508	0.00193	0.00000
48 h	0.22591	0.77337	0.00064	0.00008	0.00000	0.00000
49 c	-0.22477	2.97927	3.23819	0.00528	0.00204	0.00000
50 h	0.23299	0.76622	0.00071	0.00008	0.00000	0.00000
51 c	-0.36743	3.01125	3.34636	0.00741	0.00242	0.00000
52 c	-0.21725	2.98693	3.22284	0.00549	0.00199	0.00000
53 h	0.25517	0.74378	0.00097	0.00008	0.00000	0.00000
54 c	-0.22936	2.98909	3.23327	0.00510	0.00190	0.00000
55 h	0.23347	0.76578	0.00068	0.00008	0.00000	0.00000
56 c	-0.19849	2.99508	3.19635	0.00512	0.00194	0.00000
57 h	0.22851	0.77081	0.00060	0.00008	0.00000	0.00000
58 c	-0.22018	2.99050	3.22266	0.00506	0.00196	0.00000
59 h	0.23007	0.76923	0.00062	0.00008	0.00000	0.00000
60 c	-0.20637	2.98359	3.21531	0.00544	0.00204	0.00000
61 h	0.23904	0.76014	0.00074	0.00007	0.00000	0.00000
62 c	-0.37700	3.01700	3.34983	0.00775	0.00242	0.00000
63 c	-0.20206	2.97930	3.21531	0.00540	0.00205	0.00000
64 h	0.23401	0.76515	0.00077	0.00008	0.00000	0.00000
65 c	-0.20292	2.98791	3.20788	0.00517	0.00196	0.00000
66 h	0.22679	0.77249	0.00064	0.00007	0.00000	0.00000
67 c	-0.20394	2.99228	3.20450	0.00518	0.00198	0.00000
68 h	0.22559	0.77371	0.00062	0.00008	0.00000	0.00000
69 c	-0.21467	2.98751	3.22019	0.00504	0.00194	0.00000
70 h	0.22691	0.77239	0.00062	0.00008	0.00000	0.00000
71 c	-0.20848	2.97861	3.22238	0.00547	0.00202	0.00000
72 h	0.23780	0.76128	0.00083	0.00008	0.00000	0.00000
73 c	-0.36013	3.01701	3.33309	0.00758	0.00244	0.00000
74 c	-0.20456	2.98151	3.21551	0.00547	0.00207	0.00000
75 h	0.23261	0.76657	0.00074	0.00008	0.00000	0.00000
76 c	-0.21914	2.99051	3.22160	0.00510	0.00194	0.00000
77 h	0.22855	0.77074	0.00064	0.00008	0.00000	0.00000
78 c	-0.20523	2.99498	3.20310	0.00520	0.00195	0.00000
79 h	0.22961	0.76969	0.00062	0.00008	0.00000	0.00000
80 c	-0.22078	2.98955	3.22398	0.00535	0.00190	0.00000
81 h	0.23607	0.76315	0.00070	0.00008	0.00000	0.00000
82 c	-0.20786	2.98600	3.21431	0.00549	0.00206	0.00000
83 h	0.24079	0.75840	0.00073	0.00007	0.00000	0.00000
84 c	-0.36149	3.01127	3.34024	0.00760	0.00238	0.00000
85 c	-0.21540	2.98005	3.22797	0.00536	0.00202	0.00000
86 h	0.24732	0.75171	0.00087	0.00009	0.00000	0.00000
87 c	-0.21662	2.98968	3.21997	0.00508	0.00189	0.00000
88 h	0.23379	0.76547	0.00067	0.00007	0.00000	0.00000
89 c	-0.21271	2.99408	3.21153	0.00514	0.00195	0.00000
90 h	0.22628	0.77301	0.00063	0.00008	0.00000	0.00000
91 c	-0.21613	2.98901	3.22018	0.00501	0.00193	0.00000
92 h	0.22897	0.77034	0.00062	0.00008	0.00000	0.00000
93 c	-0.21692	2.97715	3.23241	0.00535	0.00202	0.00000

94	h	0.22910	0.77009	0.00072	0.00008	0.00000	0.00000
95	c	-0.37595	3.01471	3.35083	0.00793	0.00249	0.00000
96	c	-0.21606	2.98044	3.22825	0.00530	0.00207	0.00000
97	h	0.23022	0.76896	0.00074	0.00008	0.00000	0.00000
98	c	-0.21293	2.98873	3.21722	0.00502	0.00197	0.00000
99	h	0.22628	0.77302	0.00062	0.00008	0.00000	0.00000
100	c	-0.19671	2.99301	3.19649	0.00522	0.00199	0.00000
101	h	0.22654	0.77275	0.00063	0.00008	0.00000	0.00000
102	c	-0.19828	2.98809	3.20293	0.00529	0.00197	0.00000
103	h	0.22933	0.76994	0.00066	0.00007	0.00000	0.00000
104	c	-0.19324	2.97774	3.20801	0.00541	0.00208	0.00000
105	h	0.22787	0.77137	0.00069	0.00007	0.00000	0.00000
106	c	-0.35210	3.01297	3.32907	0.00760	0.00246	0.00000
107	c	-0.19940	2.97591	3.21593	0.00549	0.00207	0.00000
108	h	0.22127	0.77787	0.00078	0.00008	0.00000	0.00000
109	c	-0.20215	2.98730	3.20764	0.00525	0.00196	0.00000
110	h	0.22803	0.77125	0.00065	0.00007	0.00000	0.00000
111	c	-0.20202	2.99250	3.20232	0.00521	0.00199	0.00000
112	h	0.22625	0.77304	0.00063	0.00008	0.00000	0.00000
113	c	-0.21241	2.98866	3.21674	0.00504	0.00197	0.00000
114	h	0.22633	0.77296	0.00062	0.00008	0.00000	0.00000
115	c	-0.21313	2.98114	3.22465	0.00527	0.00206	0.00000
116	h	0.23403	0.76516	0.00073	0.00008	0.00000	0.00000
117	c	-0.35012	3.00861	3.33147	0.00758	0.00246	0.00000
118	c	-0.22256	2.97981	3.23538	0.00529	0.00207	0.00000
119	h	0.22815	0.77102	0.00076	0.00007	0.00000	0.00000
120	c	-0.21766	2.98745	3.22323	0.00501	0.00196	0.00000
121	h	0.22506	0.77423	0.00063	0.00008	0.00000	0.00000
122	c	-0.20372	2.99258	3.20398	0.00517	0.00199	0.00000
123	h	0.22710	0.77221	0.00062	0.00008	0.00000	0.00000
124	c	-0.19734	2.98924	3.20092	0.00522	0.00196	0.00000
125	h	0.22802	0.77126	0.00064	0.00008	0.00000	0.00000
126	c	-0.19848	2.97985	3.21109	0.00548	0.00207	0.00000
127	h	0.23356	0.76555	0.00081	0.00008	0.00000	0.00000
128	c	-0.35900	3.00985	3.33937	0.00734	0.00243	0.00000
129	c	-0.21362	2.98374	3.22246	0.00542	0.00200	0.00000
130	h	0.24470	0.75430	0.00092	0.00008	0.00000	0.00000
131	c	-0.22573	2.98863	3.23014	0.00504	0.00192	0.00000
132	h	0.22882	0.77049	0.00062	0.00008	0.00000	0.00000
133	c	-0.19217	2.99560	3.18953	0.00507	0.00197	0.00000
134	h	0.22824	0.77109	0.00059	0.00008	0.00000	0.00000
135	c	-0.21187	2.99145	3.21341	0.00501	0.00200	0.00000
136	h	0.22957	0.76974	0.00061	0.00008	0.00000	0.00000
137	c	-0.19924	2.98380	3.20797	0.00542	0.00205	0.00000
138	h	0.23350	0.76567	0.00075	0.00008	0.00000	0.00000

QTAIM Charges:

1	(Au)	Charge:	-0.179270	Volume:	183.103	Bohr^3
2	(Pt)	Charge:	-0.267843	Volume:	170.138	Bohr^3
3	(P)	Charge:	1.965226	Volume:	70.882	Bohr^3
4	(P)	Charge:	1.893579	Volume:	69.540	Bohr^3
5	(P)	Charge:	1.869956	Volume:	73.592	Bohr^3
6	(P)	Charge:	1.877654	Volume:	67.493	Bohr^3
7	(C)	Charge:	-0.646316	Volume:	79.303	Bohr^3
8	(C)	Charge:	0.003906	Volume:	79.936	Bohr^3

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 9 (H )    Charge:    0.029596     Volume:    45.878 Bohr^3
10 (C )    Charge:    0.005880     Volume:    81.820 Bohr^3
11 (H )    Charge:    0.022806     Volume:    47.849 Bohr^3
12 (C )    Charge:    0.003822     Volume:    82.748 Bohr^3
13 (H )    Charge:    0.022142     Volume:    47.852 Bohr^3
14 (C )    Charge:    0.003426     Volume:    81.442 Bohr^3
15 (H )    Charge:    0.018653     Volume:    48.995 Bohr^3
16 (C )    Charge:   -0.006460     Volume:    73.212 Bohr^3
17 (H )    Charge:    0.032296     Volume:    42.531 Bohr^3
18 (C )    Charge:   -0.648892     Volume:    76.644 Bohr^3
19 (C )    Charge:   -0.004038     Volume:    77.820 Bohr^3
20 (H )    Charge:    0.036868     Volume:    41.205 Bohr^3
21 (C )    Charge:    0.001683     Volume:    81.490 Bohr^3
22 (H )    Charge:    0.015620     Volume:    49.311 Bohr^3
23 (C )    Charge:    0.004873     Volume:    82.240 Bohr^3
24 (H )    Charge:    0.023591     Volume:    47.742 Bohr^3
25 (C )    Charge:    0.007307     Volume:    82.890 Bohr^3
26 (H )    Charge:    0.022874     Volume:    47.766 Bohr^3
27 (C )    Charge:    0.000144     Volume:    80.056 Bohr^3
28 (H )    Charge:    0.029917     Volume:    45.716 Bohr^3
29 (C )    Charge:   -0.650833     Volume:    81.536 Bohr^3
30 (C )    Charge:   -0.000984     Volume:    81.746 Bohr^3
31 (H )    Charge:    0.028520     Volume:    45.534 Bohr^3
32 (C )    Charge:    0.005725     Volume:    82.094 Bohr^3
33 (H )    Charge:    0.020515     Volume:    47.938 Bohr^3
34 (C )    Charge:    0.003996     Volume:    82.210 Bohr^3
35 (H )    Charge:    0.022257     Volume:    47.822 Bohr^3
36 (C )    Charge:    0.007388     Volume:    81.806 Bohr^3
37 (H )    Charge:    0.017855     Volume:    49.714 Bohr^3
38 (C )    Charge:   -0.010638     Volume:    71.567 Bohr^3
39 (H )    Charge:    0.032228     Volume:    40.161 Bohr^3
40 (C )    Charge:   -0.622601     Volume:    71.817 Bohr^3
41 (C )    Charge:    0.004988     Volume:    75.539 Bohr^3
42 (H )    Charge:    0.026715     Volume:    41.452 Bohr^3
43 (C )    Charge:    0.008941     Volume:    80.614 Bohr^3
44 (H )    Charge:    0.023156     Volume:    48.767 Bohr^3
45 (C )    Charge:    0.004799     Volume:    80.770 Bohr^3
46 (H )    Charge:    0.017158     Volume:    48.289 Bohr^3
47 (C )    Charge:   -0.001377     Volume:    79.413 Bohr^3
48 (H )    Charge:    0.010421     Volume:    48.877 Bohr^3
49 (C )    Charge:   -0.002619     Volume:    74.225 Bohr^3
50 (H )    Charge:    0.016368     Volume:    46.618 Bohr^3
51 (C )    Charge:   -0.624909     Volume:    74.434 Bohr^3
52 (C )    Charge:   -0.012763     Volume:    72.294 Bohr^3
53 (H )    Charge:    0.048597     Volume:    34.414 Bohr^3
54 (C )    Charge:   -0.003169     Volume:    81.362 Bohr^3
55 (H )    Charge:    0.020996     Volume:    48.898 Bohr^3
56 (C )    Charge:    0.000466     Volume:    81.838 Bohr^3
57 (H )    Charge:    0.020046     Volume:    48.020 Bohr^3
58 (C )    Charge:    0.002934     Volume:    80.991 Bohr^3
59 (H )    Charge:    0.019507     Volume:    48.145 Bohr^3
60 (C )    Charge:    0.000510     Volume:    74.139 Bohr^3
61 (H )    Charge:    0.030047     Volume:    45.824 Bohr^3
62 (C )    Charge:   -0.629739     Volume:    76.036 Bohr^3
63 (C )    Charge:    0.005842     Volume:    74.817 Bohr^3
64 (H )    Charge:    0.022640     Volume:    44.834 Bohr^3
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 65 (C )    Charge:    0.013865     Volume:    76.443 Bohr^3
 66 (H )    Charge:    0.013552     Volume:    48.947 Bohr^3
 67 (C )    Charge:    0.005439     Volume:    80.405 Bohr^3
 68 (H )    Charge:    0.013375     Volume:    48.445 Bohr^3
 69 (C )    Charge:    0.005904     Volume:    81.491 Bohr^3
 70 (H )    Charge:    0.014690     Volume:    48.611 Bohr^3
 71 (C )    Charge:   -0.004559     Volume:    74.196 Bohr^3
 72 (H )    Charge:    0.023018     Volume:    42.162 Bohr^3
 73 (C )    Charge:   -0.616733     Volume:    76.529 Bohr^3
 74 (C )    Charge:    0.004777     Volume:    75.904 Bohr^3
 75 (H )    Charge:    0.021190     Volume:    47.280 Bohr^3
 76 (C )    Charge:    0.003898     Volume:    80.547 Bohr^3
 77 (H )    Charge:    0.016603     Volume:    48.632 Bohr^3
 78 (C )    Charge:    0.001561     Volume:    79.842 Bohr^3
 79 (H )    Charge:    0.020486     Volume:    48.093 Bohr^3
 80 (C )    Charge:    0.003751     Volume:    78.259 Bohr^3
 81 (H )    Charge:    0.025903     Volume:    47.321 Bohr^3
 82 (C )    Charge:   -0.004077     Volume:    73.096 Bohr^3
 83 (H )    Charge:    0.031680     Volume:    44.074 Bohr^3
 84 (C )    Charge:   -0.634199     Volume:    74.183 Bohr^3
 85 (C )    Charge:   -0.003726     Volume:    74.963 Bohr^3
 86 (H )    Charge:    0.034168     Volume:    37.059 Bohr^3
 87 (C )    Charge:    0.001136     Volume:    82.785 Bohr^3
 88 (H )    Charge:    0.023434     Volume:    49.632 Bohr^3
 89 (C )    Charge:   -0.000013     Volume:    80.606 Bohr^3
 90 (H )    Charge:    0.013350     Volume:    48.632 Bohr^3
 91 (C )    Charge:    0.003976     Volume:    83.031 Bohr^3
 92 (H )    Charge:    0.016816     Volume:    49.593 Bohr^3
 93 (C )    Charge:    0.000941     Volume:    73.025 Bohr^3
 94 (H )    Charge:    0.010715     Volume:    45.405 Bohr^3
 95 (C )    Charge:   -0.636826     Volume:    76.878 Bohr^3
 96 (C )    Charge:   -0.005601     Volume:    78.868 Bohr^3
 97 (H )    Charge:    0.015669     Volume:    46.143 Bohr^3
 98 (C )    Charge:    0.006796     Volume:    81.646 Bohr^3
 99 (H )    Charge:    0.014041     Volume:    48.322 Bohr^3
100 (C )    Charge:    0.011245     Volume:    78.989 Bohr^3
101 (H )    Charge:    0.015656     Volume:    48.387 Bohr^3
102 (C )    Charge:    0.020619     Volume:    75.448 Bohr^3
103 (H )    Charge:    0.017545     Volume:    48.674 Bohr^3
104 (C )    Charge:    0.013419     Volume:    72.690 Bohr^3
105 (H )    Charge:    0.011662     Volume:    49.034 Bohr^3
106 (C )    Charge:   -0.626388     Volume:    77.459 Bohr^3
107 (C )    Charge:    0.011277     Volume:    72.345 Bohr^3
108 (H )    Charge:    0.002198     Volume:    46.283 Bohr^3
109 (C )    Charge:    0.017552     Volume:    76.076 Bohr^3
110 (H )    Charge:    0.014688     Volume:    48.953 Bohr^3
111 (C )    Charge:    0.008857     Volume:    79.289 Bohr^3
112 (H )    Charge:    0.014022     Volume:    48.438 Bohr^3
113 (C )    Charge:    0.006546     Volume:    81.019 Bohr^3
114 (H )    Charge:    0.013316     Volume:    48.356 Bohr^3
115 (C )    Charge:   -0.004238     Volume:    80.134 Bohr^3
116 (H )    Charge:    0.022247     Volume:    45.218 Bohr^3
117 (C )    Charge:   -0.622552     Volume:    72.784 Bohr^3
118 (C )    Charge:   -0.011450     Volume:    74.789 Bohr^3
119 (H )    Charge:    0.010496     Volume:    45.879 Bohr^3
120 (C )    Charge:    0.002898     Volume:    82.547 Bohr^3
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121 (H )    Charge:    0.011080     Volume:    48.629 Bohr^3
122 (C )    Charge:    0.007328     Volume:    81.208 Bohr^3
123 (H )    Charge:    0.016688     Volume:    48.190 Bohr^3
124 (C )    Charge:    0.015448     Volume:    76.573 Bohr^3
125 (H )    Charge:    0.016196     Volume:    48.775 Bohr^3
126 (C )    Charge:    0.013771     Volume:    74.472 Bohr^3
127 (H )    Charge:    0.021524     Volume:    44.507 Bohr^3
128 (C )    Charge:   -0.625596     Volume:    76.620 Bohr^3
129 (C )    Charge:   -0.012681     Volume:    71.909 Bohr^3
130 (H )    Charge:    0.031586     Volume:    35.999 Bohr^3
131 (C )    Charge:   -0.000455     Volume:    83.415 Bohr^3
132 (H )    Charge:    0.016334     Volume:    50.161 Bohr^3
133 (C )    Charge:    0.005617     Volume:    82.571 Bohr^3
134 (H )    Charge:    0.021494     Volume:    47.894 Bohr^3
135 (C )    Charge:    0.006582     Volume:    82.856 Bohr^3
136 (H )    Charge:    0.021355     Volume:    47.876 Bohr^3
137 (C )    Charge:    0.003193     Volume:    77.364 Bohr^3
138 (H )    Charge:    0.023942     Volume:    45.996 Bohr^3
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$[(Ph_3P)AuPt(PPh_3)_3]^+$ (1') (trigonal pyramidal form)

ZPE(BP86/def2-SVP) = 1.0737130 Hartree (optimized geometry)
E(BP86/def2-SVP) = −4398.9760260 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −4397.75189268870 Hartree (single point)

Cartesian coordinates in Å:

Au	0.87538	0.12162	0.17001
Pt	-1.68043	0.06353	-0.05572
P	3.12413	-0.03008	-0.04902
C	4.01842	0.00191	1.53364
C	5.28597	-0.60175	1.66772
H	5.74110	-1.12718	0.81433
C	5.95597	-0.53664	2.89868
H	6.94291	-1.00990	3.00922
C	5.36526	0.12700	3.98857
H	5.89285	0.17182	4.95306
C	4.10052	0.72456	3.85286
H	3.63041	1.23671	4.70444
C	3.41964	0.66078	2.62888
H	2.42072	1.11318	2.52391
C	3.57029	-1.56306	-0.93396
C	2.87334	-2.74601	-0.60469
H	2.08809	-2.72717	0.16706
C	3.15809	-3.93548	-1.28675
H	2.60956	-4.85437	-1.03380
C	4.12599	-3.95044	-2.30605
H	4.33634	-4.88314	-2.84999
C	4.81897	-2.77412	-2.63573
H	5.57651	-2.78424	-3.43344
C	4.54653	-1.57857	-1.95072
H	5.08269	-0.65516	-2.21531
C	3.74070	1.35330	-1.06596
C	4.67306	2.28309	-0.56707
H	5.09806	2.15043	0.43889
C	5.05212	3.38040	-1.35917
H	5.78087	4.10669	-0.96966
C	4.50529	3.54894	-2.64145
H	4.80238	4.41057	-3.25732
C	3.57264	2.61989	-3.13730
H	3.13809	2.75463	-4.13861
C	3.18239	1.52788	-2.35285
H	2.42771	0.82075	-2.73267
P	-1.68174	1.76623	-1.62921
C	-3.45017	2.24875	-1.75260
C	-4.17919	2.35156	-0.54503
H	-3.66772	2.19733	0.41832
C	-5.55246	2.63140	-0.57246
H	-6.10659	2.70255	0.37422
C	-6.21137	2.80525	-1.80209
H	-7.29085	3.01760	-1.82416
C	-5.48850	2.71323	-3.00363

H	-5.99944	2.85774	-3.96744
C	-4.11096	2.43977	-2.98269
H	-3.55027	2.36593	-3.92564
C	-1.18391	1.26886	-3.32544
C	-1.89893	0.22516	-3.95362
H	-2.76428	-0.22806	-3.44788
C	-1.50836	-0.24059	-5.21439
H	-2.07754	-1.04888	-5.69498
C	-0.37415	0.29905	-5.84534
H	-0.05585	-0.08234	-6.82677
C	0.34872	1.32631	-5.21942
H	1.22957	1.76037	-5.71709
C	-0.05983	1.82190	-3.96932
H	0.49361	2.64489	-3.49538
C	-0.78779	3.35615	-1.36695
C	0.56529	3.32570	-0.97241
H	1.05556	2.35300	-0.79690
C	1.28531	4.51168	-0.77866
H	2.34422	4.45919	-0.48513
C	0.64606	5.75163	-0.95331
H	1.20094	6.68796	-0.79111
C	-0.70678	5.79245	-1.33200
H	-1.21159	6.76089	-1.46677
C	-1.42164	4.60260	-1.54868
H	-2.47664	4.64317	-1.85713
P	-1.45840	0.14163	2.24100
C	-3.20027	0.56761	2.62890
C	-4.21956	-0.26093	2.09841
H	-3.95130	-1.18616	1.56864
C	-5.56583	0.10512	2.22476
H	-6.34625	-0.54325	1.80001
C	-5.91035	1.30147	2.87781
H	-6.96736	1.59066	2.97753
C	-4.90287	2.12920	3.40315
H	-5.17044	3.06570	3.91511
C	-3.55117	1.76864	3.27900
H	-2.76480	2.42414	3.68082
C	-0.44471	1.46491	3.02579
C	-0.20287	2.63710	2.27858
H	-0.64125	2.73211	1.27381
C	0.60868	3.65398	2.79986
H	0.79553	4.55687	2.19981
C	1.18694	3.50596	4.07354
H	1.83222	4.29820	4.48186
C	0.94006	2.34390	4.82501
H	1.38191	2.23082	5.82677
C	0.12826	1.32124	4.30531
H	-0.05001	0.40671	4.88954
C	-1.03185	-1.33551	3.23326
C	0.15637	-2.02573	2.91545
H	0.75097	-1.70093	2.04375
C	0.57371	-3.10824	3.69773
H	1.50231	-3.63974	3.44378
C	-0.20407	-3.52377	4.79302
H	0.11888	-4.37991	5.40396
C	-1.40021	-2.85479	5.09896

H	-2.01290	-3.18291	5.95217
C	-1.81531	-1.75826	4.32486
H	-2.74496	-1.22435	4.57311
P	-2.05900	-2.08082	-0.91846
C	-1.57795	-3.48522	0.16760
C	-2.33976	-3.74766	1.32769
H	-3.23299	-3.14431	1.54675
C	-1.97672	-4.78331	2.19604
H	-2.58454	-4.98178	3.09027
C	-0.82962	-5.55370	1.93570
H	-0.54050	-6.36197	2.62340
C	-0.05579	-5.28482	0.79674
H	0.83892	-5.89051	0.58524
C	-0.42991	-4.26100	-0.08999
H	0.16128	-4.07362	-0.99755
C	-1.11554	-2.45441	-2.45612
C	0.16014	-1.87399	-2.61072
H	0.52252	-1.16264	-1.84843
C	0.96026	-2.18583	-3.71627
H	1.96104	-1.73828	-3.80794
C	0.47701	-3.06275	-4.70128
H	1.09585	-3.30325	-5.57864
C	-0.80378	-3.62624	-4.56839
H	-1.18874	-4.30682	-5.34283
C	-1.59694	-3.33233	-3.44693
H	-2.59533	-3.78321	-3.34761
C	-3.82684	-2.40339	-1.29398
C	-4.66727	-1.28897	-1.50715
H	-4.25208	-0.27197	-1.43559
C	-6.02981	-1.47175	-1.78683
H	-6.67110	-0.59263	-1.94842
C	-6.56518	-2.76945	-1.84630
H	-7.63477	-2.91588	-2.05946
C	-5.73583	-3.88311	-1.62300
H	-6.15651	-4.89924	-1.66118
C	-4.37155	-3.70463	-1.34533
H	-3.72930	-4.57701	-1.15154

$[(Cy_3P)AuPt(PCy_3)_2]^+$ (2)

ZPE(BP86/def2-SVP) = 1.4126710 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3395.6748221 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3394.70177497158 Hartree (single point)

Cartesian coordinates in Å:

Pt	11.66499	6.36492	7.09896
Au	12.15629	4.83645	5.09850
P	13.01302	7.94673	6.08737
P	10.38149	4.75402	8.13571
P	12.66025	3.50236	3.30520
C	14.79848	7.40806	5.90565
H	14.78451	6.90752	4.91053
C	15.17812	6.33211	6.94309
H	15.11077	6.75976	7.96653
H	14.42766	5.51389	6.90573
C	16.59440	5.79284	6.70051
H	16.85488	5.05255	7.48514
H	16.61082	5.24051	5.73443
C	17.63229	6.92267	6.65265
H	18.64278	6.51474	6.44328
H	17.69251	7.40725	7.65296
C	17.25274	7.97671	5.60401
H	17.28758	7.51722	4.59087
H	17.99062	8.80523	5.59512
C	15.84243	8.53837	5.84949
H	15.83761	9.09636	6.81065
H	15.58458	9.27320	5.06040
C	12.96927	9.48562	7.13805
H	13.61510	10.26030	6.66935
C	13.50522	9.16094	8.54915
H	12.94510	8.28089	8.94355
H	14.56681	8.84622	8.49923
C	13.35020	10.34540	9.51295
H	13.71641	10.05730	10.52010
H	14.00137	11.18101	9.17147
C	11.89649	10.83036	9.58029
H	11.80778	11.70069	10.26238
H	11.26194	10.02488	10.01456
C	11.37373	11.18555	8.18268
H	10.31172	11.50428	8.22863
H	11.94358	12.05591	7.78691
C	11.51692	10.00575	7.21122
H	11.15941	10.29761	6.20327
H	10.85972	9.16602	7.53861
C	12.50883	8.41341	4.34637
H	13.05191	7.64604	3.74822
C	12.96460	9.79997	3.85823
H	12.46422	10.58778	4.46214
H	14.05440	9.93350	4.01004
C	12.61166	10.00125	2.37512
H	12.92525	11.01347	2.04641
H	13.19875	9.27822	1.76414
C	11.11423	9.78597	2.11594

H	10.88665	9.90753	1.03672
H	10.53451	10.57321	2.64787
C	10.66147	8.40505	2.61016
H	11.16993	7.62008	2.00581
H	9.57249	8.26476	2.44845
C	11.00482	8.18903	4.09031
H	10.72712	7.16385	4.41835
H	10.40828	8.88331	4.71990
C	9.90325	5.38397	9.83446
H	10.70362	4.97585	10.49348
C	10.01875	6.92337	9.87202
H	11.02543	7.22873	9.49991
H	9.28304	7.36451	9.16372
C	9.77401	7.47296	11.28325
H	10.59181	7.12617	11.95386
H	9.82652	8.58175	11.27361
C	8.42257	6.99850	11.83793
H	7.60237	7.43966	11.22804
H	8.27709	7.37220	12.87234
C	8.31006	5.46716	11.80142
H	7.31646	5.14063	12.17193
H	9.06245	5.02515	12.49232
C	8.54483	4.91612	10.38467
H	7.73317	5.27985	9.71740
H	8.48032	3.80915	10.38619
C	8.80637	4.31946	7.24135
H	8.14026	3.80285	7.96636
C	8.13340	5.62693	6.77232
H	7.90865	6.27806	7.64247
H	8.87168	6.18820	6.15497
C	6.85845	5.36071	5.96116
H	6.42863	6.32191	5.61103
H	6.09065	4.89584	6.61908
C	7.14103	4.42925	4.77539
H	6.21074	4.22538	4.20621
H	7.83570	4.93993	4.07068
C	7.77975	3.11774	5.24959
H	8.00583	2.45748	4.38610
H	7.05212	2.56043	5.88047
C	9.06102	3.37146	6.05533
H	9.83522	3.83145	5.39422
H	9.48697	2.40920	6.40562
C	11.30511	3.16407	8.41111
H	11.47517	2.79381	7.37359
C	10.55130	2.08470	9.20415
H	9.56818	1.86519	8.73778
H	10.33781	2.46433	10.22763
C	11.39302	0.80202	9.31085
H	10.84640	0.03673	9.89962
H	11.53059	0.37451	8.29164
C	12.76782	1.08459	9.93373
H	12.62886	1.41594	10.98734
H	13.37081	0.15414	9.97816
C	13.52047	2.17374	9.15593
H	13.75959	1.79466	8.13849
H	14.49255	2.40113	9.64047

C	12.68903	3.45726	9.02217
H	12.55933	3.91663	10.02797
H	13.21123	4.21465	8.39974
C	13.16660	1.80038	3.85621
H	12.18652	1.31234	4.05557
C	13.90172	0.98329	2.77738
H	13.32720	0.97466	1.82706
H	14.87631	1.46871	2.55180
C	14.15393	-0.45294	3.26547
H	13.17604	-0.97011	3.38777
H	14.71279	-1.02015	2.49299
C	14.91063	-0.46779	4.60144
H	15.93109	-0.05035	4.44789
H	15.05123	-1.51054	4.95250
C	14.18411	0.36316	5.66982
H	14.76526	0.37467	6.61508
H	13.20687	-0.11349	5.91045
C	13.93454	1.80138	5.19345
H	14.90589	2.32609	5.07544
H	13.36458	2.38100	5.95054
C	14.05624	4.24643	2.31760
H	14.30910	3.51683	1.51591
C	15.28304	4.46122	3.22645
H	15.66844	3.48722	3.58777
H	14.94831	5.01442	4.13269
C	16.40730	5.24519	2.53569
H	17.23104	5.41707	3.25971
H	16.83882	4.63101	1.71481
C	15.89952	6.57247	1.96123
H	15.54824	7.22544	2.79285
H	16.72241	7.12186	1.46042
C	14.74023	6.32748	0.98914
H	15.10743	5.74480	0.11544
H	14.35400	7.28608	0.58414
C	13.59336	5.56655	1.66774
H	12.78401	5.37460	0.93550
H	13.15378	6.21014	2.46255
C	11.24327	3.30290	2.09640
H	11.72009	3.25330	1.09054
C	10.31971	4.53958	2.15231
H	9.88383	4.59748	3.17395
H	10.89773	5.47414	2.02243
C	9.19549	4.45183	1.11203
H	8.54045	5.34369	1.19650
H	9.63779	4.48541	0.09117
C	8.37954	3.16335	1.27832
H	7.60907	3.08472	0.48435
H	7.82909	3.20556	2.24303
C	9.28445	1.92403	1.26544
H	9.73510	1.80661	0.25467
H	8.69071	1.00473	1.44874
C	10.41779	2.01868	2.30166
H	9.98755	2.02407	3.32817
H	11.05853	1.11765	2.22754

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1pt	-0.32866	2.92572	6.36656	9.01142	0.02424	0.00073
2au	-0.26632	3.10752	6.50381	9.63852	0.01619	0.00027
3p	0.03282	5.66466	8.83125	0.43035	0.04092	
4p	0.02627	5.62870	8.87165	0.43222	0.04116	
5p	0.01469	5.62807	8.88880	0.42672	0.04171	
6c	0.20659	2.93592	2.72368	0.12783	0.00597	
7h	-0.07520	1.02458	0.04832	0.00230		
8c	-0.06419	3.09166	2.85441	0.11253	0.00559	
9h	0.09052	0.86980	0.03777	0.00191		
10h	0.03516	0.91716	0.04566	0.00201		
11c	-0.15380	3.15690	2.88301	0.10851	0.00538	
12h	0.08733	0.87385	0.03697	0.00185		
13h	0.04765	0.91044	0.03999	0.00192		
14c	-0.12083	3.14186	2.86658	0.10705	0.00534	
15h	0.08756	0.87319	0.03740	0.00185		
16h	0.06615	0.89512	0.03687	0.00186		
17c	-0.13193	3.14659	2.87227	0.10771	0.00537	
18h	0.05021	0.90867	0.03923	0.00190		
19h	0.09468	0.86621	0.03725	0.00186		
20c	-0.22083	3.19491	2.90603	0.11436	0.00552	
21h	0.08098	0.87772	0.03937	0.00193		
22h	0.08993	0.86799	0.04021	0.00187		
23c	0.05696	3.04430	2.76331	0.12953	0.00590	
24h	0.09652	0.85891	0.04238	0.00218		
25c	-0.21534	3.18187	2.91376	0.11413	0.00558	
26h	0.09079	0.86706	0.04021	0.00194		
27h	0.08697	0.86982	0.04130	0.00191		
28c	-0.14196	3.16230	2.86855	0.10579	0.00531	
29h	0.08596	0.87475	0.03744	0.00185		
30h	0.07379	0.88726	0.03708	0.00187		
31c	-0.08446	3.09840	2.87223	0.10840	0.00543	
32h	0.09715	0.86425	0.03675	0.00185		
33h	0.02476	0.93483	0.03856	0.00185		
34c	-0.15193	3.16789	2.87278	0.10593	0.00532	
35h	0.08596	0.87480	0.03739	0.00185		
36h	0.07451	0.88671	0.03692	0.00186		
37c	-0.19590	3.17198	2.90521	0.11313	0.00558	
38h	0.08551	0.87131	0.04126	0.00191		
39h	0.07781	0.88018	0.04006	0.00195		
40c	0.15702	2.96403	2.74243	0.13049	0.00603	
41h	-0.01981	0.97052	0.04703	0.00226		
42c	-0.21611	3.19511	2.90183	0.11365	0.00551	
43h	0.07921	0.87991	0.03896	0.00193		
44h	0.08907	0.86899	0.04008	0.00186		
45c	-0.13515	3.14816	2.87291	0.10869	0.00539	
46h	0.09366	0.86737	0.03712	0.00185		
47h	0.05090	0.90949	0.03774	0.00186		
48c	-0.12436	3.14968	2.86247	0.10688	0.00533	
49h	0.08784	0.87290	0.03740	0.00185		
50h	0.06798	0.89319	0.03696	0.00187		
51c	-0.14279	3.14902	2.87931	0.10908	0.00538	
52h	0.05522	0.90307	0.03979	0.00192		

53h	0.08648	0.87465	0.03702	0.00185	
54c	-0.06672	3.10140	2.84798	0.11176	0.00557
55h	0.04243	0.90996	0.04558	0.00203	
56h	0.08749	0.87264	0.03799	0.00188	
57c	0.05124	3.04238	2.77194	0.12846	0.00599
58h	0.08718	0.86804	0.04258	0.00220	
59c	-0.13694	3.11761	2.89656	0.11709	0.00568
60h	0.02723	0.92687	0.04393	0.00197	
61h	0.09350	0.86768	0.03695	0.00187	
62c	-0.16825	3.17137	2.88547	0.10610	0.00531
63h	0.07297	0.88804	0.03711	0.00188	
64h	0.08479	0.87486	0.03848	0.00187	
65c	-0.12684	3.14686	2.86780	0.10685	0.00532
66h	0.06701	0.89415	0.03698	0.00187	
67h	0.09246	0.86847	0.03723	0.00185	
68c	-0.13943	3.15957	2.86764	0.10689	0.00532
69h	0.09008	0.87057	0.03750	0.00185	
70h	0.06962	0.89136	0.03715	0.00187	
71c	-0.22159	3.20383	2.89998	0.11230	0.00549
72h	0.07803	0.88116	0.03888	0.00192	
73h	0.08936	0.86913	0.03961	0.00191	
74c	0.10098	3.02194	2.74116	0.12998	0.00594
75h	0.09634	0.85703	0.04439	0.00224	
76c	-0.17930	3.16549	2.89647	0.11173	0.00561
77h	0.09133	0.86766	0.03913	0.00188	
78h	0.08605	0.87089	0.04109	0.00197	
79c	-0.14678	3.17039	2.86490	0.10617	0.00533
80h	0.08518	0.87545	0.03752	0.00185	
81h	0.07423	0.88672	0.03717	0.00187	
82c	-0.12827	3.13733	2.87654	0.10901	0.00539
83h	0.09564	0.86578	0.03675	0.00184	
84h	0.05100	0.90833	0.03878	0.00188	
85c	-0.15959	3.17109	2.87713	0.10605	0.00533
86h	0.07173	0.88590	0.04047	0.00190	
87h	0.08198	0.87923	0.03692	0.00187	
88c	-0.10123	3.07154	2.90717	0.11681	0.00571
89h	-0.01697	0.97181	0.04333	0.00183	
90h	0.08904	0.86976	0.03926	0.00194	
91c	0.10796	3.02680	2.72821	0.13107	0.00597
92h	0.06437	0.88879	0.04456	0.00228	
93c	-0.21421	3.19784	2.89907	0.11180	0.00550
94h	0.09084	0.86843	0.03883	0.00191	
95h	0.07642	0.88293	0.03872	0.00193	
96c	-0.13738	3.15207	2.87131	0.10863	0.00537
97h	0.09391	0.86710	0.03715	0.00184	
98h	0.05934	0.90177	0.03703	0.00187	
99c	-0.12844	3.14932	2.86688	0.10692	0.00532
100h	0.06919	0.89196	0.03698	0.00186	
101h	0.08712	0.87361	0.03742	0.00185	
102c	-0.10643	3.10442	2.88847	0.10813	0.00541
103h	0.02241	0.93537	0.04037	0.00186	
104h	0.08939	0.87204	0.03672	0.00185	
105c	-0.14647	3.13766	2.89031	0.11284	0.00566
106h	0.08462	0.87585	0.03764	0.00188	
107h	0.08063	0.87538	0.04207	0.00191	
108c	0.06010	3.06448	2.73823	0.13122	0.00597

109h	0.09731	0.85614	0.04426	0.00228	
110c	-0.22226	3.20640	2.89813	0.11223	0.00551
111h	0.09855	0.86108	0.03849	0.00188	
112h	0.08205	0.87785	0.03819	0.00191	
113c	-0.14718	3.16339	2.87151	0.10695	0.00533
114h	0.07150	0.88935	0.03727	0.00187	
115h	0.09427	0.86649	0.03740	0.00185	
116c	-0.12739	3.15140	2.86441	0.10627	0.00531
117h	0.06741	0.89368	0.03704	0.00187	
118h	0.09271	0.86812	0.03732	0.00185	
119c	-0.16341	3.16254	2.88855	0.10699	0.00533
120h	0.09145	0.86859	0.03809	0.00187	
121h	0.06839	0.89259	0.03716	0.00187	
122c	-0.10095	3.11067	2.87102	0.11364	0.00562
123h	0.08687	0.87156	0.03967	0.00189	
124h	0.03152	0.92198	0.04452	0.00198	
125c	0.02676	3.04656	2.78907	0.13169	0.00591
126h	0.10402	0.85142	0.04238	0.00218	
127c	-0.17098	3.13921	2.91170	0.11444	0.00563
128h	0.09594	0.86186	0.04030	0.00190	
129h	0.03864	0.91580	0.04361	0.00196	
130c	-0.14514	3.16643	2.86763	0.10575	0.00533
131h	0.08564	0.87373	0.03874	0.00189	
132h	0.08285	0.87849	0.03680	0.00186	
133c	-0.11849	3.12761	2.87727	0.10820	0.00541
134h	0.04047	0.91839	0.03924	0.00191	
135h	0.10042	0.86123	0.03652	0.00183	
136c	-0.14861	3.17181	2.86511	0.10634	0.00535
137h	0.08055	0.88067	0.03691	0.00186	
138h	0.08752	0.87267	0.03794	0.00187	
139c	-0.11795	3.09307	2.90678	0.11248	0.00562
140h	0.10478	0.85377	0.03948	0.00197	
141h	0.00248	0.95338	0.04222	0.00191	
142c	0.11995	3.00870	2.73696	0.12844	0.00595
143h	0.09328	0.86321	0.04133	0.00218	
144c	-0.10933	3.09329	2.89528	0.11510	0.00567
145h	0.04233	0.91367	0.04202	0.00198	
146h	0.05961	0.89702	0.04147	0.00190	
147c	-0.17559	3.18308	2.88037	0.10680	0.00534
148h	0.08670	0.87407	0.03739	0.00185	
149h	0.07471	0.88596	0.03745	0.00188	
150c	-0.10147	3.11870	2.86989	0.10753	0.00535
151h	0.09430	0.86664	0.03722	0.00185	
152h	0.04944	0.90795	0.04072	0.00190	
153c	-0.15269	3.16649	2.87431	0.10655	0.00533
154h	0.07359	0.88755	0.03698	0.00187	
155h	0.09024	0.87046	0.03745	0.00185	
156c	-0.21845	3.18393	2.91580	0.11318	0.00555
157h	0.07060	0.88803	0.03948	0.00188	
158h	0.08965	0.86804	0.04036	0.00194	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 pt	-0.28249	2.81840	6.00400	9.45774	0.00212	0.00023
2 au	0.24897	2.95590	6.00662	9.78669	0.00175	0.00007
3 p	1.04654	5.21731	8.70420	0.03054	0.00141	0.00000
4 p	1.05136	5.21601	8.70060	0.03061	0.00142	0.00000
5 p	1.00874	5.22907	8.72662	0.03401	0.00157	0.00000
6 c	-0.52765	3.07704	3.44030	0.00921	0.00109	0.00000
7 h	0.23198	0.76642	0.00140	0.00019	0.00000	0.00000
8 c	-0.42208	3.05068	3.36406	0.00633	0.00101	0.00000
9 h	0.20941	0.78964	0.00081	0.00014	0.00000	0.00000
10 h	0.23073	0.76830	0.00083	0.00014	0.00000	0.00000
11 c	-0.40534	3.05413	3.34421	0.00604	0.00096	0.00000
12 h	0.21916	0.78008	0.00061	0.00015	0.00000	0.00000
13 h	0.19519	0.80387	0.00080	0.00014	0.00000	0.00000
14 c	-0.40724	3.05861	3.34141	0.00625	0.00097	0.00000
15 h	0.21975	0.77946	0.00063	0.00015	0.00000	0.00000
16 h	0.20125	0.79791	0.00070	0.00015	0.00000	0.00000
17 c	-0.40220	3.05600	3.33917	0.00608	0.00096	0.00000
18 h	0.19757	0.80150	0.00079	0.00014	0.00000	0.00000
19 h	0.22240	0.77683	0.00062	0.00015	0.00000	0.00000
20 c	-0.41796	3.04885	3.36178	0.00632	0.00100	0.00000
21 h	0.20657	0.79243	0.00085	0.00015	0.00000	0.00000
22 h	0.21229	0.78685	0.00071	0.00015	0.00000	0.00000
23 c	-0.53518	3.08026	3.44365	0.01023	0.00104	0.00000
24 h	0.23462	0.76384	0.00134	0.00020	0.00000	0.00000
25 c	-0.41239	3.04941	3.35571	0.00624	0.00103	0.00000
26 h	0.20502	0.79401	0.00083	0.00014	0.00000	0.00000
27 h	0.21623	0.78281	0.00080	0.00016	0.00000	0.00000
28 c	-0.40521	3.05558	3.34256	0.00612	0.00095	0.00000
29 h	0.22010	0.77912	0.00063	0.00015	0.00000	0.00000
30 h	0.20352	0.79562	0.00071	0.00014	0.00000	0.00000
31 c	-0.40555	3.05794	3.34040	0.00623	0.00098	0.00000
32 h	0.22221	0.77702	0.00061	0.00015	0.00000	0.00000
33 h	0.19568	0.80346	0.00071	0.00015	0.00000	0.00000
34 c	-0.40493	3.05561	3.34225	0.00612	0.00095	0.00000
35 h	0.21986	0.77936	0.00063	0.00015	0.00000	0.00000
36 h	0.20310	0.79605	0.00071	0.00014	0.00000	0.00000
37 c	-0.41423	3.05021	3.35674	0.00626	0.00102	0.00000
38 h	0.21537	0.78367	0.00080	0.00016	0.00000	0.00000
39 h	0.20938	0.78963	0.00085	0.00014	0.00000	0.00000
40 c	-0.52584	3.07745	3.43812	0.00917	0.00110	0.00000
41 h	0.22982	0.76860	0.00139	0.00020	0.00000	0.00000
42 c	-0.41752	3.04919	3.36101	0.00631	0.00101	0.00000
43 h	0.20647	0.79254	0.00085	0.00014	0.00000	0.00000
44 h	0.21261	0.78653	0.00070	0.00015	0.00000	0.00000
45 c	-0.40061	3.05677	3.33681	0.00606	0.00096	0.00000
46 h	0.22285	0.77638	0.00062	0.00015	0.00000	0.00000
47 h	0.19478	0.80435	0.00073	0.00014	0.00000	0.00000
48 c	-0.40720	3.05846	3.34153	0.00624	0.00097	0.00000
49 h	0.21992	0.77929	0.00063	0.00015	0.00000	0.00000
50 h	0.20191	0.79725	0.00069	0.00015	0.00000	0.00000
51 c	-0.40397	3.05425	3.34281	0.00595	0.00096	0.00000
52 h	0.19210	0.80697	0.00079	0.00014	0.00000	0.00000

53	h	0.21909	0.78016	0.00060	0.00014	0.00000	0.00000
54	c	-0.42162	3.05071	3.36357	0.00633	0.00102	0.00000
55	h	0.23100	0.76802	0.00085	0.00014	0.00000	0.00000
56	h	0.20948	0.78957	0.00081	0.00014	0.00000	0.00000
57	c	-0.52833	3.07852	3.43946	0.00926	0.00109	0.00000
58	h	0.23322	0.76525	0.00132	0.00020	0.00000	0.00000
59	c	-0.40956	3.05201	3.35026	0.00625	0.00104	0.00000
60	h	0.20913	0.78977	0.00096	0.00014	0.00000	0.00000
61	h	0.20762	0.79138	0.00086	0.00014	0.00000	0.00000
62	c	-0.40683	3.05574	3.34407	0.00606	0.00097	0.00000
63	h	0.20165	0.79750	0.00070	0.00014	0.00000	0.00000
64	h	0.21854	0.78067	0.00065	0.00015	0.00000	0.00000
65	c	-0.40571	3.05954	3.33899	0.00620	0.00097	0.00000
66	h	0.19974	0.79942	0.00069	0.00015	0.00000	0.00000
67	h	0.22302	0.77620	0.00063	0.00016	0.00000	0.00000
68	c	-0.40218	3.05744	3.33767	0.00612	0.00096	0.00000
69	h	0.22222	0.77700	0.00063	0.00015	0.00000	0.00000
70	h	0.20038	0.79875	0.00073	0.00014	0.00000	0.00000
71	c	-0.41693	3.05122	3.35834	0.00636	0.00101	0.00000
72	h	0.20389	0.79510	0.00087	0.00014	0.00000	0.00000
73	h	0.21880	0.78032	0.00074	0.00014	0.00000	0.00000
74	c	-0.53201	3.07626	3.44473	0.00996	0.00107	0.00000
75	h	0.23537	0.76309	0.00134	0.00020	0.00000	0.00000
76	c	-0.41837	3.05178	3.35929	0.00626	0.00103	0.00000
77	h	0.21461	0.78446	0.00078	0.00015	0.00000	0.00000
78	h	0.22049	0.77852	0.00086	0.00014	0.00000	0.00000
79	c	-0.40462	3.05468	3.34289	0.00610	0.00095	0.00000
80	h	0.21999	0.77924	0.00063	0.00015	0.00000	0.00000
81	h	0.20250	0.79664	0.00072	0.00014	0.00000	0.00000
82	c	-0.41025	3.05740	3.34576	0.00611	0.00098	0.00000
83	h	0.22200	0.77724	0.00061	0.00015	0.00000	0.00000
84	h	0.19642	0.80267	0.00077	0.00014	0.00000	0.00000
85	c	-0.40585	3.05309	3.34582	0.00598	0.00096	0.00000
86	h	0.21208	0.78705	0.00072	0.00015	0.00000	0.00000
87	h	0.20698	0.79218	0.00070	0.00014	0.00000	0.00000
88	c	-0.42297	3.04743	3.36853	0.00599	0.00102	0.00000
89	h	0.20624	0.79273	0.00088	0.00015	0.00000	0.00000
90	h	0.21497	0.78412	0.00077	0.00015	0.00000	0.00000
91	c	-0.52951	3.07673	3.44208	0.00960	0.00111	0.00000
92	h	0.23708	0.76142	0.00131	0.00019	0.00000	0.00000
93	c	-0.42147	3.05047	3.36370	0.00628	0.00101	0.00000
94	h	0.21443	0.78467	0.00075	0.00015	0.00000	0.00000
95	h	0.20552	0.79347	0.00087	0.00014	0.00000	0.00000
96	c	-0.40078	3.05712	3.33664	0.00607	0.00096	0.00000
97	h	0.22215	0.77708	0.00062	0.00015	0.00000	0.00000
98	h	0.19543	0.80369	0.00073	0.00014	0.00000	0.00000
99	c	-0.40717	3.05921	3.34075	0.00624	0.00097	0.00000
100	h	0.20157	0.79760	0.00069	0.00015	0.00000	0.00000
101	h	0.22006	0.77915	0.00064	0.00016	0.00000	0.00000
102	c	-0.40399	3.05425	3.34275	0.00603	0.00096	0.00000
103	h	0.19788	0.80116	0.00081	0.00015	0.00000	0.00000
104	h	0.21959	0.77966	0.00061	0.00015	0.00000	0.00000
105	c	-0.41889	3.04988	3.36167	0.00633	0.00101	0.00000
106	h	0.20066	0.79843	0.00076	0.00014	0.00000	0.00000
107	h	0.23277	0.76634	0.00075	0.00014	0.00000	0.00000
108	c	-0.53588	3.07877	3.44661	0.00940	0.00110	0.00000

109 h	0.24264	0.75587	0.00130	0.00020	0.00000	0.00000
110 c	-0.41885	3.05212	3.35936	0.00636	0.00101	0.00000
111 h	0.21578	0.78334	0.00074	0.00015	0.00000	0.00000
112 h	0.20626	0.79272	0.00088	0.00014	0.00000	0.00000
113 c	-0.40242	3.05746	3.33786	0.00615	0.00096	0.00000
114 h	0.20080	0.79832	0.00074	0.00014	0.00000	0.00000
115 h	0.22437	0.77486	0.00062	0.00015	0.00000	0.00000
116 c	-0.40692	3.05915	3.34057	0.00623	0.00097	0.00000
117 h	0.20083	0.79833	0.00069	0.00015	0.00000	0.00000
118 h	0.22404	0.77518	0.00063	0.00015	0.00000	0.00000
119 c	-0.40780	3.05686	3.34397	0.00600	0.00097	0.00000
120 h	0.22202	0.77719	0.00064	0.00015	0.00000	0.00000
121 h	0.19937	0.79976	0.00073	0.00014	0.00000	0.00000
122 c	-0.41412	3.04982	3.35705	0.00623	0.00102	0.00000
123 h	0.20667	0.79236	0.00083	0.00015	0.00000	0.00000
124 h	0.22351	0.77559	0.00077	0.00014	0.00000	0.00000
125 c	-0.52689	3.07963	3.43594	0.01029	0.00103	0.00000
126 h	0.23558	0.76290	0.00132	0.00020	0.00000	0.00000
127 c	-0.42666	3.04876	3.37062	0.00625	0.00103	0.00000
128 h	0.21882	0.78025	0.00078	0.00015	0.00000	0.00000
129 h	0.21393	0.78503	0.00089	0.00014	0.00000	0.00000
130 c	-0.40834	3.05427	3.34705	0.00608	0.00095	0.00000
131 h	0.22013	0.77903	0.00070	0.00014	0.00000	0.00000
132 h	0.20789	0.79127	0.00070	0.00014	0.00000	0.00000
133 c	-0.40891	3.05653	3.34524	0.00617	0.00097	0.00000
134 h	0.19386	0.80521	0.00079	0.00014	0.00000	0.00000
135 h	0.22557	0.77367	0.00061	0.00015	0.00000	0.00000
136 c	-0.40555	3.05434	3.34419	0.00608	0.00094	0.00000
137 h	0.20730	0.79187	0.00070	0.00014	0.00000	0.00000
138 h	0.21967	0.77952	0.00066	0.00015	0.00000	0.00000
139 c	-0.41980	3.04834	3.36424	0.00620	0.00102	0.00000
140 h	0.22065	0.77844	0.00076	0.00015	0.00000	0.00000
141 h	0.20644	0.79253	0.00088	0.00015	0.00000	0.00000
142 c	-0.52573	3.08009	3.43512	0.00946	0.00106	0.00000
143 h	0.23120	0.76726	0.00133	0.00020	0.00000	0.00000
144 c	-0.41968	3.05079	3.36166	0.00620	0.00103	0.00000
145 h	0.21213	0.78686	0.00087	0.00014	0.00000	0.00000
146 h	0.22400	0.77506	0.00079	0.00015	0.00000	0.00000
147 c	-0.40817	3.05515	3.34597	0.00610	0.00094	0.00000
148 h	0.22114	0.77807	0.00065	0.00015	0.00000	0.00000
149 h	0.20286	0.79627	0.00073	0.00014	0.00000	0.00000
150 c	-0.40883	3.05696	3.34462	0.00627	0.00098	0.00000
151 h	0.22360	0.77564	0.00061	0.00015	0.00000	0.00000
152 h	0.20245	0.79660	0.00080	0.00015	0.00000	0.00000
153 c	-0.40305	3.05672	3.33926	0.00613	0.00095	0.00000
154 h	0.20338	0.79576	0.00072	0.00014	0.00000	0.00000
155 h	0.22248	0.77674	0.00063	0.00015	0.00000	0.00000
156 c	-0.41421	3.05050	3.35638	0.00631	0.00101	0.00000
157 h	0.20625	0.79281	0.00081	0.00014	0.00000	0.00000
158 h	0.21681	0.78227	0.00077	0.00015	0.00000	0.00000

QTAIM Charges:

1 (Pt)	Charge:	-0.328719	Volume:	184.954	Bohr^3
2 (Au)	Charge:	-0.116929	Volume:	194.974	Bohr^3
3 (P)	Charge:	1.584658	Volume:	69.675	Bohr^3

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 4 (P )    Charge:    1.614615     Volume:    69.661 Bohr^3
 5 (P )    Charge:    1.642414     Volume:    70.750 Bohr^3
 6 (C )    Charge:   -0.496773     Volume:    58.440 Bohr^3
 7 (H )    Charge:    0.003993     Volume:    37.585 Bohr^3
 8 (C )    Charge:    0.023013     Volume:    55.818 Bohr^3
 9 (H )    Charge:   -0.006521     Volume:    47.484 Bohr^3
10 (H )    Charge:    0.012029     Volume:    42.527 Bohr^3
11 (C )    Charge:    0.030846     Volume:    58.183 Bohr^3
12 (H )    Charge:    0.000798     Volume:    49.420 Bohr^3
13 (H )    Charge:   -0.017536     Volume:    47.961 Bohr^3
14 (C )    Charge:    0.032208     Volume:    58.495 Bohr^3
15 (H )    Charge:    0.003627     Volume:    49.195 Bohr^3
16 (H )    Charge:   -0.009628     Volume:    50.138 Bohr^3
17 (C )    Charge:    0.031881     Volume:    58.206 Bohr^3
18 (H )    Charge:   -0.012717     Volume:    48.636 Bohr^3
19 (H )    Charge:    0.006399     Volume:    48.965 Bohr^3
20 (C )    Charge:    0.029737     Volume:    55.942 Bohr^3
21 (H )    Charge:   -0.004438     Volume:    45.446 Bohr^3
22 (H )    Charge:   -0.006768     Volume:    46.008 Bohr^3
23 (C )    Charge:   -0.515184     Volume:    58.610 Bohr^3
24 (H )    Charge:    0.016068     Volume:    46.025 Bohr^3
25 (C )    Charge:    0.024495     Volume:    55.617 Bohr^3
26 (H )    Charge:   -0.011157     Volume:    45.200 Bohr^3
27 (H )    Charge:   -0.003006     Volume:    43.947 Bohr^3
28 (C )    Charge:    0.033012     Volume:    58.384 Bohr^3
29 (H )    Charge:    0.004119     Volume:    49.110 Bohr^3
30 (H )    Charge:   -0.005837     Volume:    49.941 Bohr^3
31 (C )    Charge:    0.032365     Volume:    58.429 Bohr^3
32 (H )    Charge:    0.006357     Volume:    48.966 Bohr^3
33 (H )    Charge:   -0.014613     Volume:    50.779 Bohr^3
34 (C )    Charge:    0.033092     Volume:    58.385 Bohr^3
35 (H )    Charge:    0.003739     Volume:    49.130 Bohr^3
36 (H )    Charge:   -0.006802     Volume:    49.989 Bohr^3
37 (C )    Charge:    0.022613     Volume:    55.774 Bohr^3
38 (H )    Charge:   -0.004144     Volume:    44.154 Bohr^3
39 (H )    Charge:   -0.004604     Volume:    47.078 Bohr^3
40 (C )    Charge:   -0.501974     Volume:    58.435 Bohr^3
41 (H )    Charge:    0.003104     Volume:    38.754 Bohr^3
42 (C )    Charge:    0.032276     Volume:    56.092 Bohr^3
43 (H )    Charge:   -0.004008     Volume:    46.045 Bohr^3
44 (H )    Charge:   -0.006534     Volume:    45.692 Bohr^3
45 (C )    Charge:    0.032116     Volume:    58.262 Bohr^3
46 (H )    Charge:    0.007281     Volume:    48.925 Bohr^3
47 (H )    Charge:   -0.016210     Volume:    52.153 Bohr^3
48 (C )    Charge:    0.032158     Volume:    58.481 Bohr^3
49 (H )    Charge:    0.004363     Volume:    49.130 Bohr^3
50 (H )    Charge:   -0.008304     Volume:    50.052 Bohr^3
51 (C )    Charge:    0.032446     Volume:    58.181 Bohr^3
52 (H )    Charge:   -0.022307     Volume:    47.223 Bohr^3
53 (H )    Charge:   -0.000421     Volume:    50.108 Bohr^3
54 (C )    Charge:    0.023459     Volume:    56.104 Bohr^3
55 (H )    Charge:    0.013105     Volume:    43.105 Bohr^3
56 (H )    Charge:   -0.005763     Volume:    47.321 Bohr^3
57 (C )    Charge:   -0.496921     Volume:    59.255 Bohr^3
58 (H )    Charge:    0.013564     Volume:    44.678 Bohr^3
59 (C )    Charge:    0.024673     Volume:    55.440 Bohr^3
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60	(H)	Charge:	-0.014880	Volume:	43.516 Bohr^3
61	(H)	Charge:	-0.006326	Volume:	48.890 Bohr^3
62	(C)	Charge:	0.030419	Volume:	58.458 Bohr^3
63	(H)	Charge:	-0.008119	Volume:	50.009 Bohr^3
64	(H)	Charge:	0.000427	Volume:	49.757 Bohr^3
65	(C)	Charge:	0.030857	Volume:	58.514 Bohr^3
66	(H)	Charge:	-0.009972	Volume:	50.131 Bohr^3
67	(H)	Charge:	0.008352	Volume:	48.854 Bohr^3
68	(C)	Charge:	0.033048	Volume:	58.350 Bohr^3
69	(H)	Charge:	0.007243	Volume:	48.916 Bohr^3
70	(H)	Charge:	-0.008881	Volume:	50.024 Bohr^3
71	(C)	Charge:	0.032556	Volume:	55.429 Bohr^3
72	(H)	Charge:	-0.007117	Volume:	46.153 Bohr^3
73	(H)	Charge:	-0.002121	Volume:	46.821 Bohr^3
74	(C)	Charge:	-0.516271	Volume:	58.644 Bohr^3
75	(H)	Charge:	0.016056	Volume:	44.532 Bohr^3
76	(C)	Charge:	0.021669	Volume:	56.069 Bohr^3
77	(H)	Charge:	-0.007276	Volume:	46.439 Bohr^3
78	(H)	Charge:	0.010458	Volume:	46.810 Bohr^3
79	(C)	Charge:	0.032789	Volume:	58.430 Bohr^3
80	(H)	Charge:	0.004043	Volume:	49.113 Bohr^3
81	(H)	Charge:	-0.007051	Volume:	50.055 Bohr^3
82	(C)	Charge:	0.030708	Volume:	57.556 Bohr^3
83	(H)	Charge:	0.003404	Volume:	49.628 Bohr^3
84	(H)	Charge:	-0.017072	Volume:	48.374 Bohr^3
85	(C)	Charge:	0.031384	Volume:	57.586 Bohr^3
86	(H)	Charge:	-0.009826	Volume:	47.074 Bohr^3
87	(H)	Charge:	-0.004492	Volume:	49.785 Bohr^3
88	(C)	Charge:	0.014509	Volume:	55.932 Bohr^3
89	(H)	Charge:	0.000377	Volume:	38.840 Bohr^3
90	(H)	Charge:	-0.006700	Volume:	46.586 Bohr^3
91	(C)	Charge:	-0.525527	Volume:	58.062 Bohr^3
92	(H)	Charge:	0.009889	Volume:	42.412 Bohr^3
93	(C)	Charge:	0.030060	Volume:	56.042 Bohr^3
94	(H)	Charge:	-0.005588	Volume:	47.736 Bohr^3
95	(H)	Charge:	-0.006189	Volume:	46.935 Bohr^3
96	(C)	Charge:	0.032424	Volume:	58.357 Bohr^3
97	(H)	Charge:	0.006383	Volume:	48.982 Bohr^3
98	(H)	Charge:	-0.016073	Volume:	52.448 Bohr^3
99	(C)	Charge:	0.032211	Volume:	58.498 Bohr^3
100	(H)	Charge:	-0.008750	Volume:	50.055 Bohr^3
101	(H)	Charge:	0.003430	Volume:	49.222 Bohr^3
102	(C)	Charge:	0.031528	Volume:	58.282 Bohr^3
103	(H)	Charge:	-0.012204	Volume:	46.801 Bohr^3
104	(H)	Charge:	0.002091	Volume:	49.329 Bohr^3
105	(C)	Charge:	0.022016	Volume:	56.362 Bohr^3
106	(H)	Charge:	-0.014667	Volume:	48.337 Bohr^3
107	(H)	Charge:	0.016365	Volume:	45.111 Bohr^3
108	(C)	Charge:	-0.522701	Volume:	58.864 Bohr^3
109	(H)	Charge:	0.022452	Volume:	42.826 Bohr^3
110	(C)	Charge:	0.029118	Volume:	55.782 Bohr^3
111	(H)	Charge:	-0.003654	Volume:	48.150 Bohr^3
112	(H)	Charge:	-0.004620	Volume:	46.597 Bohr^3
113	(C)	Charge:	0.032383	Volume:	58.398 Bohr^3
114	(H)	Charge:	-0.008219	Volume:	50.148 Bohr^3
115	(H)	Charge:	0.009999	Volume:	48.711 Bohr^3

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116 (C )    Charge:    0.032312     Volume:    58.485 Bohr^3
117 (H )    Charge:   -0.008836     Volume:    50.039 Bohr^3
118 (H )    Charge:    0.010065     Volume:    48.732 Bohr^3
119 (C )    Charge:    0.028923     Volume:    57.980 Bohr^3
120 (H )    Charge:    0.003808     Volume:    48.511 Bohr^3
121 (H )    Charge:   -0.012466     Volume:    52.347 Bohr^3
122 (C )    Charge:    0.026300     Volume:    56.191 Bohr^3
123 (H )    Charge:   -0.004081     Volume:    45.927 Bohr^3
124 (H )    Charge:    0.005149     Volume:    44.404 Bohr^3
125 (C )    Charge:   -0.506934     Volume:    59.025 Bohr^3
126 (H )    Charge:    0.019133     Volume:    46.627 Bohr^3
127 (C )    Charge:    0.020207     Volume:    55.511 Bohr^3
128 (H )    Charge:   -0.002175     Volume:    44.579 Bohr^3
129 (H )    Charge:   -0.000042     Volume:    39.439 Bohr^3
130 (C )    Charge:    0.031243     Volume:    57.928 Bohr^3
131 (H )    Charge:    0.002367     Volume:    49.167 Bohr^3
132 (H )    Charge:   -0.002614     Volume:    49.714 Bohr^3
133 (C )    Charge:    0.031083     Volume:    58.329 Bohr^3
134 (H )    Charge:   -0.020184     Volume:    48.831 Bohr^3
135 (H )    Charge:    0.009488     Volume:    48.884 Bohr^3
136 (C )    Charge:    0.034251     Volume:    58.382 Bohr^3
137 (H )    Charge:   -0.002100     Volume:    49.675 Bohr^3
138 (H )    Charge:    0.002059     Volume:    50.696 Bohr^3
139 (C )    Charge:    0.022168     Volume:    55.123 Bohr^3
140 (H )    Charge:    0.002121     Volume:    45.026 Bohr^3
141 (H )    Charge:   -0.009115     Volume:    39.913 Bohr^3
142 (C )    Charge:   -0.488265     Volume:    59.117 Bohr^3
143 (H )    Charge:    0.014247     Volume:    46.780 Bohr^3
144 (C )    Charge:    0.024895     Volume:    55.280 Bohr^3
145 (H )    Charge:   -0.001015     Volume:    43.165 Bohr^3
146 (H )    Charge:    0.004777     Volume:    41.558 Bohr^3
147 (C )    Charge:    0.030486     Volume:    58.366 Bohr^3
148 (H )    Charge:    0.003922     Volume:    50.318 Bohr^3
149 (H )    Charge:   -0.008219     Volume:    50.172 Bohr^3
150 (C )    Charge:    0.030657     Volume:    58.361 Bohr^3
151 (H )    Charge:    0.008849     Volume:    48.805 Bohr^3
152 (H )    Charge:   -0.006481     Volume:    46.048 Bohr^3
153 (C )    Charge:    0.032869     Volume:    58.316 Bohr^3
154 (H )    Charge:   -0.006287     Volume:    49.778 Bohr^3
155 (H )    Charge:    0.007344     Volume:    48.964 Bohr^3
156 (C )    Charge:    0.029432     Volume:    55.279 Bohr^3
157 (H )    Charge:   -0.006393     Volume:    47.403 Bohr^3
158 (H )    Charge:   -0.000108     Volume:    44.876 Bohr^3
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$[(Ph_3P)AuPt(nbe)_3]^+$ (3) (trigonal pyramidal form)

ZPE(BP86/def2-SVP) = 0.7193132 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2108.9953146 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2108.28154628079 Hartree (single point)

Cartesian coordinates in Å:

Au	0.69383	-0.02764	-0.02186
Pt	-1.91831	-0.02232	-0.03889
P	2.96800	-0.01767	-0.01389
C	-3.07985	2.80882	-1.10601
H	-3.31229	3.42553	-0.21971
C	-1.79815	1.98598	-1.03496
H	-0.84296	2.45677	-0.75329
C	-1.91028	0.98260	-2.03686
H	-1.05578	0.60788	-2.62040
C	-3.27127	1.19819	-2.69548
H	-3.68289	0.34267	-3.25982
C	-3.08424	2.50528	-3.53640
H	-2.20487	2.44418	-4.20709
H	-3.97328	2.67281	-4.17611
C	-2.94739	3.61261	-2.44300
H	-3.76157	4.36045	-2.51661
H	-1.98901	4.16514	-2.50031
C	-4.11483	1.74181	-1.52034
H	-5.08311	2.17181	-1.84285
H	-4.30752	0.99184	-0.72668
C	-3.09378	-2.34721	-1.96672
H	-3.31288	-1.88574	-2.94607
C	-1.81158	-1.88963	-1.27990
H	-0.85208	-1.89319	-1.82075
C	-1.93870	-2.25403	0.08917
H	-1.09293	-2.58326	0.71154
C	-3.30919	-2.91484	0.22155
H	-3.72945	-2.96989	1.24137
C	-3.13376	-4.29927	-0.48784
H	-2.26411	-4.85998	-0.09251
H	-4.03176	-4.92611	-0.31961
C	-2.98053	-3.90850	-1.99260
H	-2.02283	-4.24651	-2.43484
H	-3.79536	-4.33643	-2.60947
C	-4.13515	-2.15906	-0.84364
H	-5.10774	-2.64166	-1.06203
H	-4.31659	-1.09433	-0.59344
C	-3.12022	-0.51398	2.92954
H	-3.35282	-1.59012	3.01786
C	-1.82857	-0.16356	2.19896
H	-0.87682	-0.64181	2.47966
C	-1.93672	1.20569	1.82861
H	-1.08249	1.89918	1.80834
C	-3.30507	1.66735	2.32547
H	-3.71107	2.58289	1.86016

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C         -3.13930        1.74333        3.88021
H         -2.26390        2.35524        4.17383
H         -4.03448        2.21375        4.33302
C         -3.00750        0.24306        4.29540
H         -2.05632        0.01731        4.81627
H         -3.83111       -0.06713        4.96852
C         -4.14587        0.37711        2.19785
H         -5.12143        0.44094        2.71813
H         -4.32404        0.06374        1.14922
C          3.64919       -0.32715        1.64749
C          4.78285       -1.14491        1.82857
H          5.25009       -1.64159        0.96537
C          5.30877       -1.32324        3.11821
H          6.19225       -1.96258        3.26219
C          4.70921       -0.69038        4.21951
H          5.12390       -0.83517        5.22812
C          3.57595        0.12257        4.03761
H          3.10424        0.61367        4.90153
C          3.04080        0.30243        2.75494
H          2.14782        0.93049        2.60718
C          3.66196       -1.29334       -1.11437
C          3.07549       -2.57751       -1.11273
H          2.19204       -2.77693       -0.48553
C          3.62041       -3.59181       -1.91158
H          3.16591       -4.59354       -1.91024
C          4.74161       -3.32624       -2.71834
H          5.16405       -4.12241       -3.34912
C          5.31920       -2.04597       -2.72584
H          6.19319       -1.83802       -3.36057
C          4.78334       -1.02463       -1.92491
H          5.23327       -0.02084       -1.93110
C          3.64106        1.58172       -0.57037
C          4.75438        2.16543        0.06713
H          5.21166        1.67568        0.93953
C          5.27286        3.37722       -0.41725
H          6.14037        3.83558        0.08005
C          4.68610        4.00233       -1.52981
H          5.09478        4.95270       -1.90396
C          3.57306        3.42023       -2.16297
H          3.11124        3.91319       -3.03115
C          3.04538        2.21377       -1.68345
H          2.16807        1.75780       -2.16931

# Raman Activity Spectrum
# X-Axis:  Frequency (cm-1) (Scaled by 0.9694)
# Y-Axis:  Intensity

# Peak information
#                  X                  Y
#       3.3056540000       0.0018000000
#       9.6295349000       0.0721000000
#      10.1441893600       0.0796000000
#      14.6313480800       0.0701000000
#      22.2199082200       2.3608000000
#      23.5809458200       2.2767000000
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#      37.1037850000        6.9038000000
#      37.4188400000        6.7681000000
#      40.2991212800        7.4810000000
#      46.3721214600        0.8167000000
#      48.0863114800        3.1341000000
#      48.2601249000        3.2166000000
#      56.9403263800        1.3039000000
#      58.2791647200        1.2334000000
#      69.5373885600        0.5651000000
#      70.0736606400        0.6400000000
#      70.8334763600        0.5891000000
#      89.0897018600        1.1215000000
#      89.2777654600        1.0782000000
#     116.2081821600        5.9296000000
#     127.2813475400        0.5062000000
#     128.5572718200        0.5024000000
#     162.1559003000        0.1640000000
#     163.5131572400        0.0825000000
#     164.5012666600        0.1462000000
#     173.7602968800        3.1757000000
#     186.2498526000       10.9112000000
#     200.1024816600        6.0268000000
#     208.2897432400        1.8678000000
#     208.9476750200        1.1037000000
#     209.7784508200        3.1222000000
#     209.9876473400        3.3365000000
#     233.3419474400        0.1927000000
#     248.0376636800        6.0868000000
#     250.3193404600        0.0070000000
#     252.0380866600        0.1743000000
#     252.3656469200        0.1796000000
#     263.9717884200        1.8524000000
#     264.3304664200        1.8637000000
#     392.5363307400        0.2643000000
#     392.7810073000        0.2696000000
#     397.3863358800        1.5598000000
#     438.2261884800        4.1814000000
#     440.9549525400        1.3652000000
#     441.1942974000        0.6592000000
#     441.4951991600        0.5773000000
#     442.2417341000        0.8494000000
#     461.1140133000        8.6991000000
#     501.9332176800        0.0721000000
#     502.2065884800        0.0613000000
#     505.2537035000        2.0147000000
#     505.7495516000        2.0184000000
#     524.2364943000        0.0366000000
#     527.8435347600        3.4771000000
#     528.1213648000        3.4865000000
#     531.0030032400       18.9602000000
#     540.0342244600        5.9351000000
#     615.7330224800        4.0129000000
#     615.7724770600        4.0641000000
#     616.5890026800        2.1412000000
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#     662.2871972600        0.5731000000
#     662.4810772600        0.5807000000
#     667.1074418200        0.0144000000
#     689.5297607600        4.6376000000
#     690.1120793400        0.6036000000
#     690.3609243200        0.5949000000
#     691.2264046400        0.7144000000
#     710.5108727200        3.5413000000
#     710.6295272800        3.5759000000
#     743.6053162600        0.0271000000
#     746.2480945400        1.2589000000
#     746.3744073600        1.2422000000
#     748.6958295400        0.4454000000
#     748.8958167600        0.4477000000
#     753.7460157800        0.3400000000
#     766.4878093800        0.0020000000
#     770.3018167400        0.9087000000
#     770.5046152200        0.9095000000
#     796.3162473800        0.1173000000
#     796.5254439000        0.1123000000
#     798.8356210400        0.5307000000
#     824.7610607600        0.0258000000
#     830.0289742400        2.5532000000
#     830.2049203400        3.0113000000
#     831.2497396600        4.4413000000
#     831.8691862600        7.0359000000
#     838.6781549200        0.5277000000
#     838.7321505000        0.5132000000
#     841.7765512000        1.5261000000
#     851.7298657000       43.8247000000
#     854.5121406400        3.3620000000
#     854.8152720200        3.4215000000
#     868.9929409000        6.7122000000
#     879.1115381000        0.0983000000
#     883.6368911800        1.7744000000
#     883.7660152600        1.8241000000
#     887.8960470200        0.4913000000
#     888.2275818200        0.4780000000
#     895.1382405400        9.8502000000
#     911.5667592800        2.9073000000
#     911.6606941400        2.9361000000
#     916.3230234400       11.1919000000
#     919.9828962000        0.8757000000
#     920.0644227400        0.8779000000
#     920.8984945000        0.2781000000
#     932.3391594200        0.0510000000
#     937.5855522200        1.6635000000
#     937.9195105200        1.6685000000
#     950.1869767000        5.6373000000
#     950.4408625600        5.6503000000
#     953.7614453200       11.1696000000
#     958.7517226400        0.2385000000
#     958.8275297200        0.2270000000
#     959.3649650800        0.6747000000
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#     981.9290103000        0.6114000000
#     981.9705006200        0.6048000000
#     982.0731600800        0.7830000000
#     985.0021052400        0.0712000000
#     994.1955070800       20.1380000000
#     994.2152828400       20.1848000000
#     994.8641992000      136.6671000000
#     995.2446887000        0.4926000000
#     995.5917339000        0.5763000000
#    1002.5369032600        7.7840000000
#    1002.9363930000        7.8428000000
#    1008.4423911200       11.1871000000
#    1019.2011800800        0.5629000000
#    1020.5668708000       56.1008000000
#    1021.1892256000        7.7752000000
#    1021.2025063800        7.7714000000
#    1029.0029773600        5.4300000000
#    1029.5974134400        5.4770000000
#    1064.9417374400        3.1583000000
#    1065.7211350400        3.4607000000
#    1072.2856210200       58.2307000000
#    1076.3197791200        0.2523000000
#    1076.4069281800        0.1300000000
#    1076.4454133600        2.6892000000
#    1091.8562559800       65.9435000000
#    1092.4616462800       25.1883000000
#    1092.6634753600       26.9613000000
#    1093.4544088200        0.1011000000
#    1106.9718193600       14.1092000000
#    1107.7110838000       13.8716000000
#    1111.9126572800        0.8266000000
#    1112.0096942200        0.8367000000
#    1119.9527639400       14.2760000000
#    1153.5952093000        0.0882000000
#    1156.3548002800        1.5857000000
#    1156.7110547800        3.3230000000
#    1156.7242386200        3.3114000000
#    1157.0834013200        3.6832000000
#    1157.2805772800        3.7109000000
#    1161.7551338000        5.6198000000
#    1161.7933281600        6.2138000000
#    1164.9627814600       24.8687000000
#    1177.0991847600        2.9725000000
#    1177.1657825400        3.0088000000
#    1178.6509033400        4.3602000000
#    1198.2593449000        0.1002000000
#    1201.1501926400       10.8118000000
#    1201.3426185400       10.8241000000
#    1237.8751361200        0.0112000000
#    1247.9170537800        0.6078000000
#    1248.4445043200        0.5536000000
#    1253.2458455800        0.0173000000
#    1255.8781543400        1.0551000000
#    1256.4029875000        1.0746000000
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#    1264.7721085200        1.7797000000
#    1264.9742284200        1.7540000000
#    1268.3057654000        0.4820000000
#    1269.5129592200       13.4648000000
#    1269.7111045800        0.9189000000
#    1269.9054692800        0.9169000000
#    1277.9567240400        3.3394000000
#    1282.5082509200        0.2539000000
#    1282.7677593000        0.2581000000
#    1289.4619510000        0.8313000000
#    1289.9341457400        0.8004000000
#    1295.2232890800        4.3454000000
#    1313.7759571000        0.0832000000
#    1315.3004355400        2.5988000000
#    1315.7128183000        2.5897000000
#    1320.3971529800        3.6981000000
#    1320.6269977200        2.4198000000
#    1320.7231622000        2.4912000000
#    1405.4297219600       22.5822000000
#    1405.7737620200       37.6380000000
#    1406.5797211800       50.2807000000
#    1430.4829925000        5.7078000000
#    1432.0673798600        2.9125000000
#    1432.1746924400        2.9458000000
#    1448.6728141000        2.5897000000
#    1449.3877466000        2.7277000000
#    1449.8421043800        3.4727000000
#    1449.8601352200       16.4346000000
#    1449.9313861200       13.2638000000
#    1455.2012384000       13.7486000000
#    1473.1939809800        2.6452000000
#    1473.4436014800        2.6414000000
#    1475.7662838800        2.9507000000
#    1476.2851067600        1.4455000000
#    1476.3213623200        1.5093000000
#    1476.6285651800        7.2807000000
#    1567.4343958600        7.0314000000
#    1568.6151250600        6.9671000000
#    1568.6846310400        7.0181000000
#    1582.3347524400       69.1375000000
#    1582.3649007800       69.8738000000
#    1582.8835297800       41.6427000000
#    2966.2038551200        9.1702000000
#    2966.3012798200      101.3534000000
#    2966.3323006200      109.3063000000
#    2972.7986833200        0.8945000000
#    2973.2601177200        4.8663000000
#    2974.9099395800      620.8827000000
#    2976.4924850800      198.7662000000
#    2976.9912413800      195.2784000000
#    2985.1552373600      605.1470000000
#    2998.3573990200       22.2869000000
#    2998.4043179800       45.4960000000
#    2998.4252570200       59.6902000000
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#    3015.0532782800      123.4335000000
#    3015.3249041600      146.8641000000
#    3016.4762605400       76.3236000000
#    3019.6341779800      154.6250000000
#    3020.3181866200      130.8571000000
#    3032.6964552200       50.8197000000
#    3032.8750187000       13.5863000000
#    3035.1233481200       15.5962000000
#    3035.4367551400       15.5584000000
#    3041.8568005200       58.9692000000
#    3042.2090804800       57.0708000000
#    3044.2675044400      366.6760000000
#    3071.5227670800       29.4839000000
#    3071.5580532400       29.5979000000
#    3071.6517942200       28.8049000000
#    3077.3496366000       12.7571000000
#    3078.0612731400       32.9200000000
#    3078.1989279400       32.5031000000
#    3085.8770606400       55.5106000000
#    3085.9676995400       55.2808000000
#    3086.0237308600       60.7617000000
#    3093.6464138800      120.7016000000
#    3093.7995790800      130.5549000000
#    3093.9820201600       37.5899000000
#    3094.2140945200      209.6925000000
#    3094.6811514400        4.4706000000
#    3094.9226289800       10.0839000000
#    3101.2636682600       41.9458000000
#    3101.4822679600       40.5938000000
#    3101.6126522600       56.3128000000
#    3108.1385561200      165.3594000000
#    3108.2357869400      139.6502000000
#    3108.4700909200      736.1678000000
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MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	-0.08515	3.41421	6.02313	9.63317	0.01434	0.00029
2pt	-0.38659	2.75967	6.76756	8.81756	0.04094	0.00086
3p	0.30298	5.53596	8.65998	0.45769	0.04338	
4c	0.13034	3.01284	2.71159	0.13724	0.00800	
5h	0.08956	0.86943	0.03900	0.00201		
6c	-0.17255	3.17393	2.86828	0.12269	0.00765	
7h	0.15680	0.80186	0.03946	0.00189		
8c	-0.16987	3.18524	2.85428	0.12270	0.00764	
9h	0.15188	0.80769	0.03856	0.00187		
10c	0.12139	3.01663	2.71650	0.13748	0.00799	
11h	0.09338	0.86550	0.03912	0.00200		
12c	-0.20953	3.21907	2.88742	0.09758	0.00546	
13h	0.08629	0.87437	0.03748	0.00186		
14h	0.10260	0.85818	0.03733	0.00189		
15c	-0.20302	3.21409	2.88629	0.09719	0.00545	
16h	0.10150	0.85929	0.03733	0.00189		
17h	0.08576	0.87480	0.03757	0.00187		

18c	-0.23018	3.20555	2.91308	0.10553	0.00603
19h	0.10208	0.85860	0.03744	0.00188	
20h	0.06673	0.88640	0.04489	0.00199	
21c	0.12701	3.01426	2.71326	0.13747	0.00800
22h	0.08981	0.86913	0.03905	0.00201	
23c	-0.17399	3.17717	2.86655	0.12262	0.00765
24h	0.15556	0.80323	0.03933	0.00188	
25c	-0.16274	3.18043	2.85177	0.12289	0.00765
26h	0.15099	0.80857	0.03856	0.00188	
27c	0.11919	3.01828	2.71726	0.13728	0.00798
28h	0.09245	0.86643	0.03912	0.00200	
29c	-0.20891	3.21835	2.88744	0.09766	0.00546
30h	0.08655	0.87404	0.03754	0.00187	
31h	0.10234	0.85842	0.03735	0.00189	
32c	-0.20316	3.21422	2.88620	0.09729	0.00545
33h	0.08573	0.87487	0.03753	0.00187	
34h	0.10228	0.85862	0.03722	0.00188	
35c	-0.22672	3.20267	2.91244	0.10559	0.00602
36h	0.10183	0.85886	0.03743	0.00188	
37h	0.06843	0.88473	0.04487	0.00197	
38c	0.12690	3.01806	2.70966	0.13738	0.00800
39h	0.08853	0.87044	0.03902	0.00201	
40c	-0.17246	3.17130	2.87071	0.12281	0.00765
41h	0.15591	0.80274	0.03946	0.00189	
42c	-0.16607	3.18451	2.85080	0.12310	0.00766
43h	0.15027	0.80931	0.03855	0.00187	
44c	0.12397	3.01621	2.71460	0.13723	0.00799
45h	0.09197	0.86706	0.03899	0.00199	
46c	-0.20953	3.21961	2.88689	0.09756	0.00546
47h	0.08582	0.87472	0.03759	0.00187	
48h	0.10288	0.85799	0.03725	0.00189	
49c	-0.20308	3.21364	2.88674	0.09725	0.00546
50h	0.08627	0.87449	0.03737	0.00186	
51h	0.10264	0.85835	0.03713	0.00188	
52c	-0.23415	3.20678	2.91546	0.10587	0.00603
53h	0.10273	0.85809	0.03730	0.00188	
54h	0.07034	0.88290	0.04478	0.00197	
55c	0.02456	3.20033	2.63231	0.13489	0.00791
56c	-0.12366	3.16927	2.83699	0.11010	0.00730
57h	0.14185	0.81629	0.04000	0.00187	
58c	-0.13841	3.18339	2.83771	0.11013	0.00718
59h	0.14600	0.81717	0.03505	0.00178	
60c	-0.08990	3.16669	2.80615	0.10990	0.00716
61h	0.14621	0.81724	0.03480	0.00176	
62c	-0.14226	3.18386	2.84177	0.10946	0.00717
63h	0.14167	0.82147	0.03508	0.00178	
64c	-0.14124	3.17944	2.84346	0.11095	0.00739
65h	0.12063	0.83835	0.03916	0.00187	
66c	0.02287	3.19989	2.63423	0.13510	0.00792
67c	-0.14197	3.17947	2.84406	0.11105	0.00739
68h	0.12014	0.83888	0.03912	0.00186	
69c	-0.14352	3.18462	2.84200	0.10973	0.00718
70h	0.14151	0.82163	0.03507	0.00178	
71c	-0.08932	3.16678	2.80533	0.11005	0.00716
72h	0.14618	0.81730	0.03476	0.00176	
73c	-0.13825	3.18352	2.83726	0.11029	0.00718

74h	0.14553	0.81761	0.03508	0.00178	
75c	-0.11991	3.16591	2.83657	0.11013	0.00730
76h	0.14105	0.81700	0.04008	0.00187	
77c	0.02367	3.20028	2.63313	0.13500	0.00793
78c	-0.11748	3.16413	2.83570	0.11036	0.00729
79h	0.13936	0.81843	0.04033	0.00188	
80c	-0.13850	3.18392	2.83682	0.11058	0.00718
81h	0.14535	0.81778	0.03509	0.00178	
82c	-0.09021	3.16721	2.80547	0.11036	0.00717
83h	0.14607	0.81742	0.03476	0.00176	
84c	-0.14230	3.18373	2.84149	0.10991	0.00717
85h	0.14128	0.82185	0.03509	0.00178	
86c	-0.13853	3.18012	2.83988	0.11114	0.00738
87h	0.11756	0.84139	0.03918	0.00187	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.31204	2.90131	6.00179	9.78337	0.00140	0.00009
2 pt	0.51011	2.48818	6.01046	8.98841	0.00275	0.00009
3 p	1.03294	5.17392	8.74806	0.04347	0.00162	0.00000
4 c	-0.26292	3.01486	3.24179	0.00537	0.00090	0.00000
5 h	0.23085	0.76816	0.00080	0.00019	0.00000	0.00000
6 c	-0.29504	3.03516	3.24910	0.00936	0.00141	0.00000
7 h	0.24066	0.75828	0.00093	0.00013	0.00000	0.00000
8 c	-0.29977	3.03571	3.25325	0.00942	0.00139	0.00000
9 h	0.24039	0.75851	0.00097	0.00013	0.00000	0.00000
10 c	-0.26257	3.01623	3.24011	0.00534	0.00089	0.00000
11 h	0.23177	0.76724	0.00081	0.00019	0.00000	0.00000
12 c	-0.41157	3.07694	3.32771	0.00597	0.00095	0.00000
13 h	0.21599	0.78312	0.00074	0.00015	0.00000	0.00000
14 h	0.22692	0.77214	0.00079	0.00015	0.00000	0.00000
15 c	-0.41155	3.07690	3.32774	0.00597	0.00095	0.00000
16 h	0.22685	0.77222	0.00079	0.00015	0.00000	0.00000
17 h	0.21562	0.78349	0.00074	0.00015	0.00000	0.00000
18 c	-0.40401	3.06533	3.33113	0.00652	0.00103	0.00000
19 h	0.22978	0.76934	0.00072	0.00015	0.00000	0.00000
20 h	0.20453	0.79426	0.00104	0.00017	0.00000	0.00000
21 c	-0.26298	3.01489	3.24183	0.00537	0.00090	0.00000
22 h	0.23088	0.76814	0.00080	0.00019	0.00000	0.00000
23 c	-0.29508	3.03520	3.24912	0.00935	0.00141	0.00000
24 h	0.24056	0.75838	0.00093	0.00013	0.00000	0.00000
25 c	-0.29990	3.03574	3.25335	0.00942	0.00139	0.00000
26 h	0.24049	0.75841	0.00097	0.00013	0.00000	0.00000
27 c	-0.26245	3.01622	3.24000	0.00534	0.00089	0.00000
28 h	0.23173	0.76727	0.00081	0.00019	0.00000	0.00000
29 c	-0.41167	3.07695	3.32780	0.00597	0.00095	0.00000
30 h	0.21607	0.78304	0.00074	0.00015	0.00000	0.00000
31 h	0.22695	0.77211	0.00079	0.00015	0.00000	0.00000
32 c	-0.41165	3.07689	3.32784	0.00597	0.00095	0.00000
33 h	0.21572	0.78339	0.00074	0.00015	0.00000	0.00000
34 h	0.22686	0.77220	0.00078	0.00015	0.00000	0.00000
35 c	-0.40383	3.06526	3.33102	0.00652	0.00103	0.00000

36 h	0.22970	0.76943	0.00072	0.00015	0.00000	0.00000
37 h	0.20441	0.79437	0.00104	0.00017	0.00000	0.00000
38 c	-0.26300	3.01486	3.24187	0.00537	0.00090	0.00000
39 h	0.23093	0.76809	0.00080	0.00019	0.00000	0.00000
40 c	-0.29520	3.03513	3.24930	0.00936	0.00141	0.00000
41 h	0.24060	0.75834	0.00093	0.00013	0.00000	0.00000
42 c	-0.30019	3.03577	3.25361	0.00942	0.00139	0.00000
43 h	0.24034	0.75856	0.00097	0.00013	0.00000	0.00000
44 c	-0.26236	3.01618	3.23995	0.00534	0.00089	0.00000
45 h	0.23165	0.76735	0.00081	0.00019	0.00000	0.00000
46 c	-0.41164	3.07693	3.32779	0.00597	0.00095	0.00000
47 h	0.21597	0.78314	0.00074	0.00015	0.00000	0.00000
48 h	0.22696	0.77210	0.00079	0.00015	0.00000	0.00000
49 c	-0.41173	3.07691	3.32790	0.00597	0.00095	0.00000
50 h	0.21573	0.78338	0.00074	0.00015	0.00000	0.00000
51 h	0.22689	0.77218	0.00078	0.00015	0.00000	0.00000
52 c	-0.40399	3.06531	3.33113	0.00653	0.00103	0.00000
53 h	0.22983	0.76930	0.00072	0.00015	0.00000	0.00000
54 h	0.20438	0.79441	0.00104	0.00017	0.00000	0.00000
55 c	-0.38607	3.01090	3.36501	0.00756	0.00260	0.00000
56 c	-0.19578	2.98537	3.20295	0.00533	0.00212	0.00000
57 h	0.23862	0.76054	0.00076	0.00008	0.00000	0.00000
58 c	-0.20263	2.99324	3.20228	0.00510	0.00201	0.00000
59 h	0.23430	0.76502	0.00060	0.00008	0.00000	0.00000
60 c	-0.18379	2.99836	3.17826	0.00515	0.00202	0.00000
61 h	0.23370	0.76562	0.00059	0.00008	0.00000	0.00000
62 c	-0.20534	2.99257	3.20566	0.00509	0.00202	0.00000
63 h	0.23220	0.76711	0.00061	0.00008	0.00000	0.00000
64 c	-0.19407	2.98190	3.20481	0.00521	0.00215	0.00000
65 h	0.22843	0.77084	0.00066	0.00008	0.00000	0.00000
66 c	-0.38605	3.01091	3.36497	0.00756	0.00260	0.00000
67 c	-0.19404	2.98187	3.20482	0.00521	0.00215	0.00000
68 h	0.22847	0.77079	0.00066	0.00008	0.00000	0.00000
69 c	-0.20529	2.99259	3.20559	0.00509	0.00202	0.00000
70 h	0.23224	0.76707	0.00061	0.00008	0.00000	0.00000
71 c	-0.18391	2.99836	3.17839	0.00515	0.00202	0.00000
72 h	0.23370	0.76563	0.00059	0.00008	0.00000	0.00000
73 c	-0.20263	2.99323	3.20229	0.00510	0.00201	0.00000
74 h	0.23426	0.76505	0.00060	0.00008	0.00000	0.00000
75 c	-0.19594	2.98538	3.20311	0.00533	0.00212	0.00000
76 h	0.23862	0.76054	0.00076	0.00008	0.00000	0.00000
77 c	-0.38590	3.01099	3.36476	0.00756	0.00260	0.00000
78 c	-0.19576	2.98535	3.20296	0.00533	0.00212	0.00000
79 h	0.23857	0.76059	0.00076	0.00008	0.00000	0.00000
80 c	-0.20258	2.99324	3.20222	0.00510	0.00201	0.00000
81 h	0.23429	0.76503	0.00060	0.00008	0.00000	0.00000
82 c	-0.18401	2.99835	3.17849	0.00515	0.00202	0.00000
83 h	0.23371	0.76562	0.00059	0.00008	0.00000	0.00000
84 c	-0.20542	2.99256	3.20574	0.00509	0.00202	0.00000
85 h	0.23218	0.76713	0.00061	0.00008	0.00000	0.00000
86 c	-0.19438	2.98185	3.20517	0.00521	0.00215	0.00000
87 h	0.22837	0.77089	0.00066	0.00008	0.00000	0.00000

QTAIM Charges:

1	(Au)	Charge:	-0.043629	Volume:	226.659 Bohr^3
2	(Pt)	Charge:	0.156251	Volume:	122.094 Bohr^3
3	(P)	Charge:	1.994578	Volume:	66.509 Bohr^3
4	(C)	Charge:	0.045317	Volume:	53.644 Bohr^3
5	(H)	Charge:	0.015653	Volume:	47.797 Bohr^3
6	(C)	Charge:	-0.103708	Volume:	60.451 Bohr^3
7	(H)	Charge:	0.046637	Volume:	47.450 Bohr^3
8	(C)	Charge:	-0.103702	Volume:	60.613 Bohr^3
9	(H)	Charge:	0.047920	Volume:	47.656 Bohr^3
10	(C)	Charge:	0.042175	Volume:	53.882 Bohr^3
11	(H)	Charge:	0.017438	Volume:	47.777 Bohr^3
12	(C)	Charge:	0.009925	Volume:	60.617 Bohr^3
13	(H)	Charge:	0.005842	Volume:	49.173 Bohr^3
14	(H)	Charge:	0.015369	Volume:	48.514 Bohr^3
15	(C)	Charge:	0.009237	Volume:	60.653 Bohr^3
16	(H)	Charge:	0.015585	Volume:	48.527 Bohr^3
17	(H)	Charge:	0.004797	Volume:	49.232 Bohr^3
18	(C)	Charge:	0.007556	Volume:	59.197 Bohr^3
19	(H)	Charge:	0.018303	Volume:	48.151 Bohr^3
20	(H)	Charge:	-0.011726	Volume:	40.242 Bohr^3
21	(C)	Charge:	0.045900	Volume:	53.669 Bohr^3
22	(H)	Charge:	0.015551	Volume:	47.800 Bohr^3
23	(C)	Charge:	-0.103743	Volume:	60.480 Bohr^3
24	(H)	Charge:	0.046467	Volume:	47.406 Bohr^3
25	(C)	Charge:	-0.105117	Volume:	60.605 Bohr^3
26	(H)	Charge:	0.047681	Volume:	47.639 Bohr^3
27	(C)	Charge:	0.042747	Volume:	53.852 Bohr^3
28	(H)	Charge:	0.017160	Volume:	47.783 Bohr^3
29	(C)	Charge:	0.009179	Volume:	60.641 Bohr^3
30	(H)	Charge:	0.005373	Volume:	49.183 Bohr^3
31	(H)	Charge:	0.016424	Volume:	48.482 Bohr^3
32	(C)	Charge:	0.008292	Volume:	60.682 Bohr^3
33	(H)	Charge:	0.005029	Volume:	49.208 Bohr^3
34	(H)	Charge:	0.015541	Volume:	48.520 Bohr^3
35	(C)	Charge:	0.008502	Volume:	59.174 Bohr^3
36	(H)	Charge:	0.018383	Volume:	48.158 Bohr^3
37	(H)	Charge:	-0.012275	Volume:	40.217 Bohr^3
38	(C)	Charge:	0.044800	Volume:	53.672 Bohr^3
39	(H)	Charge:	0.015813	Volume:	47.807 Bohr^3
40	(C)	Charge:	-0.104767	Volume:	60.485 Bohr^3
41	(H)	Charge:	0.046606	Volume:	47.456 Bohr^3
42	(C)	Charge:	-0.104535	Volume:	60.582 Bohr^3
43	(H)	Charge:	0.047448	Volume:	47.639 Bohr^3
44	(C)	Charge:	0.042788	Volume:	53.859 Bohr^3
45	(H)	Charge:	0.017352	Volume:	47.760 Bohr^3
46	(C)	Charge:	0.009633	Volume:	60.637 Bohr^3
47	(H)	Charge:	0.005196	Volume:	49.188 Bohr^3
48	(H)	Charge:	0.015834	Volume:	48.509 Bohr^3
49	(C)	Charge:	0.009731	Volume:	60.671 Bohr^3
50	(H)	Charge:	0.004638	Volume:	49.223 Bohr^3
51	(H)	Charge:	0.015637	Volume:	48.521 Bohr^3
52	(C)	Charge:	0.007797	Volume:	59.205 Bohr^3
53	(H)	Charge:	0.018663	Volume:	48.130 Bohr^3

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54 (H )    Charge:   -0.012250     Volume:    40.241 Bohr^3
55 (C )    Charge:   -0.657230     Volume:    80.796 Bohr^3
56 (C )    Charge:   -0.020027     Volume:    81.515 Bohr^3
57 (H )    Charge:    0.066103     Volume:    44.859 Bohr^3
58 (C )    Charge:   -0.016682     Volume:    82.954 Bohr^3
59 (H )    Charge:    0.062227     Volume:    46.618 Bohr^3
60 (C )    Charge:   -0.015446     Volume:    82.500 Bohr^3
61 (H )    Charge:    0.063476     Volume:    46.509 Bohr^3
62 (C )    Charge:   -0.016777     Volume:    83.005 Bohr^3
63 (H )    Charge:    0.057808     Volume:    46.881 Bohr^3
64 (C )    Charge:   -0.021290     Volume:    81.617 Bohr^3
65 (H )    Charge:    0.047400     Volume:    47.903 Bohr^3
66 (C )    Charge:   -0.657105     Volume:    80.789 Bohr^3
67 (C )    Charge:   -0.021251     Volume:    81.589 Bohr^3
68 (H )    Charge:    0.047213     Volume:    47.898 Bohr^3
69 (C )    Charge:   -0.016902     Volume:    83.021 Bohr^3
70 (H )    Charge:    0.058126     Volume:    46.872 Bohr^3
71 (C )    Charge:   -0.015087     Volume:    82.513 Bohr^3
72 (H )    Charge:    0.062972     Volume:    46.507 Bohr^3
73 (C )    Charge:   -0.016379     Volume:    82.954 Bohr^3
74 (H )    Charge:    0.061987     Volume:    46.625 Bohr^3
75 (C )    Charge:   -0.020342     Volume:    81.534 Bohr^3
76 (H )    Charge:    0.066357     Volume:    44.852 Bohr^3
77 (C )    Charge:   -0.657196     Volume:    80.757 Bohr^3
78 (C )    Charge:   -0.020133     Volume:    81.559 Bohr^3
79 (H )    Charge:    0.066443     Volume:    44.833 Bohr^3
80 (C )    Charge:   -0.016265     Volume:    82.958 Bohr^3
81 (H )    Charge:    0.061947     Volume:    46.610 Bohr^3
82 (C )    Charge:   -0.015818     Volume:    82.525 Bohr^3
83 (H )    Charge:    0.063628     Volume:    46.510 Bohr^3
84 (C )    Charge:   -0.016421     Volume:    83.021 Bohr^3
85 (H )    Charge:    0.057499     Volume:    46.884 Bohr^3
86 (C )    Charge:   -0.020786     Volume:    81.568 Bohr^3
87 (H )    Charge:    0.046655     Volume:    47.973 Bohr^3
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$[(Ph_3P)AuPt(nbe)_3]^+$ (3') (square planar form)

ZPE(BP86/def2-SVP) = 0.7184060 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2108.9823414 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2108.25590780595 Hartree (single point)

Cartesian coordinates in Å:

Au	0.39724	0.42326	0.02202
Pt	-2.20286	0.63377	-0.06301
P	2.79440	0.15131	-0.00944
C	3.42317	0.21970	-1.72319
C	4.11224	-0.85914	-2.31160
H	4.34933	-1.75184	-1.71455
C	4.48696	-0.79276	-3.66382
H	5.02332	-1.63712	-4.12173
C	4.18318	0.34585	-4.42750
H	4.47747	0.39276	-5.48642
C	3.50688	1.42927	-3.83770
H	3.27681	2.32635	-4.43157
C	3.12116	1.36617	-2.49173
H	2.58751	2.21251	-2.02977
C	3.23737	-1.50462	0.62542
C	2.38436	-2.58916	0.32369
H	1.47719	-2.42164	-0.27631
C	2.68772	-3.87336	0.79580
H	2.02138	-4.71549	0.55715
C	3.83540	-4.08002	1.58168
H	4.06853	-5.08641	1.95997
C	4.68228	-3.00168	1.88777
H	5.57963	-3.16260	2.50348
C	4.38909	-1.71403	1.41025
H	5.05145	-0.86966	1.65212
C	3.79144	1.33565	0.95491
C	4.97561	1.90426	0.44363
H	5.31244	1.65480	-0.57333
C	5.72225	2.78913	1.23829
H	6.64511	3.23394	0.83745
C	5.29630	3.10276	2.53942
H	5.88458	3.79657	3.15806
C	4.11701	2.53313	3.05165
H	3.78238	2.77873	4.07039
C	3.36158	1.65651	2.26103
H	2.43764	1.21068	2.65980
C	-5.15525	-0.08284	1.01560
H	-5.05102	-0.40841	2.06675
C	-4.27091	1.08052	0.57837
H	-4.22183	2.01628	1.15969
C	-4.23895	1.04371	-0.83635
H	-4.15874	1.94765	-1.46260
C	-5.10875	-0.13792	-1.25248
H	-4.96451	-0.51361	-2.28175
C	-6.56944	0.33562	-0.93908

H	-6.79641	1.31575	-1.40206
H	-7.29630	-0.39528	-1.34531
C	-6.60205	0.37135	0.62100
H	-6.84907	1.37094	1.02870
H	-7.34466	-0.34230	1.02946
C	-4.87384	-1.12788	-0.08885
H	-5.59435	-1.96927	-0.08285
H	-3.83566	-1.51919	-0.05959
C	-1.98948	-1.24174	-2.63368
H	-3.00777	-1.59628	-2.40349
C	-1.64411	0.16377	-2.14857
H	-2.20533	1.02815	-2.55085
C	-0.20666	0.23202	-2.15315
H	0.29853	1.15659	-2.48413
C	0.27869	-1.13218	-2.63983
H	1.33500	-1.37525	-2.43106
C	-0.08086	-1.14082	-4.16263
H	0.31554	-0.24798	-4.68357
H	0.37712	-2.02930	-4.64095
C	-1.63617	-1.22371	-4.15868
H	-2.12107	-0.38035	-4.68770
H	-1.99474	-2.15879	-4.63268
C	-0.81147	-2.06619	-2.07096
H	-0.76393	-3.09304	-2.48278
H	-0.81593	-2.11281	-0.96372
C	0.14461	-1.02677	2.70368
H	1.21981	-1.23849	2.56760
C	-0.36315	0.30650	2.14877
H	0.06497	1.26691	2.48928
C	-1.79527	0.17498	2.05221
H	-2.41771	1.01192	2.41974
C	-2.11014	-1.24134	2.52523
H	-3.09162	-1.64462	2.22447
C	-1.87735	-1.18900	4.07242
H	-2.44097	-0.36472	4.55109
H	-2.22650	-2.13538	4.53066
C	-0.33257	-1.03192	4.19446
H	-0.02585	-0.11438	4.73350
H	0.12686	-1.89145	4.72185
C	-0.85543	-2.01726	2.06957
H	-0.79142	-3.03455	2.50184
H	-0.76420	-2.08072	0.96788

[Pt(nbe)$_3$] (4) (up-up-down isomer)

ZPE(BP86/def2-SVP) = 0.4495098 Hartree (optimized geometry)
E(BP86/def2-SVP) = −937.3429845 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −937.00976680704 Hartree (single point)

Cartesian coordinates in Å:

Pt	0.27665	0.35105	-0.02861
C	-0.20635	1.67544	2.85230
C	-0.82307	0.71378	1.83540
C	-0.09439	-0.50777	1.95984
C	0.94469	-0.26785	3.05483
C	0.12026	-0.20688	4.38266
C	-0.67169	1.13507	4.24422
C	1.27364	1.22909	2.85854
C	0.95095	2.61978	-2.20411
C	-0.09005	1.56845	-1.82050
C	-0.81952	2.12009	-0.72403
C	-0.20136	3.49342	-0.45739
C	-0.66381	4.37853	-1.66096
C	0.12903	3.77413	-2.86647
C	1.27877	3.25724	-0.83519
C	1.20227	-1.61531	-2.39388
C	1.73550	-0.61422	-1.36962
C	1.73741	-1.29697	-0.11766
C	1.20586	-2.70096	-0.40331
C	2.35360	-3.41155	-1.19345
C	2.35101	-2.66266	-2.56668
C	0.20006	-2.43194	-1.54604
H	1.85905	4.19848	-0.92281
H	1.79233	2.55739	-0.14612
H	1.80488	2.25971	-2.80896
H	-0.40030	3.92947	0.53933
H	-0.39106	5.43982	-1.48883
H	-1.76229	4.34029	-1.80346
H	0.81000	4.52340	-3.31956
H	-0.53121	3.39946	-3.67399
H	-0.55351	0.94003	-2.59801
H	-1.90223	1.96942	-0.58853
H	1.78897	1.43429	1.89907
H	1.85232	1.66037	3.70076
H	-0.40469	2.75057	2.68505
H	1.79812	-0.97197	3.07718
H	-0.40028	1.84975	5.04795
H	-1.77034	0.99485	4.28625
H	0.79953	-0.18729	5.25931
H	-0.54060	-1.08907	4.49864
H	-1.90526	0.74802	1.63311
H	-0.55813	-1.50085	1.84578
H	2.50990	-1.14204	0.65244
H	2.50715	0.11721	-1.65819
H	0.82581	-1.18501	-3.34116

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H           0.83276       -3.26502        0.47244
H          -0.14060       -3.35897       -2.05095
H          -0.67271       -1.83144       -1.21698
H           3.32077       -2.17766       -2.79655
H           2.12228       -3.35336       -3.40395
H           3.32472       -3.34034       -0.66403
H           2.12635       -4.48984       -1.31996

# Raman Activity Spectrum
# X-Axis:  Frequency (cm-1) (Scaled by 0.9694)
# Y-Axis:  Intensity

# Peak information
#                  X                  Y
#      23.5458535400        0.8830000000
#      30.8059809600        0.3739000000
#      37.0675294400        0.8666000000
#      54.0318355600        0.4108000000
#      66.5314730400        0.6150000000
#      67.6313542800        0.6383000000
#     147.2186095800        5.6849000000
#     152.7038625400        0.7213000000
#     169.0920542400        0.0749000000
#     172.8169737400        0.2357000000
#     178.3534110200        0.0193000000
#     203.7070016800        4.3161000000
#     222.1871585800        7.1365000000
#     227.1321649200        3.1551000000
#     233.0738114000        1.7111000000
#     250.8275968800        0.1207000000
#     252.6410534600        0.1671000000
#     253.5231105200        0.0575000000
#     449.0168707000        1.4339000000
#     451.1237646600        1.5976000000
#     461.3497713800        5.5533000000
#     519.2863501400        0.2919000000
#     526.2041824200        0.1698000000
#     527.9544341200        0.1020000000
#     536.1700021800        2.6404000000
#     539.0846002200        2.9334000000
#     548.3563295800        4.2521000000
#     666.5343325400        0.0725000000
#     668.6894056800        0.6259000000
#     672.9327603000        0.8461000000
#     748.3019623200        0.4438000000
#     749.1342891600        1.2315000000
#     752.4199735200        0.3087000000
#     764.2917306200        0.3851000000
#     766.5564429000        0.4513000000
#     767.5103325000        0.7828000000
#     796.8424377000        0.3411000000
#     797.2005340600        0.6068000000
#     797.9022827200        0.8455000000
#     825.7023481600        0.3151000000
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#     827.3036030800        0.3758000000
#     827.7320778800        0.5824000000
#     828.2080532800        5.2204000000
#     834.2933648400        5.1642000000
#     851.3499578400       40.8981000000
#     854.7685469400        2.9017000000
#     855.4620557000        4.3164000000
#     866.4362453400       11.3454000000
#     883.6702385400        1.4094000000
#     886.9705608400        1.7000000000
#     887.4913225200        0.0167000000
#     892.9470087800       11.2264000000
#     894.1291920800        1.7787000000
#     895.2559257000        0.1021000000
#     910.9154194200        4.1512000000
#     912.6370738200        5.6889000000
#     916.0880408800       11.9778000000
#     931.9914356400        1.5006000000
#     934.0169969400        1.1493000000
#     935.2225427800        2.6285000000
#     946.2006100200        5.4165000000
#     947.7818953000       15.5893000000
#     948.5699205600        6.5103000000
#     981.7519009200        0.1615000000
#     984.2798053000        0.0472000000
#     991.2981643600        0.1103000000
#    1003.5662121800        7.4531000000
#    1006.0402179200        7.4801000000
#    1007.1585177600        5.8775000000
#    1025.5206017400        2.4562000000
#    1029.2010257800        2.4514000000
#    1030.3413310000        4.5623000000
#    1059.0051318400        1.7777000000
#    1062.4344812800        1.8900000000
#    1066.4141591000       68.8783000000
#    1102.5197529200        3.1571000000
#    1107.7637222200        0.6300000000
#    1108.8078629600        1.1665000000
#    1108.9788651200        9.8995000000
#    1109.8153603800       12.8433000000
#    1114.3963570200        7.5462000000
#    1150.0351847400        0.3990000000
#    1152.5539767600        0.6910000000
#    1153.2059952000        1.4292000000
#    1160.1996345600        4.6484000000
#    1161.3942261800       15.1544000000
#    1162.2334357600       19.0431000000
#    1199.7601699800        3.0849000000
#    1200.5289041800        6.4790000000
#    1200.8415356800        9.5244000000
#    1245.2334637600        1.0219000000
#    1249.2069374200        0.9159000000
#    1249.3890876800        1.6479000000
#    1251.6112433000        0.3991000000
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#    1253.4315826200        1.0417000000
#    1253.8485215600        0.2677000000
#    1258.5133713000        2.9054000000
#    1260.1412847200        3.1626000000
#    1262.3488024000       13.3275000000
#    1266.7767307800        0.3511000000
#    1268.0225067200        0.7810000000
#    1268.1534726600        1.0656000000
#    1286.8070552200        1.7025000000
#    1288.4026876200        5.2102000000
#    1289.3519241000        3.2519000000
#    1307.2312468800        0.1021000000
#    1308.4610277200        3.8454000000
#    1311.0323612200        4.2075000000
#    1392.3217859800       15.6575000000
#    1393.0399175000       54.6470000000
#    1397.1780922200       24.7537000000
#    1438.9572934200        1.8909000000
#    1441.2137658000        1.3665000000
#    1444.1505631000       12.8117000000
#    1447.5113759600        5.7828000000
#    1447.5247536800       17.4128000000
#    1447.9106718200       12.8875000000
#    1469.3898615000        2.5468000000
#    1469.9120772800        3.0450000000
#    1470.4593035800        8.7528000000
#    2950.3725837200       36.3141000000
#    2950.4550796600      123.9219000000
#    2950.7317464200       93.1288000000
#    2955.9159037400       45.9707000000
#    2957.8263003200        6.5635000000
#    2959.1923788000       76.3410000000
#    2962.2460857400      293.5197000000
#    2962.3826742000      182.3125000000
#    2963.7413852400      878.0228000000
#    2983.6835912200       28.9950000000
#    2983.7163569400       64.3121000000
#    2983.7275050400       31.8327000000
#    3002.1277833800      119.7986000000
#    3002.2055292600      178.6816000000
#    3002.4472006800       90.4726000000
#    3006.9608240200       82.0114000000
#    3007.7203489200      112.0823000000
#    3007.9817961000       21.1979000000
#    3009.6350108600      125.2352000000
#    3012.2997945200       46.9820000000
#    3012.3380858200      137.4854000000
#    3016.3388965600       20.5645000000
#    3017.9639987200      155.0540000000
#    3021.5636717400      138.8330000000
#    3063.3924092800       27.5707000000
#    3063.8805021800       74.3855000000
#    3066.8186566400       32.5101000000
#    3080.0169407000      260.1824000000
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#    3080.2798419800       12.6344000000
#    3083.2628796600       80.3532000000
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MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1pt	0.06695	2.90038	6.32635	8.66632	0.03880	0.00121
2c	0.10305	3.03807	2.71152	0.13931	0.00805	
3c	-0.20285	3.19222	2.87425	0.12840	0.00797	
4c	-0.22064	3.20886	2.87446	0.12934	0.00798	
5c	0.11281	3.02071	2.71993	0.13851	0.00804	
6c	-0.19927	3.19796	2.89709	0.09873	0.00549	
7c	-0.19707	3.19872	2.89412	0.09875	0.00548	
8c	-0.22067	3.19400	2.91758	0.10315	0.00594	
9c	0.10938	3.02306	2.72095	0.13855	0.00805	
10c	-0.21637	3.20795	2.87112	0.12932	0.00798	
11c	-0.20340	3.19238	2.87479	0.12826	0.00797	
12c	0.10818	3.03431	2.71009	0.13937	0.00805	
13c	-0.19510	3.19755	2.89338	0.09870	0.00548	
14c	-0.19897	3.19764	2.89722	0.09863	0.00548	
15c	-0.22822	3.19753	2.92092	0.10381	0.00595	
16c	0.11146	3.02501	2.71670	0.13877	0.00805	
17c	-0.24431	3.21532	2.89186	0.12920	0.00794	
18c	-0.24677	3.21597	2.89325	0.12960	0.00795	
19c	0.10793	3.02641	2.71908	0.13854	0.00804	
20c	-0.19817	3.19928	2.89480	0.09861	0.00548	
21c	-0.19923	3.20000	2.89517	0.09858	0.00548	
22c	-0.22012	3.19376	2.91837	0.10206	0.00592	
23h	0.07153	0.88886	0.03771	0.00190		
24h	0.09468	0.85975	0.04357	0.00200		
25h	0.06735	0.89235	0.03829	0.00201		
26h	0.06736	0.89234	0.03830	0.00200		
27h	0.07920	0.88168	0.03723	0.00189		
28h	0.07264	0.88799	0.03748	0.00189		
29h	0.07911	0.88161	0.03738	0.00190		
30h	0.07306	0.88775	0.03731	0.00188		
31h	0.10902	0.84974	0.03937	0.00187		
32h	0.10788	0.85177	0.03847	0.00188		
33h	0.09041	0.86373	0.04384	0.00202		
34h	0.07157	0.88889	0.03765	0.00189		
35h	0.06826	0.89164	0.03810	0.00199		
36h	0.06771	0.89206	0.03822	0.00201		
37h	0.07926	0.88156	0.03728	0.00190		
38h	0.07292	0.88765	0.03754	0.00189		
39h	0.07919	0.88177	0.03715	0.00189		
40h	0.07353	0.88725	0.03734	0.00188		
41h	0.10526	0.85390	0.03895	0.00189		
42h	0.11062	0.84842	0.03909	0.00187		
43h	0.11239	0.84659	0.03915	0.00187		
44h	0.11297	0.84647	0.03870	0.00186		
45h	0.06862	0.89120	0.03817	0.00200		
46h	0.06999	0.88992	0.03809	0.00201		
47h	0.07134	0.88925	0.03753	0.00188		
48h	0.09187	0.86240	0.04369	0.00204		
49h	0.07195	0.88874	0.03743	0.00188		

50h	0.07995	0.88094	0.03721	0.00189
51h	0.07177	0.88884	0.03751	0.00189
52h	0.07998	0.88090	0.03723	0.00189

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 pt	0.53902	2.46072	6.00227	8.99570	0.00204	0.00025
2 c	-0.25386	3.01612	3.23149	0.00535	0.00090	0.00000
3 c	-0.31365	3.03439	3.26901	0.00890	0.00134	0.00000
4 c	-0.30651	3.03367	3.26262	0.00887	0.00136	0.00000
5 c	-0.25504	3.01520	3.23361	0.00533	0.00090	0.00000
6 c	-0.41199	3.07530	3.32980	0.00592	0.00096	0.00000
7 c	-0.41273	3.07580	3.33003	0.00594	0.00096	0.00000
8 c	-0.40975	3.06821	3.33404	0.00648	0.00102	0.00000
9 c	-0.25511	3.01523	3.23365	0.00532	0.00090	0.00000
10 c	-0.30630	3.03361	3.26246	0.00887	0.00136	0.00000
11 c	-0.31392	3.03441	3.26927	0.00890	0.00134	0.00000
12 c	-0.25377	3.01610	3.23142	0.00535	0.00090	0.00000
13 c	-0.41271	3.07579	3.33003	0.00594	0.00096	0.00000
14 c	-0.41192	3.07532	3.32972	0.00593	0.00096	0.00000
15 c	-0.40979	3.06822	3.33407	0.00648	0.00102	0.00000
16 c	-0.25525	3.01566	3.23335	0.00534	0.00090	0.00000
17 c	-0.30670	3.03360	3.26290	0.00884	0.00136	0.00000
18 c	-0.30620	3.03354	3.26245	0.00885	0.00136	0.00000
19 c	-0.25533	3.01561	3.23347	0.00535	0.00090	0.00000
20 c	-0.41238	3.07561	3.32989	0.00593	0.00096	0.00000
21 c	-0.41245	3.07564	3.32993	0.00592	0.00096	0.00000
22 c	-0.41062	3.06954	3.33356	0.00651	0.00102	0.00000
23 h	0.20994	0.78918	0.00072	0.00016	0.00000	0.00000
24 h	0.22384	0.77515	0.00086	0.00016	0.00000	0.00000
25 h	0.22016	0.77887	0.00078	0.00019	0.00000	0.00000
26 h	0.22133	0.77767	0.00081	0.00019	0.00000	0.00000
27 h	0.21194	0.78711	0.00080	0.00016	0.00000	0.00000
28 h	0.20971	0.78938	0.00076	0.00015	0.00000	0.00000
29 h	0.21201	0.78704	0.00080	0.00016	0.00000	0.00000
30 h	0.20971	0.78938	0.00075	0.00015	0.00000	0.00000
31 h	0.23146	0.76748	0.00093	0.00014	0.00000	0.00000
32 h	0.23014	0.76881	0.00091	0.00014	0.00000	0.00000
33 h	0.22387	0.77511	0.00086	0.00016	0.00000	0.00000
34 h	0.20992	0.78919	0.00072	0.00016	0.00000	0.00000
35 h	0.22139	0.77761	0.00081	0.00019	0.00000	0.00000
36 h	0.22015	0.77888	0.00078	0.00019	0.00000	0.00000
37 h	0.21194	0.78711	0.00080	0.00016	0.00000	0.00000
38 h	0.20973	0.78936	0.00076	0.00015	0.00000	0.00000
39 h	0.21205	0.78700	0.00080	0.00016	0.00000	0.00000
40 h	0.20970	0.78940	0.00075	0.00015	0.00000	0.00000
41 h	0.23011	0.76884	0.00091	0.00014	0.00000	0.00000
42 h	0.23154	0.76740	0.00092	0.00014	0.00000	0.00000
43 h	0.23151	0.76742	0.00093	0.00014	0.00000	0.00000
44 h	0.23153	0.76740	0.00093	0.00014	0.00000	0.00000
45 h	0.22089	0.77815	0.00077	0.00019	0.00000	0.00000
46 h	0.22091	0.77813	0.00077	0.00019	0.00000	0.00000

47 h	0.20981	0.78931	0.00072	0.00016	0.00000	0.00000
48 h	0.22770	0.77130	0.00084	0.00015	0.00000	0.00000
49 h	0.20967	0.78942	0.00075	0.00015	0.00000	0.00000
50 h	0.21231	0.78674	0.00079	0.00016	0.00000	0.00000
51 h	0.20965	0.78945	0.00075	0.00015	0.00000	0.00000
52 h	0.21230	0.78675	0.00079	0.00016	0.00000	0.00000

QTAIM Charges:

1 (Pt)	Charge:	0.140241	Volume:	147.392 Bohr^3
2 (C)	Charge:	0.044136	Volume:	54.074 Bohr^3
3 (C)	Charge:	-0.101310	Volume:	61.190 Bohr^3
4 (C)	Charge:	-0.102306	Volume:	60.761 Bohr^3
5 (C)	Charge:	0.043461	Volume:	53.565 Bohr^3
6 (C)	Charge:	0.009658	Volume:	60.628 Bohr^3
7 (C)	Charge:	0.010105	Volume:	60.590 Bohr^3
8 (C)	Charge:	0.004621	Volume:	59.915 Bohr^3
9 (C)	Charge:	0.043280	Volume:	53.610 Bohr^3
10 (C)	Charge:	-0.102451	Volume:	60.734 Bohr^3
11 (C)	Charge:	-0.100623	Volume:	61.213 Bohr^3
12 (C)	Charge:	0.044724	Volume:	54.046 Bohr^3
13 (C)	Charge:	0.009928	Volume:	60.592 Bohr^3
14 (C)	Charge:	0.010557	Volume:	60.605 Bohr^3
15 (C)	Charge:	0.003138	Volume:	59.899 Bohr^3
16 (C)	Charge:	0.044646	Volume:	53.828 Bohr^3
17 (C)	Charge:	-0.100964	Volume:	60.732 Bohr^3
18 (C)	Charge:	-0.100241	Volume:	60.705 Bohr^3
19 (C)	Charge:	0.043274	Volume:	53.817 Bohr^3
20 (C)	Charge:	0.010422	Volume:	60.615 Bohr^3
21 (C)	Charge:	0.009734	Volume:	60.622 Bohr^3
22 (C)	Charge:	0.001855	Volume:	60.049 Bohr^3
23 (H)	Charge:	-0.009192	Volume:	49.971 Bohr^3
24 (H)	Charge:	0.012228	Volume:	44.549 Bohr^3
25 (H)	Charge:	-0.001866	Volume:	50.429 Bohr^3
26 (H)	Charge:	0.000951	Volume:	50.198 Bohr^3
27 (H)	Charge:	-0.006585	Volume:	50.122 Bohr^3
28 (H)	Charge:	-0.006592	Volume:	50.039 Bohr^3
29 (H)	Charge:	-0.007340	Volume:	50.126 Bohr^3
30 (H)	Charge:	-0.006073	Volume:	50.039 Bohr^3
31 (H)	Charge:	0.034148	Volume:	49.066 Bohr^3
32 (H)	Charge:	0.031834	Volume:	48.808 Bohr^3
33 (H)	Charge:	0.011423	Volume:	44.516 Bohr^3
34 (H)	Charge:	-0.009280	Volume:	49.952 Bohr^3
35 (H)	Charge:	0.000988	Volume:	50.189 Bohr^3
36 (H)	Charge:	-0.001841	Volume:	50.440 Bohr^3
37 (H)	Charge:	-0.007161	Volume:	50.150 Bohr^3
38 (H)	Charge:	-0.006149	Volume:	50.053 Bohr^3
39 (H)	Charge:	-0.006656	Volume:	50.124 Bohr^3
40 (H)	Charge:	-0.005788	Volume:	50.024 Bohr^3
41 (H)	Charge:	0.032251	Volume:	48.815 Bohr^3
42 (H)	Charge:	0.034207	Volume:	49.036 Bohr^3
43 (H)	Charge:	0.034715	Volume:	48.523 Bohr^3
44 (H)	Charge:	0.034545	Volume:	48.498 Bohr^3

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45 (H )    Charge:   -0.000591     Volume:    50.622 Bohr^3
46 (H )    Charge:   -0.000318     Volume:    50.614 Bohr^3
47 (H )    Charge:   -0.009260     Volume:    49.989 Bohr^3
48 (H )    Charge:    0.016686     Volume:    45.300 Bohr^3
49 (H )    Charge:   -0.005769     Volume:    50.058 Bohr^3
50 (H )    Charge:   -0.006749     Volume:    50.097 Bohr^3
51 (H )    Charge:   -0.005967     Volume:    50.068 Bohr^3
52 (H )    Charge:   -0.006683     Volume:    50.096 Bohr^3
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[Pt(nbe)$_3$] (4) (up-up-up isomer)

ZPE(BP86/def2-SVP) = 0.4498140 Hartree (optimized geometry)
E(BP86/def2-SVP) = −937.3423936 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −937.00860662708 Hartree (single point)

Cartesian coordinates in Å:

Pt	-1.92517	-1.26832	-1.30927
C	-3.02682	-0.15808	-4.12952
H	-4.02320	0.28291	-3.94181
C	-1.96986	0.07929	-3.04958
H	-1.73680	1.10620	-2.72736
C	-0.96761	-0.91473	-3.25955
H	0.10600	-0.72479	-3.10051
C	-1.42738	-1.72905	-4.46838
H	-0.95976	-2.72340	-4.59142
C	-1.24123	-0.76829	-5.68885
H	-0.21900	-0.34172	-5.72607
H	-1.40422	-1.31561	-6.63970
C	-2.34630	0.31387	-5.45654
H	-3.08280	0.32446	-6.28581
H	-1.93592	1.33961	-5.36802
C	-2.96315	-1.69076	-4.31308
H	-3.50065	-2.04161	-5.21744
H	-3.31859	-2.24850	-3.42568
C	-1.00885	-4.30076	-1.91005
H	-0.87467	-4.39203	-3.00377
C	-0.54734	-2.98498	-1.28143
H	0.48368	-2.63291	-1.44169
C	-1.20850	-2.90260	-0.01954
H	-0.73594	-2.46889	0.87635
C	-2.04942	-4.17312	0.10035
H	-2.86497	-4.14788	0.84651
C	-1.00787	-5.32041	0.31539
H	-0.31160	-5.09518	1.14783
H	-1.52464	-6.26921	0.56646
C	-0.29187	-5.41025	-1.07233
H	0.80093	-5.23724	-1.00750
H	-0.44049	-6.40464	-1.54066
C	-2.45013	-4.42964	-1.36859
H	-2.88571	-5.43646	-1.53114
H	-3.13354	-3.65609	-1.76785
C	-4.54497	-1.54277	0.55092
H	-4.53617	-2.56146	0.98075
C	-3.18836	-0.84422	0.44377
H	-2.55459	-0.73751	1.33793
C	-3.36163	0.19931	-0.51384
H	-2.86166	1.17755	-0.43043
C	-4.82080	0.12340	-0.96190
H	-5.06420	0.63023	-1.91399
C	-5.64174	0.62771	0.27068
H	-5.27602	1.60769	0.63709

H	-6.70909	0.75610	-0.00236
C	-5.45373	-0.52301	1.31329
H	-4.98652	-0.17936	2.25773
H	-6.42354	-0.99205	1.57740
C	-5.09984	-1.39317	-0.88319
H	-6.17802	-1.64149	-0.95880
H	-4.52775	-1.97390	-1.63177

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1pt	-0.05258	3.06551	6.31124	8.63651	0.03812	0.00120
2c	0.12174	3.01528	2.71575	0.13918	0.00804	
3h	0.06991	0.88938	0.03871	0.00201		
4c	-0.21404	3.21150	2.86505	0.12956	0.00793	
5h	0.10856	0.85041	0.03914	0.00189		
6c	-0.21239	3.20310	2.87081	0.13054	0.00793	
7h	0.11176	0.84698	0.03937	0.00189		
8c	0.12292	3.01827	2.71164	0.13912	0.00804	
9h	0.06600	0.89313	0.03885	0.00202		
10c	-0.19113	3.19352	2.89352	0.09861	0.00548	
11h	0.07339	0.88733	0.03740	0.00188		
12h	0.07845	0.88250	0.03716	0.00189		
13c	-0.19759	3.19914	2.89418	0.09878	0.00548	
14h	0.07817	0.88266	0.03727	0.00190		
15h	0.07350	0.88717	0.03745	0.00188		
16c	-0.22930	3.19804	2.91997	0.10530	0.00600	
17h	0.07340	0.88684	0.03786	0.00190		
18h	0.08567	0.86696	0.04536	0.00201		
19c	0.12185	3.01609	2.71518	0.13884	0.00803	
20h	0.07007	0.88922	0.03870	0.00201		
21c	-0.21957	3.21676	2.86557	0.12933	0.00792	
22h	0.10615	0.85243	0.03953	0.00190		
23c	-0.20837	3.19917	2.87053	0.13072	0.00794	
24h	0.11263	0.84627	0.03921	0.00188		
25c	0.12344	3.01850	2.71094	0.13907	0.00805	
26h	0.06577	0.89346	0.03876	0.00201		
27c	-0.19299	3.19527	2.89342	0.09881	0.00548	
28h	0.07364	0.88694	0.03753	0.00189		
29h	0.07844	0.88246	0.03721	0.00190		
30c	-0.19863	3.19871	2.89531	0.09912	0.00549	
31h	0.07358	0.88711	0.03743	0.00188		
32h	0.07977	0.88122	0.03712	0.00189		
33c	-0.23046	3.19858	2.92062	0.10527	0.00600	
34h	0.07420	0.88631	0.03760	0.00189		
35h	0.08737	0.86573	0.04490	0.00200		
36c	0.12151	3.01502	2.71625	0.13917	0.00804	
37h	0.07173	0.88787	0.03840	0.00200		
38c	-0.21919	3.21626	2.86576	0.12924	0.00792	
39h	0.10718	0.85171	0.03923	0.00189		
40c	-0.21274	3.20298	2.87167	0.13017	0.00792	
41h	0.11071	0.84802	0.03939	0.00189		
42c	0.12521	3.01486	2.71272	0.13916	0.00805	
43h	0.06795	0.89141	0.03864	0.00201		

44c	-0.19320	3.19595	2.89312	0.09865	0.00548
45h	0.07319	0.88742	0.03750	0.00189	
46h	0.07881	0.88215	0.03715	0.00189	
47c	-0.19939	3.19896	2.89590	0.09904	0.00549
48h	0.07373	0.88700	0.03739	0.00188	
49h	0.07989	0.88105	0.03717	0.00189	
50c	-0.23074	3.19954	2.91985	0.10535	0.00600
51h	0.07287	0.88744	0.03779	0.00190	
52h	0.08913	0.86402	0.04486	0.00199	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 pt	0.53655	2.46122	6.00176	8.99819	0.00203	0.00025
2 c	-0.25457	3.01564	3.23270	0.00533	0.00090	0.00000
3 h	0.22142	0.77757	0.00082	0.00019	0.00000	0.00000
4 c	-0.30892	3.03428	3.26439	0.00890	0.00135	0.00000
5 h	0.23061	0.76832	0.00093	0.00014	0.00000	0.00000
6 c	-0.30704	3.03415	3.26265	0.00889	0.00135	0.00000
7 h	0.23068	0.76827	0.00091	0.00014	0.00000	0.00000
8 c	-0.25420	3.01506	3.23289	0.00534	0.00090	0.00000
9 h	0.22095	0.77804	0.00081	0.00019	0.00000	0.00000
10 c	-0.41237	3.07559	3.32990	0.00593	0.00095	0.00000
11 h	0.20977	0.78933	0.00075	0.00015	0.00000	0.00000
12 h	0.21209	0.78696	0.00080	0.00016	0.00000	0.00000
13 c	-0.41222	3.07560	3.32974	0.00592	0.00096	0.00000
14 h	0.21210	0.78694	0.00080	0.00016	0.00000	0.00000
15 h	0.20979	0.78930	0.00075	0.00015	0.00000	0.00000
16 c	-0.40865	3.06612	3.33507	0.00643	0.00103	0.00000
17 h	0.21037	0.78875	0.00072	0.00016	0.00000	0.00000
18 h	0.22090	0.77802	0.00091	0.00017	0.00000	0.00000
19 c	-0.25450	3.01563	3.23264	0.00533	0.00090	0.00000
20 h	0.22141	0.77758	0.00082	0.00019	0.00000	0.00000
21 c	-0.30874	3.03426	3.26423	0.00891	0.00135	0.00000
22 h	0.23056	0.76836	0.00093	0.00014	0.00000	0.00000
23 c	-0.30679	3.03413	3.26242	0.00889	0.00135	0.00000
24 h	0.23070	0.76825	0.00091	0.00014	0.00000	0.00000
25 c	-0.25427	3.01508	3.23295	0.00534	0.00090	0.00000
26 h	0.22099	0.77801	0.00081	0.00019	0.00000	0.00000
27 c	-0.41254	3.07562	3.33003	0.00593	0.00096	0.00000
28 h	0.20980	0.78929	0.00075	0.00015	0.00000	0.00000
29 h	0.21218	0.78686	0.00080	0.00016	0.00000	0.00000
30 c	-0.41239	3.07560	3.32991	0.00592	0.00096	0.00000
31 h	0.20985	0.78925	0.00075	0.00015	0.00000	0.00000
32 h	0.21219	0.78686	0.00080	0.00016	0.00000	0.00000
33 c	-0.40890	3.06619	3.33525	0.00643	0.00103	0.00000
34 h	0.21042	0.78870	0.00072	0.00016	0.00000	0.00000
35 h	0.22115	0.77777	0.00091	0.00017	0.00000	0.00000
36 c	-0.25470	3.01566	3.23281	0.00533	0.00090	0.00000
37 h	0.22152	0.77747	0.00082	0.00019	0.00000	0.00000
38 c	-0.30867	3.03428	3.26414	0.00890	0.00135	0.00000
39 h	0.23064	0.76829	0.00093	0.00014	0.00000	0.00000
40 c	-0.30651	3.03409	3.26218	0.00888	0.00135	0.00000

41 h	0.23077	0.76817	0.00091	0.00014	0.00000	0.00000
42 c	-0.25440	3.01507	3.23308	0.00534	0.00090	0.00000
43 h	0.22107	0.77792	0.00081	0.00019	0.00000	0.00000
44 c	-0.41246	3.07563	3.32995	0.00593	0.00096	0.00000
45 h	0.20977	0.78932	0.00075	0.00015	0.00000	0.00000
46 h	0.21217	0.78688	0.00080	0.00016	0.00000	0.00000
47 c	-0.41240	3.07564	3.32988	0.00592	0.00096	0.00000
48 h	0.20986	0.78923	0.00075	0.00015	0.00000	0.00000
49 h	0.21221	0.78684	0.00080	0.00016	0.00000	0.00000
50 c	-0.40875	3.06615	3.33514	0.00643	0.00103	0.00000
51 h	0.21038	0.78874	0.00072	0.00016	0.00000	0.00000
52 h	0.22113	0.77779	0.00091	0.00017	0.00000	0.00000

QTAIM Charges:

1 (Pt)	Charge:	0.135682	Volume:	151.020 Bohr^3
2 (C)	Charge:	0.044465	Volume:	53.834 Bohr^3
3 (H)	Charge:	0.000959	Volume:	49.227 Bohr^3
4 (C)	Charge:	-0.100837	Volume:	60.932 Bohr^3
5 (H)	Charge:	0.032814	Volume:	48.626 Bohr^3
6 (C)	Charge:	-0.101460	Volume:	60.868 Bohr^3
7 (H)	Charge:	0.032539	Volume:	48.908 Bohr^3
8 (C)	Charge:	0.045312	Volume:	53.668 Bohr^3
9 (H)	Charge:	0.000189	Volume:	49.159 Bohr^3
10 (C)	Charge:	0.008913	Volume:	60.592 Bohr^3
11 (H)	Charge:	-0.005388	Volume:	50.034 Bohr^3
12 (H)	Charge:	-0.006598	Volume:	50.106 Bohr^3
13 (C)	Charge:	0.009332	Volume:	60.559 Bohr^3
14 (H)	Charge:	-0.006512	Volume:	50.100 Bohr^3
15 (H)	Charge:	-0.005805	Volume:	50.020 Bohr^3
16 (C)	Charge:	0.007235	Volume:	59.695 Bohr^3
17 (H)	Charge:	-0.008694	Volume:	49.909 Bohr^3
18 (H)	Charge:	0.008074	Volume:	41.408 Bohr^3
19 (C)	Charge:	0.043650	Volume:	53.838 Bohr^3
20 (H)	Charge:	0.001572	Volume:	49.215 Bohr^3
21 (C)	Charge:	-0.100321	Volume:	60.928 Bohr^3
22 (H)	Charge:	0.032353	Volume:	48.616 Bohr^3
23 (C)	Charge:	-0.100821	Volume:	60.878 Bohr^3
24 (H)	Charge:	0.032600	Volume:	48.892 Bohr^3
25 (C)	Charge:	0.045516	Volume:	53.679 Bohr^3
26 (H)	Charge:	-0.000220	Volume:	49.179 Bohr^3
27 (C)	Charge:	0.009047	Volume:	60.587 Bohr^3
28 (H)	Charge:	-0.006019	Volume:	50.060 Bohr^3
29 (H)	Charge:	-0.006546	Volume:	50.127 Bohr^3
30 (C)	Charge:	0.010008	Volume:	60.575 Bohr^3
31 (H)	Charge:	-0.005821	Volume:	50.010 Bohr^3
32 (H)	Charge:	-0.006576	Volume:	50.093 Bohr^3
33 (C)	Charge:	0.005485	Volume:	59.753 Bohr^3
34 (H)	Charge:	-0.008005	Volume:	49.886 Bohr^3
35 (H)	Charge:	0.008745	Volume:	41.408 Bohr^3
36 (C)	Charge:	0.043639	Volume:	53.868 Bohr^3
37 (H)	Charge:	0.001438	Volume:	49.238 Bohr^3
38 (C)	Charge:	-0.099845	Volume:	60.938 Bohr^3

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39 (H )    Charge:    0.032464     Volume:    48.589 Bohr^3
40 (C )    Charge:   -0.101039     Volume:    60.888 Bohr^3
41 (H )    Charge:    0.032430     Volume:    48.898 Bohr^3
42 (C )    Charge:    0.045622     Volume:    53.689 Bohr^3
43 (H )    Charge:    0.000256     Volume:    49.141 Bohr^3
44 (C )    Charge:    0.009052     Volume:    60.604 Bohr^3
45 (H )    Charge:   -0.005811     Volume:    50.027 Bohr^3
46 (H )    Charge:   -0.006342     Volume:    50.105 Bohr^3
47 (C )    Charge:    0.009616     Volume:    60.574 Bohr^3
48 (H )    Charge:   -0.005773     Volume:    50.005 Bohr^3
49 (H )    Charge:   -0.006691     Volume:    50.101 Bohr^3
50 (C )    Charge:    0.006008     Volume:    59.729 Bohr^3
51 (H )    Charge:   -0.008499     Volume:    49.900 Bohr^3
52 (H )    Charge:    0.008606     Volume:    41.386 Bohr^3
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[Pt(PPh$_3$)$_3$] (5)

ZPE(BP86/def2-SVP) = 0.8027286 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3227.2590028 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3226.42967213039 Hartree (single point)

Cartesian coordinates in Å:

Pt	-1.71898	2.41839	-1.13772
P	-1.21538	2.39195	1.08223
P	-3.53712	3.51349	-1.97671
P	-0.78096	0.87683	-2.54293
C	-0.78215	-0.79679	-1.76662
C	0.21977	-1.76091	-1.98905
H	1.04605	-1.54453	-2.68232
C	0.17578	-2.99078	-1.31167
H	0.96944	-3.73491	-1.48085
C	-0.87037	-3.26964	-0.41716
H	-0.89516	-4.22963	0.12043
C	-1.87528	-2.31252	-0.19523
H	-2.68498	-2.51593	0.52115
C	-1.82615	-1.08045	-0.85923
H	-2.57779	-0.29936	-0.66252
C	0.97849	1.16840	-3.00567
C	1.74727	1.98694	-2.15070
H	1.25579	2.44355	-1.27491
C	3.10179	2.22652	-2.42818
H	3.69140	2.86704	-1.75472
C	3.69623	1.66098	-3.56929
H	4.75721	1.85276	-3.79146
C	2.93082	0.85974	-4.43471
H	3.39216	0.42358	-5.33417
C	1.57642	0.61450	-4.15719
H	0.97399	-0.00215	-4.84157
C	-1.58008	0.57258	-4.17584
C	-2.31593	-0.59514	-4.45600
H	-2.37817	-1.39448	-3.70330
C	-2.96807	-0.73989	-5.69180
H	-3.54606	-1.65417	-5.89568
C	-2.88433	0.27002	-6.66216
H	-3.39121	0.14982	-7.63171
C	-2.16159	1.44404	-6.38272
H	-2.10154	2.24946	-7.13072
C	-1.52541	1.59935	-5.14516
H	-0.97737	2.52730	-4.92401
C	-0.64872	0.77724	1.77380
C	-1.31657	0.10284	2.81376
H	-2.18405	0.57213	3.30089
C	-0.87947	-1.16933	3.22465
H	-1.41388	-1.69377	4.03192
C	0.23382	-1.76631	2.61434
H	0.57147	-2.76362	2.93463
C	0.90935	-1.09173	1.58065

H	1.77193	-1.56018	1.08454
C	0.46145	0.16237	1.15289
H	0.95857	0.66919	0.31192
C	0.13139	3.54631	1.56665
C	0.98660	3.31332	2.66299
H	0.85626	2.40542	3.27135
C	2.00492	4.23116	2.96791
H	2.67137	4.04375	3.82392
C	2.17578	5.38441	2.18270
H	2.97684	6.10017	2.42296
C	1.32865	5.61804	1.08496
H	1.46572	6.51481	0.46159
C	0.31371	4.70075	0.77437
H	-0.34568	4.85072	-0.09736
C	-2.62125	2.83877	2.18875
C	-2.50678	3.71216	3.28727
H	-1.52481	4.13110	3.55346
C	-3.64621	4.05636	4.03543
H	-3.55021	4.74939	4.88559
C	-4.90099	3.52179	3.70319
H	-5.79180	3.79957	4.28648
C	-5.02067	2.64607	2.60934
H	-6.00475	2.24361	2.32721
C	-3.89084	2.31970	1.85099
H	-3.98092	1.67557	0.96215
C	-4.69871	4.32666	-0.79585
C	-4.12089	5.14782	0.19658
H	-3.02485	5.25347	0.23030
C	-4.92546	5.78480	1.14773
H	-4.46250	6.41591	1.92055
C	-6.31761	5.58302	1.13943
H	-6.94881	6.06465	1.90167
C	-6.89730	4.75149	0.16848
H	-7.98590	4.58592	0.16274
C	-6.09334	4.12946	-0.80316
H	-6.54992	3.48061	-1.56585
C	-4.58442	2.28199	-2.85065
C	-5.00570	1.15058	-2.11377
H	-4.77200	1.09020	-1.03966
C	-5.70474	0.11193	-2.74111
H	-6.02810	-0.76137	-2.15425
C	-5.97889	0.17980	-4.11882
H	-6.51692	-0.64108	-4.61647
C	-5.54809	1.29124	-4.85844
H	-5.74290	1.34275	-5.93985
C	-4.85528	2.33951	-4.23123
H	-4.51267	3.20131	-4.82125
C	-3.24311	4.83644	-3.22231
C	-1.94301	4.96170	-3.75196
H	-1.15827	4.28434	-3.37463
C	-1.66576	5.93551	-4.72442
H	-0.64786	6.02866	-5.13305
C	-2.68609	6.79422	-5.16722
H	-2.47042	7.56000	-5.92811
C	-3.98118	6.68372	-4.62979
H	-4.77823	7.36291	-4.96948

C	-4.25986	5.71112	-3.65713
H	-5.27067	5.62868	-3.22859

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1pt	-0.67090	2.99141	6.67574	8.98370	0.01945	0.00060
2p	0.37634	5.55647	8.54538	0.47901	0.04280	
3p	0.36437	5.56312	8.55450	0.47527	0.04273	
4p	0.26520	5.56860	8.65019	0.47384	0.04218	
5c	-0.01532	3.24591	2.62880	0.13272	0.00789	
6c	-0.08592	3.14399	2.82153	0.11311	0.00729	
7h	0.11807	0.83951	0.04052	0.00190		
8c	-0.17581	3.20253	2.85463	0.11140	0.00724	
9h	0.12101	0.84279	0.03441	0.00179		
10c	-0.09985	3.16394	2.81825	0.11041	0.00725	
11h	0.11534	0.84807	0.03481	0.00178		
12c	-0.13487	3.18233	2.83547	0.10984	0.00723	
13h	0.11411	0.84880	0.03527	0.00182		
14c	-0.00664	3.16293	2.72312	0.11310	0.00749	
15h	0.06767	0.88681	0.04353	0.00199		
16c	-0.02938	3.27263	2.61580	0.13314	0.00782	
17c	-0.08346	3.19135	2.77178	0.11294	0.00739	
18h	0.11124	0.84316	0.04369	0.00190		
19c	-0.18226	3.19646	2.86696	0.11166	0.00717	
20h	0.12669	0.83688	0.03466	0.00177		
21c	-0.09333	3.15293	2.82315	0.11005	0.00720	
22h	0.12264	0.84074	0.03486	0.00176		
23c	-0.15244	3.18309	2.85034	0.11182	0.00719	
24h	0.12392	0.83958	0.03473	0.00177		
25c	-0.14386	3.16740	2.85425	0.11494	0.00727	
26h	0.13994	0.81915	0.03903	0.00188		
27c	0.05614	3.25045	2.55141	0.13421	0.00779	
28c	-0.09342	3.15372	2.82320	0.10917	0.00733	
29h	0.11740	0.83929	0.04139	0.00193		
30c	-0.14218	3.19362	2.82860	0.11265	0.00730	
31h	0.11248	0.85104	0.03468	0.00180		
32c	-0.13187	3.17451	2.83931	0.11080	0.00725	
33h	0.11875	0.84516	0.03433	0.00176		
34c	-0.14738	3.18468	2.84417	0.11130	0.00723	
35h	0.11985	0.84392	0.03445	0.00178		
36c	-0.17787	3.21945	2.83708	0.11389	0.00744	
37h	0.10098	0.85696	0.04016	0.00190		
38c	-0.01262	3.26897	2.60148	0.13436	0.00782	
39c	-0.09030	3.14143	2.83141	0.11020	0.00727	
40h	0.12481	0.83209	0.04119	0.00191		
41c	-0.17578	3.20193	2.85446	0.11216	0.00723	
42h	0.11877	0.84487	0.03457	0.00179		
43c	-0.10102	3.16347	2.81940	0.11091	0.00724	
44h	0.11427	0.84921	0.03475	0.00178		
45c	-0.14126	3.18895	2.83318	0.11188	0.00725	
46h	0.11546	0.84757	0.03517	0.00181		
47c	-0.08099	3.18241	2.77607	0.11500	0.00751	
48h	0.07785	0.87743	0.04278	0.00194		

49c	-0.04243	3.26229	2.63903	0.13326	0.00785
50c	-0.14167	3.17384	2.84715	0.11341	0.00727
51h	0.13211	0.82662	0.03938	0.00189	
52c	-0.14286	3.17836	2.84593	0.11139	0.00718
53h	0.12370	0.83967	0.03486	0.00178	
54c	-0.09748	3.15571	2.82449	0.11008	0.00719
55h	0.12287	0.84055	0.03482	0.00176	
56c	-0.18070	3.19799	2.86416	0.11138	0.00717
57h	0.12484	0.83859	0.03479	0.00178	
58c	-0.09576	3.17102	2.80488	0.11249	0.00737
59h	0.13145	0.82527	0.04136	0.00192	
60c	-0.02709	3.27295	2.61285	0.13341	0.00788
61c	-0.08162	3.12973	2.83281	0.11181	0.00727
62h	0.12724	0.83052	0.04034	0.00190	
63c	-0.17517	3.20314	2.85291	0.11190	0.00723
64h	0.12084	0.84293	0.03444	0.00179	
65c	-0.10620	3.16744	2.82089	0.11062	0.00725
66h	0.11582	0.84767	0.03473	0.00178	
67c	-0.13158	3.18585	2.82769	0.11079	0.00725
68h	0.11258	0.85019	0.03542	0.00182	
69c	-0.06859	3.16274	2.78414	0.11418	0.00753
70h	0.09718	0.86006	0.04082	0.00194	
71c	0.01723	3.24209	2.59945	0.13341	0.00782
72c	-0.10515	3.18212	2.80236	0.11315	0.00753
73h	0.09061	0.86673	0.04074	0.00193	
74c	-0.13295	3.18822	2.82612	0.11135	0.00726
75h	0.11276	0.85018	0.03524	0.00181	
76c	-0.10654	3.16664	2.82221	0.11046	0.00723
77h	0.11533	0.84809	0.03481	0.00178	
78c	-0.16808	3.19280	2.85555	0.11250	0.00723
79h	0.12042	0.84331	0.03448	0.00179	
80c	-0.12337	3.15418	2.85072	0.11121	0.00726
81h	0.13123	0.82696	0.03991	0.00189	
82c	0.03235	3.27101	2.55530	0.13348	0.00786
83c	-0.10435	3.17664	2.80699	0.11327	0.00745
84h	0.10077	0.85807	0.03928	0.00188	
85c	-0.17026	3.19341	2.85833	0.11130	0.00722
86h	0.11676	0.84660	0.03485	0.00179	
87c	-0.09479	3.15160	2.82569	0.11026	0.00723
88h	0.11448	0.84889	0.03486	0.00177	
89c	-0.15122	3.19741	2.83320	0.11329	0.00732
90h	0.11188	0.85154	0.03478	0.00180	
91c	-0.05519	3.12004	2.81743	0.11037	0.00735
92h	0.11888	0.83756	0.04160	0.00195	
93c	-0.04765	3.27470	2.63054	0.13454	0.00787
94c	-0.11506	3.17873	2.81672	0.11224	0.00737
95h	0.14422	0.81200	0.04185	0.00193	
96c	-0.15614	3.18226	2.85582	0.11091	0.00716
97h	0.12454	0.83887	0.03481	0.00177	
98c	-0.10181	3.15915	2.82537	0.11008	0.00721
99h	0.12194	0.84143	0.03487	0.00176	
100c	-0.12663	3.16609	2.84259	0.11077	0.00717
101h	0.12340	0.83991	0.03490	0.00178	
102c	-0.15250	3.19042	2.83919	0.11558	0.00731
103h	0.12282	0.83675	0.03857	0.00187	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 pt	-0.11012	2.61507	6.00048	9.49155	0.00290	0.00012
2 p	0.89637	5.23880	8.82394	0.03967	0.00121	0.00000
3 p	0.89653	5.24220	8.82088	0.03918	0.00122	0.00000
4 p	0.88959	5.24542	8.82495	0.03885	0.00119	0.00000
5 c	-0.34538	3.01835	3.31732	0.00733	0.00239	0.00000
6 c	-0.21341	2.98190	3.22415	0.00527	0.00209	0.00000
7 h	0.22784	0.77134	0.00074	0.00008	0.00000	0.00000
8 c	-0.22015	2.98762	3.22557	0.00497	0.00198	0.00000
9 h	0.21733	0.78194	0.00065	0.00008	0.00000	0.00000
10 c	-0.20770	2.99066	3.20991	0.00515	0.00200	0.00000
11 h	0.21737	0.78189	0.00066	0.00008	0.00000	0.00000
12 c	-0.21357	2.98648	3.21997	0.00516	0.00196	0.00000
13 h	0.22111	0.77816	0.00066	0.00008	0.00000	0.00000
14 c	-0.19774	2.98334	3.20684	0.00549	0.00207	0.00000
15 h	0.23591	0.76326	0.00076	0.00007	0.00000	0.00000
16 c	-0.34534	3.01767	3.31806	0.00721	0.00241	0.00000
17 c	-0.20447	2.98869	3.20831	0.00538	0.00210	0.00000
18 h	0.24056	0.75861	0.00074	0.00008	0.00000	0.00000
19 c	-0.21652	2.98986	3.21968	0.00496	0.00201	0.00000
20 h	0.22177	0.77752	0.00063	0.00008	0.00000	0.00000
21 c	-0.20758	2.99318	3.20740	0.00499	0.00202	0.00000
22 h	0.21830	0.78099	0.00063	0.00009	0.00000	0.00000
23 c	-0.21797	2.98940	3.22158	0.00497	0.00202	0.00000
24 h	0.21913	0.78015	0.00063	0.00008	0.00000	0.00000
25 c	-0.21095	2.98550	3.21793	0.00543	0.00209	0.00000
26 h	0.23256	0.76661	0.00075	0.00008	0.00000	0.00000
27 c	-0.34773	3.02415	3.31363	0.00757	0.00238	0.00000
28 c	-0.21216	2.98167	3.22309	0.00532	0.00208	0.00000
29 h	0.23212	0.76705	0.00075	0.00008	0.00000	0.00000
30 c	-0.20628	2.98655	3.21266	0.00509	0.00197	0.00000
31 h	0.21730	0.78195	0.00066	0.00008	0.00000	0.00000
32 c	-0.22219	2.98947	3.22560	0.00512	0.00200	0.00000
33 h	0.21599	0.78326	0.00067	0.00008	0.00000	0.00000
34 c	-0.21759	2.98627	3.22432	0.00502	0.00198	0.00000
35 h	0.21833	0.78094	0.00065	0.00008	0.00000	0.00000
36 c	-0.20568	2.97786	3.22039	0.00535	0.00207	0.00000
37 h	0.22584	0.77332	0.00076	0.00008	0.00000	0.00000
38 c	-0.35156	3.02290	3.31889	0.00739	0.00237	0.00000
39 c	-0.22074	2.98285	3.23053	0.00528	0.00208	0.00000
40 h	0.23145	0.76773	0.00074	0.00008	0.00000	0.00000
41 c	-0.22024	2.98728	3.22604	0.00494	0.00198	0.00000
42 h	0.21663	0.78265	0.00065	0.00008	0.00000	0.00000
43 c	-0.21322	2.99027	3.21585	0.00511	0.00200	0.00000
44 h	0.21639	0.78287	0.00066	0.00008	0.00000	0.00000
45 c	-0.20956	2.98650	3.21587	0.00522	0.00196	0.00000
46 h	0.22243	0.77681	0.00068	0.00008	0.00000	0.00000
47 c	-0.19773	2.98005	3.21001	0.00558	0.00208	0.00000
48 h	0.23249	0.76672	0.00072	0.00008	0.00000	0.00000
49 c	-0.34682	3.01671	3.32040	0.00729	0.00242	0.00000

50	c	-0.20796	2.98532	3.21514	0.00541	0.00210	0.00000
51	h	0.23357	0.76561	0.00073	0.00008	0.00000	0.00000
52	c	-0.21630	2.98965	3.21965	0.00498	0.00201	0.00000
53	h	0.21964	0.77965	0.00063	0.00008	0.00000	0.00000
54	c	-0.20966	2.99319	3.20945	0.00500	0.00203	0.00000
55	h	0.21853	0.78076	0.00063	0.00009	0.00000	0.00000
56	c	-0.21812	2.98962	3.22150	0.00498	0.00201	0.00000
57	h	0.22054	0.77875	0.00063	0.00008	0.00000	0.00000
58	c	-0.20215	2.98688	3.20783	0.00532	0.00212	0.00000
59	h	0.23720	0.76201	0.00072	0.00008	0.00000	0.00000
60	c	-0.35127	3.02201	3.31952	0.00736	0.00239	0.00000
61	c	-0.21704	2.98248	3.22722	0.00526	0.00209	0.00000
62	h	0.22944	0.76974	0.00074	0.00008	0.00000	0.00000
63	c	-0.21830	2.98793	3.22341	0.00498	0.00198	0.00000
64	h	0.21750	0.78177	0.00065	0.00008	0.00000	0.00000
65	c	-0.21113	2.99045	3.21354	0.00515	0.00200	0.00000
66	h	0.21782	0.78145	0.00066	0.00008	0.00000	0.00000
67	c	-0.21166	2.98630	3.21819	0.00520	0.00196	0.00000
68	h	0.22233	0.77693	0.00067	0.00007	0.00000	0.00000
69	c	-0.19956	2.97918	3.21285	0.00544	0.00209	0.00000
70	h	0.22363	0.77557	0.00072	0.00008	0.00000	0.00000
71	c	-0.34840	3.02300	3.31557	0.00743	0.00239	0.00000
72	c	-0.19516	2.98175	3.20581	0.00550	0.00210	0.00000
73	h	0.23132	0.76791	0.00069	0.00007	0.00000	0.00000
74	c	-0.20821	2.98690	3.21413	0.00521	0.00197	0.00000
75	h	0.22209	0.77716	0.00067	0.00008	0.00000	0.00000
76	c	-0.21309	2.99059	3.21540	0.00510	0.00200	0.00000
77	h	0.21647	0.78279	0.00066	0.00008	0.00000	0.00000
78	c	-0.22127	2.98773	3.22661	0.00495	0.00198	0.00000
79	h	0.21684	0.78244	0.00064	0.00008	0.00000	0.00000
80	c	-0.22323	2.98358	3.23223	0.00533	0.00209	0.00000
81	h	0.23058	0.76861	0.00074	0.00008	0.00000	0.00000
82	c	-0.34476	3.01757	3.31745	0.00735	0.00239	0.00000
83	c	-0.21030	2.97689	3.22609	0.00524	0.00208	0.00000
84	h	0.21875	0.78046	0.00072	0.00008	0.00000	0.00000
85	c	-0.21817	2.98601	3.22522	0.00496	0.00198	0.00000
86	h	0.21754	0.78172	0.00065	0.00008	0.00000	0.00000
87	c	-0.21801	2.98913	3.22180	0.00508	0.00200	0.00000
88	h	0.21640	0.78286	0.00066	0.00008	0.00000	0.00000
89	c	-0.20192	2.98654	3.20824	0.00518	0.00196	0.00000
90	h	0.21911	0.78013	0.00068	0.00008	0.00000	0.00000
91	c	-0.21196	2.98052	3.22398	0.00538	0.00208	0.00000
92	h	0.23229	0.76685	0.00078	0.00008	0.00000	0.00000
93	c	-0.34693	3.01737	3.31984	0.00730	0.00243	0.00000
94	c	-0.19879	2.98779	3.20347	0.00541	0.00211	0.00000
95	h	0.23738	0.76180	0.00074	0.00008	0.00000	0.00000
96	c	-0.22198	2.98931	3.22569	0.00497	0.00201	0.00000
97	h	0.21989	0.77940	0.00063	0.00008	0.00000	0.00000
98	c	-0.20629	2.99315	3.20612	0.00500	0.00202	0.00000
99	h	0.21830	0.78099	0.00063	0.00009	0.00000	0.00000
100	c	-0.21767	2.98982	3.22085	0.00498	0.00202	0.00000
101	h	0.21945	0.77983	0.00063	0.00008	0.00000	0.00000
102	c	-0.19850	2.98467	3.20635	0.00539	0.00209	0.00000
103	h	0.23023	0.76897	0.00072	0.00008	0.00000	0.00000

QTAIM Charges:

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 1 (Pt)    Charge:   -0.518088     Volume:   192.891 Bohr^3
 2 (P )    Charge:    1.805299     Volume:    71.568 Bohr^3
 3 (P )    Charge:    1.810467     Volume:    72.237 Bohr^3
 4 (P )    Charge:    1.803371     Volume:    72.783 Bohr^3
 5 (C )    Charge:   -0.592022     Volume:    73.963 Bohr^3
 6 (C )    Charge:   -0.027902     Volume:    81.794 Bohr^3
 7 (H )    Charge:    0.046212     Volume:    45.342 Bohr^3
 8 (C )    Charge:   -0.034512     Volume:    82.821 Bohr^3
 9 (H )    Charge:    0.029795     Volume:    48.870 Bohr^3
10 (C )    Charge:   -0.028985     Volume:    81.480 Bohr^3
11 (H )    Charge:    0.030395     Volume:    49.028 Bohr^3
12 (C )    Charge:   -0.021729     Volume:    80.173 Bohr^3
13 (H )    Charge:    0.034777     Volume:    49.578 Bohr^3
14 (C )    Charge:   -0.023160     Volume:    75.826 Bohr^3
15 (H )    Charge:    0.054871     Volume:    45.500 Bohr^3
16 (C )    Charge:   -0.597862     Volume:    80.495 Bohr^3
17 (C )    Charge:   -0.035748     Volume:    81.697 Bohr^3
18 (H )    Charge:    0.064659     Volume:    44.261 Bohr^3
19 (C )    Charge:   -0.031907     Volume:    83.862 Bohr^3
20 (H )    Charge:    0.038730     Volume:    48.227 Bohr^3
21 (C )    Charge:   -0.032674     Volume:    83.706 Bohr^3
22 (H )    Charge:    0.034880     Volume:    48.433 Bohr^3
23 (C )    Charge:   -0.033081     Volume:    83.891 Bohr^3
24 (H )    Charge:    0.034034     Volume:    48.462 Bohr^3
25 (C )    Charge:   -0.031249     Volume:    78.911 Bohr^3
26 (H )    Charge:    0.052762     Volume:    46.216 Bohr^3
27 (C )    Charge:   -0.596721     Volume:    77.649 Bohr^3
28 (C )    Charge:   -0.021882     Volume:    81.370 Bohr^3
29 (H )    Charge:    0.052755     Volume:    45.870 Bohr^3
30 (C )    Charge:   -0.024654     Volume:    80.098 Bohr^3
31 (H )    Charge:    0.028544     Volume:    49.416 Bohr^3
32 (C )    Charge:   -0.033096     Volume:    81.334 Bohr^3
33 (H )    Charge:    0.026375     Volume:    49.223 Bohr^3
34 (C )    Charge:   -0.029807     Volume:    82.607 Bohr^3
35 (H )    Charge:    0.030276     Volume:    48.832 Bohr^3
36 (C )    Charge:   -0.026409     Volume:    78.291 Bohr^3
37 (H )    Charge:    0.039614     Volume:    46.671 Bohr^3
38 (C )    Charge:   -0.598410     Volume:    76.994 Bohr^3
39 (C )    Charge:   -0.034416     Volume:    83.186 Bohr^3
40 (H )    Charge:    0.050928     Volume:    45.065 Bohr^3
41 (C )    Charge:   -0.035335     Volume:    84.240 Bohr^3
42 (H )    Charge:    0.028404     Volume:    48.874 Bohr^3
43 (C )    Charge:   -0.031060     Volume:    82.282 Bohr^3
44 (H )    Charge:    0.028196     Volume:    49.160 Bohr^3
45 (C )    Charge:   -0.018839     Volume:    78.160 Bohr^3
46 (H )    Charge:    0.035544     Volume:    49.234 Bohr^3
47 (C )    Charge:   -0.020491     Volume:    74.252 Bohr^3
48 (H )    Charge:    0.048083     Volume:    45.205 Bohr^3
49 (C )    Charge:   -0.602071     Volume:    79.282 Bohr^3
50 (C )    Charge:   -0.027640     Volume:    80.441 Bohr^3
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 51 (H )    Charge:    0.055346     Volume:    46.231 Bohr^3
 52 (C )    Charge:   -0.033518     Volume:    83.865 Bohr^3
 53 (H )    Charge:    0.035391     Volume:    48.393 Bohr^3
 54 (C )    Charge:   -0.033270     Volume:    83.770 Bohr^3
 55 (H )    Charge:    0.034937     Volume:    48.407 Bohr^3
 56 (C )    Charge:   -0.033211     Volume:    83.968 Bohr^3
 57 (H )    Charge:    0.036571     Volume:    48.306 Bohr^3
 58 (C )    Charge:   -0.032794     Volume:    82.568 Bohr^3
 59 (H )    Charge:    0.059211     Volume:    46.493 Bohr^3
 60 (C )    Charge:   -0.594660     Volume:    75.166 Bohr^3
 61 (C )    Charge:   -0.029770     Volume:    82.712 Bohr^3
 62 (H )    Charge:    0.048602     Volume:    45.628 Bohr^3
 63 (C )    Charge:   -0.034133     Volume:    83.300 Bohr^3
 64 (H )    Charge:    0.029625     Volume:    48.824 Bohr^3
 65 (C )    Charge:   -0.028722     Volume:    81.324 Bohr^3
 66 (H )    Charge:    0.030121     Volume:    49.123 Bohr^3
 67 (C )    Charge:   -0.019572     Volume:    79.302 Bohr^3
 68 (H )    Charge:    0.036232     Volume:    49.623 Bohr^3
 69 (C )    Charge:   -0.022538     Volume:    74.566 Bohr^3
 70 (H )    Charge:    0.035489     Volume:    46.322 Bohr^3
 71 (C )    Charge:   -0.594099     Volume:    77.062 Bohr^3
 72 (C )    Charge:   -0.017377     Volume:    75.365 Bohr^3
 73 (H )    Charge:    0.046103     Volume:    48.031 Bohr^3
 74 (C )    Charge:   -0.018294     Volume:    78.342 Bohr^3
 75 (H )    Charge:    0.035400     Volume:    49.369 Bohr^3
 76 (C )    Charge:   -0.031224     Volume:    82.368 Bohr^3
 77 (H )    Charge:    0.028564     Volume:    49.089 Bohr^3
 78 (C )    Charge:   -0.037009     Volume:    84.180 Bohr^3
 79 (H )    Charge:    0.029192     Volume:    48.881 Bohr^3
 80 (C )    Charge:   -0.035184     Volume:    82.131 Bohr^3
 81 (H )    Charge:    0.047759     Volume:    45.795 Bohr^3
 82 (C )    Charge:   -0.602608     Volume:    76.610 Bohr^3
 83 (C )    Charge:   -0.027717     Volume:    79.731 Bohr^3
 84 (H )    Charge:    0.028648     Volume:    46.911 Bohr^3
 85 (C )    Charge:   -0.030863     Volume:    84.643 Bohr^3
 86 (H )    Charge:    0.030273     Volume:    48.789 Bohr^3
 87 (C )    Charge:   -0.029740     Volume:    82.746 Bohr^3
 88 (H )    Charge:    0.028214     Volume:    49.096 Bohr^3
 89 (C )    Charge:   -0.019637     Volume:    78.054 Bohr^3
 90 (H )    Charge:    0.030269     Volume:    49.270 Bohr^3
 91 (C )    Charge:   -0.017253     Volume:    78.032 Bohr^3
 92 (H )    Charge:    0.050407     Volume:    45.690 Bohr^3
 93 (C )    Charge:   -0.594675     Volume:    79.830 Bohr^3
 94 (C )    Charge:   -0.030060     Volume:    81.058 Bohr^3
 95 (H )    Charge:    0.059534     Volume:    44.275 Bohr^3
 96 (C )    Charge:   -0.035203     Volume:    84.289 Bohr^3
 97 (H )    Charge:    0.035195     Volume:    48.471 Bohr^3
 98 (C )    Charge:   -0.032984     Volume:    83.648 Bohr^3
 99 (H )    Charge:    0.034973     Volume:    48.417 Bohr^3
100 (C )    Charge:   -0.031030     Volume:    83.864 Bohr^3
101 (H )    Charge:    0.035167     Volume:    48.416 Bohr^3
102 (C )    Charge:   -0.024729     Volume:    79.872 Bohr^3
103 (H )    Charge:    0.051432     Volume:    47.120 Bohr^3
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$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (6) (square planar form)
(The nbe ligand is bound in the position *trans* to the Au atom.)

ZPE(BP86/def2-SVP) = 0.9573377 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3635.6697656 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3634.61529146367 Hartree (single point)

Cartesian coordinates in Å:

Au	0.39061	0.39276	-0.05115
Pt	-1.80392	1.68360	-0.80002
P	2.04160	-1.02990	0.71096
P	-1.31410	2.35084	1.39068
P	-0.79651	0.76876	-2.71029
C	3.18780	-1.55699	-0.60802
C	3.59851	-2.89822	-0.73815
H	3.25219	-3.65313	-0.01710
C	4.43471	-3.26923	-1.80323
H	4.75077	-4.31790	-1.90821
C	4.86550	-2.30715	-2.73277
H	5.51754	-2.60376	-3.56786
C	4.46062	-0.96744	-2.59835
H	4.78717	-0.21015	-3.32521
C	3.61679	-0.59123	-1.54370
H	3.26752	0.44931	-1.46245
C	1.27040	-2.54846	1.36918
C	0.08063	-2.99321	0.75660
H	-0.35225	-2.41771	-0.07487
C	-0.55377	-4.15397	1.21920
H	-1.47995	-4.49624	0.73438
C	-0.01311	-4.86697	2.30379
H	-0.51743	-5.77177	2.67482
C	1.17154	-4.42313	2.91669
H	1.59650	-4.98127	3.76424
C	1.81947	-3.26859	2.44908
H	2.74517	-2.92134	2.93121
C	3.05450	-0.34956	2.06817
C	4.39305	0.04153	1.87492
H	4.88527	-0.13446	0.90714
C	5.09797	0.65413	2.92460
H	6.14512	0.95564	2.77290
C	4.47364	0.87547	4.16331
H	5.03045	1.35324	4.98308
C	3.13757	0.47889	4.35643
H	2.64246	0.64650	5.32451
C	2.42558	-0.12713	3.31323
H	1.37833	-0.42695	3.46428
C	-0.64384	-1.06447	-2.64441
C	0.56626	-1.74461	-2.88693
H	1.48091	-1.18414	-3.12022
C	0.61434	-3.14534	-2.80218
H	1.57003	-3.66035	-2.97615
C	-0.54353	-3.87836	-2.49696

H	-0.50288	-4.97601	-2.43983
C	-1.75170	-3.20322	-2.24782
H	-2.66198	-3.76962	-1.99988
C	-1.80080	-1.80226	-2.30505
H	-2.74043	-1.27397	-2.08484
C	0.86312	1.42829	-3.15500
C	1.52535	2.32616	-2.29617
H	1.03940	2.64175	-1.36087
C	2.79424	2.82307	-2.63290
H	3.29588	3.52420	-1.94978
C	3.40749	2.42599	-3.83246
H	4.40230	2.81389	-4.09880
C	2.74041	1.54541	-4.70389
H	3.21138	1.24462	-5.65169
C	1.46709	1.05697	-4.37545
H	0.93755	0.38973	-5.07204
C	-1.68656	1.07050	-4.29840
C	-2.34342	0.05878	-5.02319
H	-2.30165	-0.98484	-4.68069
C	-3.04863	0.37978	-6.19645
H	-3.55726	-0.41729	-6.75918
C	-3.09945	1.70583	-6.65216
H	-3.65298	1.95338	-7.57005
C	-2.43241	2.71708	-5.93715
H	-2.45881	3.75679	-6.29624
C	-1.72994	2.40224	-4.76647
H	-1.20215	3.19441	-4.21151
C	-1.16839	1.09873	2.73041
C	-0.85556	1.50698	4.04557
H	-0.72395	2.57549	4.27317
C	-0.71554	0.55051	5.06219
H	-0.46324	0.87276	6.08349
C	-0.90096	-0.81523	4.77798
H	-0.78445	-1.56374	5.57576
C	-1.24519	-1.22288	3.47902
H	-1.39584	-2.28790	3.25135
C	-1.38493	-0.26765	2.45900
H	-1.66154	-0.57751	1.43925
C	0.28350	3.26366	1.32868
C	1.39967	2.88763	2.10047
H	1.31634	2.08223	2.83995
C	2.64059	3.51197	1.90167
H	3.50491	3.18606	2.49864
C	2.77264	4.53554	0.94919
H	3.74368	5.03136	0.80140
C	1.66005	4.92226	0.18144
H	1.75686	5.71712	-0.57313
C	0.42539	4.27851	0.35479
H	-0.42412	4.53569	-0.29683
C	-2.50773	3.52907	2.15959
C	-2.38217	4.92696	2.03887
H	-1.49933	5.36638	1.55466
C	-3.37742	5.77164	2.55851
H	-3.26618	6.86227	2.46476
C	-4.50172	5.23070	3.20188
H	-5.27873	5.89503	3.60818

C	-4.62456	3.83703	3.33558
H	-5.49595	3.40570	3.85064
C	-3.63481	2.99006	2.81753
H	-3.73131	1.90021	2.93541
C	-4.94831	1.77618	-0.14426
H	-5.05665	1.71192	0.95208
C	-3.80940	2.65689	-0.65511
H	-3.68481	3.68675	-0.28653
C	-3.58316	2.26481	-1.99915
H	-3.26627	2.95647	-2.79377
C	-4.57977	1.14548	-2.29264
H	-4.34341	0.51012	-3.16553
C	-5.96423	1.86865	-2.37004
H	-5.94429	2.71792	-3.08061
H	-6.74388	1.16413	-2.72245
C	-6.21547	2.30868	-0.89148
H	-6.33103	3.40423	-0.77645
H	-7.12852	1.83685	-0.47658
C	-4.69520	0.45982	-0.91114
H	-5.54134	-0.25307	-0.84693
H	-3.75536	-0.03943	-0.59027

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	-0.19559	2.93881	6.57375	9.66790	0.01490	0.00024
2pt	-0.35490	3.04071	6.52769	8.75603	0.02959	0.00088
3p	0.42074	5.56168	8.53037	0.44525	0.04196	
4p	0.24103	5.55655	8.68028	0.48056	0.04159	
5p	0.25281	5.56042	8.65468	0.49052	0.04157	
6c	0.03773	3.27152	2.54897	0.13390	0.00788	
7c	-0.14329	3.18602	2.83841	0.11153	0.00733	
8h	0.14018	0.81807	0.03987	0.00188		
9c	-0.16043	3.19946	2.84347	0.11033	0.00717	
10h	0.14329	0.82020	0.03473	0.00178		
11c	-0.09765	3.16118	2.81917	0.11017	0.00712	
12h	0.14318	0.82027	0.03479	0.00176		
13c	-0.11135	3.15944	2.83482	0.10993	0.00715	
14h	0.13641	0.82599	0.03582	0.00178		
15c	-0.20636	3.26633	2.81840	0.11423	0.00741	
16h	0.14813	0.80775	0.04227	0.00185		
17c	-0.01780	3.26432	2.61203	0.13356	0.00789	
18c	-0.02810	3.20867	2.69864	0.11332	0.00747	
19h	0.10753	0.84244	0.04800	0.00203		
20c	-0.19994	3.22380	2.85940	0.10958	0.00716	
21h	0.13415	0.82947	0.03461	0.00178		
22c	-0.09532	3.15830	2.81981	0.11007	0.00713	
23h	0.14405	0.81952	0.03467	0.00176		
24c	-0.14462	3.18647	2.84121	0.10978	0.00717	
25h	0.14297	0.82035	0.03490	0.00178		
26c	-0.10030	3.14943	2.83208	0.11151	0.00728	
27h	0.14687	0.81225	0.03901	0.00187		
28c	0.08437	3.24053	2.53162	0.13566	0.00781	
29c	-0.14855	3.17659	2.85371	0.11091	0.00734	

30h	0.14264	0.81525	0.04024	0.00187	
31c	-0.14385	3.18655	2.83958	0.11053	0.00719
32h	0.14074	0.82260	0.03487	0.00179	
33c	-0.13061	3.18249	2.83107	0.10992	0.00713
34h	0.14282	0.82074	0.03468	0.00176	
35c	-0.08699	3.14804	2.82124	0.11053	0.00718
36h	0.13740	0.82647	0.03437	0.00176	
37c	-0.21350	3.27785	2.81166	0.11653	0.00747
38h	0.09598	0.85950	0.04272	0.00181	
39c	0.04849	3.23809	2.57249	0.13305	0.00789
40c	-0.02018	3.17115	2.73005	0.11169	0.00730
41h	0.10894	0.84427	0.04480	0.00200	
42c	-0.14023	3.20126	2.82084	0.11096	0.00718
43h	0.13176	0.83051	0.03592	0.00181	
44c	-0.11161	3.18019	2.81418	0.11011	0.00713
45h	0.13565	0.82770	0.03487	0.00178	
46c	-0.17704	3.19752	2.86149	0.11090	0.00713
47h	0.14054	0.82284	0.03483	0.00179	
48c	-0.11975	3.21116	2.78710	0.11412	0.00737
49h	0.11303	0.84317	0.04192	0.00188	
50c	0.00496	3.27960	2.57896	0.12867	0.00781
51c	-0.03806	3.22599	2.68701	0.11755	0.00750
52h	0.13762	0.81202	0.04839	0.00198	
53c	-0.18857	3.19903	2.87006	0.11231	0.00717
54h	0.13311	0.82972	0.03540	0.00177	
55c	-0.10562	3.17123	2.81686	0.11040	0.00713
56h	0.14482	0.81924	0.03420	0.00175	
57c	-0.19845	3.23274	2.84817	0.11036	0.00718
58h	0.14172	0.82211	0.03440	0.00177	
59c	-0.10668	3.14845	2.83574	0.11513	0.00735
60h	0.15142	0.80859	0.03813	0.00186	
61c	0.07693	3.23207	2.54712	0.13600	0.00787
62c	-0.19042	3.20527	2.86522	0.11260	0.00732
63h	0.13858	0.81796	0.04158	0.00189	
64c	-0.11489	3.16324	2.83349	0.11096	0.00720
65h	0.13896	0.82454	0.03472	0.00178	
66c	-0.12097	3.17667	2.82766	0.10947	0.00718
67h	0.13933	0.82401	0.03491	0.00176	
68c	-0.12731	3.17322	2.83627	0.11064	0.00719
69h	0.13778	0.82563	0.03481	0.00177	
70c	-0.22631	3.21553	2.88807	0.11523	0.00748
71h	0.13316	0.82691	0.03810	0.00183	
72c	0.00626	3.21909	2.63690	0.12992	0.00784
73c	-0.10687	3.14890	2.83474	0.11588	0.00735
74h	0.15139	0.80916	0.03758	0.00187	
75c	-0.22731	3.24900	2.86053	0.11066	0.00712
76h	0.14100	0.82230	0.03491	0.00179	
77c	-0.05345	3.13066	2.80526	0.11044	0.00709
78h	0.13962	0.82381	0.03479	0.00178	
79c	-0.14095	3.21360	2.80866	0.11155	0.00715
80h	0.12940	0.83117	0.03759	0.00184	
81c	-0.07624	3.16025	2.79376	0.11480	0.00743
82h	0.16528	0.79092	0.04179	0.00201	
83c	0.10835	3.18956	2.56263	0.13161	0.00785
84c	-0.06135	3.19933	2.74195	0.11271	0.00737
85h	0.09469	0.85666	0.04668	0.00197	

86c	-0.14988	3.22046	2.81118	0.11104	0.00721
87h	0.12945	0.83220	0.03657	0.00177	
88c	-0.11187	3.16202	2.83333	0.10940	0.00713
89h	0.14295	0.82095	0.03435	0.00175	
90c	-0.20010	3.23654	2.84439	0.11198	0.00719
91h	0.14145	0.82259	0.03420	0.00176	
92c	-0.15843	3.14429	2.89082	0.11588	0.00744
93h	0.15131	0.80883	0.03801	0.00185	
94c	0.07780	3.23521	2.54288	0.13628	0.00783
95c	-0.17792	3.19274	2.86510	0.11275	0.00733
96h	0.13036	0.82513	0.04261	0.00190	
97c	-0.12986	3.17459	2.83730	0.11078	0.00719
98h	0.13807	0.82531	0.03484	0.00178	
99c	-0.10369	3.16687	2.81998	0.10966	0.00717
100h	0.13930	0.82405	0.03490	0.00176	
101c	-0.14806	3.18684	2.84375	0.11028	0.00719
102h	0.13698	0.82646	0.03479	0.00177	
103c	-0.19331	3.20314	2.87000	0.11274	0.00744
104h	0.13584	0.82220	0.04006	0.00190	
105c	0.15886	2.98457	2.70961	0.13890	0.00806
106h	0.07416	0.88261	0.04120	0.00203	
107c	-0.27938	3.24724	2.89518	0.12921	0.00774
108h	0.15130	0.80664	0.04021	0.00186	
109c	-0.25092	3.21731	2.89321	0.13257	0.00783
110h	0.15587	0.80082	0.04144	0.00188	
111c	0.14141	3.00717	2.70560	0.13778	0.00803
112h	0.08775	0.86956	0.04068	0.00200	
113c	-0.21446	3.22418	2.88698	0.09783	0.00548
114h	0.08662	0.87405	0.03747	0.00187	
115h	0.09361	0.86750	0.03700	0.00188	
116c	-0.20993	3.21497	2.89246	0.09705	0.00546
117h	0.08600	0.87461	0.03752	0.00187	
118h	0.09305	0.86816	0.03690	0.00188	
119c	-0.22330	3.20760	2.90708	0.10264	0.00598
120h	0.08977	0.87074	0.03760	0.00189	
121h	0.06482	0.88759	0.04550	0.00209	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.30821	2.89220	6.00569	9.79228	0.00156	0.00006
2 pt	0.10627	2.58892	6.00462	9.29732	0.00264	0.00023
3 p	0.95156	5.19803	8.81036	0.03865	0.00140	0.00000
4 p	1.00057	5.19016	8.76907	0.03890	0.00130	0.00000
5 p	0.99168	5.19167	8.77636	0.03900	0.00129	0.00000
6 c	-0.36883	3.00839	3.35058	0.00737	0.00248	0.00000
7 c	-0.19555	2.98355	3.20464	0.00529	0.00207	0.00000
8 h	0.23620	0.76298	0.00073	0.00008	0.00000	0.00000
9 c	-0.21158	2.99221	3.21231	0.00508	0.00197	0.00000
10 h	0.23094	0.76837	0.00061	0.00008	0.00000	0.00000
11 c	-0.19451	2.99628	3.19112	0.00512	0.00198	0.00000
12 h	0.23018	0.76915	0.00059	0.00008	0.00000	0.00000
13 c	-0.21330	2.99081	3.21541	0.00515	0.00193	0.00000

14 h	0.23222	0.76701	0.00069	0.00008	0.00000	0.00000
15 c	-0.20958	2.98335	3.21881	0.00540	0.00202	0.00000
16 h	0.24324	0.75588	0.00080	0.00008	0.00000	0.00000
17 c	-0.37178	3.00840	3.35356	0.00732	0.00249	0.00000
18 c	-0.19494	2.98235	3.20503	0.00552	0.00204	0.00000
19 h	0.24529	0.75370	0.00093	0.00008	0.00000	0.00000
20 c	-0.22077	2.98990	3.22380	0.00513	0.00194	0.00000
21 h	0.22886	0.77043	0.00064	0.00008	0.00000	0.00000
22 c	-0.19557	2.99636	3.19208	0.00515	0.00197	0.00000
23 h	0.23078	0.76854	0.00060	0.00008	0.00000	0.00000
24 c	-0.21209	2.99201	3.21304	0.00506	0.00198	0.00000
25 h	0.23161	0.76771	0.00060	0.00008	0.00000	0.00000
26 c	-0.20039	2.98386	3.20912	0.00536	0.00206	0.00000
27 h	0.23769	0.76151	0.00072	0.00008	0.00000	0.00000
28 c	-0.36770	3.00902	3.34874	0.00745	0.00249	0.00000
29 c	-0.19845	2.98241	3.20877	0.00520	0.00207	0.00000
30 h	0.23648	0.76273	0.00071	0.00008	0.00000	0.00000
31 c	-0.20945	2.99192	3.21047	0.00508	0.00197	0.00000
32 h	0.23079	0.76852	0.00061	0.00008	0.00000	0.00000
33 c	-0.20229	2.99596	3.19920	0.00516	0.00197	0.00000
34 h	0.23103	0.76829	0.00060	0.00008	0.00000	0.00000
35 c	-0.21320	2.98969	3.21649	0.00509	0.00193	0.00000
36 h	0.22949	0.76980	0.00063	0.00008	0.00000	0.00000
37 c	-0.21516	2.98116	3.22649	0.00547	0.00203	0.00000
38 h	0.24519	0.75379	0.00093	0.00009	0.00000	0.00000
39 c	-0.36225	3.01047	3.34190	0.00747	0.00243	0.00000
40 c	-0.21604	2.98210	3.22642	0.00550	0.00203	0.00000
41 h	0.24537	0.75369	0.00086	0.00008	0.00000	0.00000
42 c	-0.20590	2.98965	3.20916	0.00519	0.00189	0.00000
43 h	0.23373	0.76553	0.00066	0.00007	0.00000	0.00000
44 c	-0.20347	2.99381	3.20245	0.00525	0.00196	0.00000
45 h	0.23006	0.76925	0.00062	0.00008	0.00000	0.00000
46 c	-0.22107	2.98942	3.22462	0.00510	0.00193	0.00000
47 h	0.22878	0.77051	0.00063	0.00008	0.00000	0.00000
48 c	-0.23086	2.97926	3.24428	0.00530	0.00203	0.00000
49 h	0.23568	0.76349	0.00075	0.00008	0.00000	0.00000
50 c	-0.36869	3.01237	3.34643	0.00744	0.00245	0.00000
51 c	-0.21285	2.98563	3.21979	0.00541	0.00203	0.00000
52 h	0.25179	0.74725	0.00087	0.00009	0.00000	0.00000
53 c	-0.22758	2.98959	3.23099	0.00510	0.00191	0.00000
54 h	0.23248	0.76677	0.00067	0.00008	0.00000	0.00000
55 c	-0.19827	2.99567	3.19549	0.00516	0.00195	0.00000
56 h	0.22923	0.77009	0.00061	0.00008	0.00000	0.00000
57 c	-0.21429	2.99097	3.21629	0.00506	0.00197	0.00000
58 h	0.23088	0.76843	0.00062	0.00008	0.00000	0.00000
59 c	-0.20054	2.98354	3.20952	0.00544	0.00204	0.00000
60 h	0.23729	0.76192	0.00072	0.00008	0.00000	0.00000
61 c	-0.36251	3.01807	3.33427	0.00771	0.00246	0.00000
62 c	-0.22067	2.98187	3.23141	0.00532	0.00208	0.00000
63 h	0.23421	0.76498	0.00073	0.00008	0.00000	0.00000
64 c	-0.20533	2.99045	3.20789	0.00502	0.00198	0.00000
65 h	0.22833	0.77098	0.00061	0.00008	0.00000	0.00000
66 c	-0.20025	2.99514	3.19801	0.00509	0.00201	0.00000
67 h	0.22944	0.76989	0.00060	0.00008	0.00000	0.00000
68 c	-0.20602	2.98986	3.20913	0.00504	0.00199	0.00000
69 h	0.22845	0.77085	0.00061	0.00008	0.00000	0.00000

70	c	-0.21566	2.97937	3.22882	0.00538	0.00209	0.00000
71	h	0.22803	0.77120	0.00070	0.00008	0.00000	0.00000
72	c	-0.37102	3.01093	3.35023	0.00741	0.00245	0.00000
73	c	-0.20591	2.98320	3.21520	0.00548	0.00204	0.00000
74	h	0.23863	0.76060	0.00070	0.00007	0.00000	0.00000
75	c	-0.21855	2.99095	3.22055	0.00511	0.00194	0.00000
76	h	0.23141	0.76789	0.00062	0.00008	0.00000	0.00000
77	c	-0.20010	2.99581	3.19715	0.00521	0.00194	0.00000
78	h	0.23139	0.76792	0.00061	0.00008	0.00000	0.00000
79	c	-0.22176	2.98999	3.22452	0.00536	0.00189	0.00000
80	h	0.23852	0.76070	0.00071	0.00008	0.00000	0.00000
81	c	-0.20582	2.98520	3.21312	0.00546	0.00204	0.00000
82	h	0.24266	0.75652	0.00074	0.00007	0.00000	0.00000
83	c	-0.35928	3.01128	3.33781	0.00776	0.00243	0.00000
84	c	-0.21640	2.98008	3.22887	0.00539	0.00206	0.00000
85	h	0.24364	0.75541	0.00086	0.00009	0.00000	0.00000
86	c	-0.20494	2.98979	3.20817	0.00509	0.00190	0.00000
87	h	0.23396	0.76528	0.00069	0.00008	0.00000	0.00000
88	c	-0.20866	2.99381	3.20779	0.00509	0.00197	0.00000
89	h	0.22750	0.77180	0.00061	0.00008	0.00000	0.00000
90	c	-0.21462	2.98895	3.21860	0.00512	0.00194	0.00000
91	h	0.22989	0.76941	0.00062	0.00008	0.00000	0.00000
92	c	-0.23575	2.98033	3.24811	0.00528	0.00204	0.00000
93	h	0.23446	0.76476	0.00071	0.00007	0.00000	0.00000
94	c	-0.36867	3.01750	3.34092	0.00779	0.00245	0.00000
95	c	-0.21561	2.98034	3.22796	0.00522	0.00209	0.00000
96	h	0.23088	0.76828	0.00075	0.00008	0.00000	0.00000
97	c	-0.20389	2.99089	3.20600	0.00501	0.00199	0.00000
98	h	0.22845	0.77086	0.00061	0.00008	0.00000	0.00000
99	c	-0.19973	2.99510	3.19751	0.00510	0.00201	0.00000
100	h	0.22948	0.76984	0.00059	0.00008	0.00000	0.00000
101	c	-0.20609	2.98964	3.20939	0.00506	0.00200	0.00000
102	h	0.22835	0.77094	0.00062	0.00008	0.00000	0.00000
103	c	-0.21102	2.97956	3.22389	0.00548	0.00209	0.00000
104	h	0.22965	0.76948	0.00079	0.00008	0.00000	0.00000
105	c	-0.25828	3.01546	3.23665	0.00527	0.00090	0.00000
106	h	0.23123	0.76777	0.00081	0.00018	0.00000	0.00000
107	c	-0.32072	3.04168	3.26860	0.00910	0.00135	0.00000
108	h	0.24620	0.75263	0.00105	0.00013	0.00000	0.00000
109	c	-0.32897	3.04178	3.27656	0.00927	0.00135	0.00000
110	h	0.24581	0.75303	0.00103	0.00013	0.00000	0.00000
111	c	-0.26483	3.01602	3.24264	0.00527	0.00090	0.00000
112	h	0.23457	0.76441	0.00085	0.00017	0.00000	0.00000
113	c	-0.41255	3.07582	3.32987	0.00592	0.00094	0.00000
114	h	0.21708	0.78203	0.00075	0.00015	0.00000	0.00000
115	h	0.22081	0.77827	0.00078	0.00015	0.00000	0.00000
116	c	-0.41336	3.07676	3.32970	0.00595	0.00095	0.00000
117	h	0.21717	0.78194	0.00075	0.00015	0.00000	0.00000
118	h	0.22098	0.77809	0.00078	0.00015	0.00000	0.00000
119	c	-0.41325	3.06777	3.33801	0.00646	0.00101	0.00000
120	h	0.22102	0.77810	0.00073	0.00016	0.00000	0.00000
121	h	0.21138	0.78759	0.00088	0.00015	0.00000	0.00000

QTAIM Charges:

1	(Au)	Charge:	-0.114519	Volume:	174.606 Bohr^3
2	(Pt)	Charge:	-0.181021	Volume:	164.465 Bohr^3
3	(P)	Charge:	1.925757	Volume:	68.823 Bohr^3
4	(P)	Charge:	1.839756	Volume:	67.179 Bohr^3
5	(P)	Charge:	1.836744	Volume:	66.197 Bohr^3
6	(C)	Charge:	-0.641437	Volume:	78.191 Bohr^3
7	(C)	Charge:	-0.018547	Volume:	80.194 Bohr^3
8	(H)	Charge:	0.061768	Volume:	45.139 Bohr^3
9	(C)	Charge:	-0.025135	Volume:	83.539 Bohr^3
10	(H)	Charge:	0.053316	Volume:	47.162 Bohr^3
11	(C)	Charge:	-0.023982	Volume:	83.532 Bohr^3
12	(H)	Charge:	0.055567	Volume:	47.025 Bohr^3
13	(C)	Charge:	-0.026653	Volume:	83.171 Bohr^3
14	(H)	Charge:	0.052721	Volume:	47.685 Bohr^3
15	(C)	Charge:	-0.036319	Volume:	75.559 Bohr^3
16	(H)	Charge:	0.068085	Volume:	41.577 Bohr^3
17	(C)	Charge:	-0.641116	Volume:	76.207 Bohr^3
18	(C)	Charge:	-0.023554	Volume:	75.657 Bohr^3
19	(H)	Charge:	0.071182	Volume:	36.899 Bohr^3
20	(C)	Charge:	-0.029904	Volume:	82.356 Bohr^3
21	(H)	Charge:	0.047590	Volume:	49.013 Bohr^3
22	(C)	Charge:	-0.027157	Volume:	83.034 Bohr^3
23	(H)	Charge:	0.055773	Volume:	47.040 Bohr^3
24	(C)	Charge:	-0.024750	Volume:	83.820 Bohr^3
25	(H)	Charge:	0.055234	Volume:	47.077 Bohr^3
26	(C)	Charge:	-0.024344	Volume:	80.081 Bohr^3
27	(H)	Charge:	0.061965	Volume:	45.155 Bohr^3
28	(C)	Charge:	-0.645542	Volume:	81.062 Bohr^3
29	(C)	Charge:	-0.019971	Volume:	82.027 Bohr^3
30	(H)	Charge:	0.061875	Volume:	44.877 Bohr^3
31	(C)	Charge:	-0.024491	Volume:	82.667 Bohr^3
32	(H)	Charge:	0.053456	Volume:	47.185 Bohr^3
33	(C)	Charge:	-0.027068	Volume:	82.657 Bohr^3
34	(H)	Charge:	0.055302	Volume:	47.057 Bohr^3
35	(C)	Charge:	-0.025847	Volume:	82.347 Bohr^3
36	(H)	Charge:	0.048918	Volume:	49.153 Bohr^3
37	(C)	Charge:	-0.035698	Volume:	73.055 Bohr^3
38	(H)	Charge:	0.069848	Volume:	38.669 Bohr^3
39	(C)	Charge:	-0.623795	Volume:	72.841 Bohr^3
40	(C)	Charge:	-0.023864	Volume:	75.937 Bohr^3
41	(H)	Charge:	0.068717	Volume:	39.495 Bohr^3
42	(C)	Charge:	-0.022099	Volume:	81.162 Bohr^3
43	(H)	Charge:	0.054808	Volume:	48.225 Bohr^3
44	(C)	Charge:	-0.023142	Volume:	80.764 Bohr^3
45	(H)	Charge:	0.050770	Volume:	47.618 Bohr^3
46	(C)	Charge:	-0.033043	Volume:	80.927 Bohr^3
47	(H)	Charge:	0.046579	Volume:	48.108 Bohr^3
48	(C)	Charge:	-0.041500	Volume:	76.391 Bohr^3
49	(H)	Charge:	0.054620	Volume:	43.531 Bohr^3
50	(C)	Charge:	-0.616207	Volume:	75.449 Bohr^3
51	(C)	Charge:	-0.038645	Volume:	75.372 Bohr^3
52	(H)	Charge:	0.079147	Volume:	34.346 Bohr^3
53	(C)	Charge:	-0.035057	Volume:	81.465 Bohr^3

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 54 (H )    Charge:    0.051627     Volume:    48.597 Bohr^3
 55 (C )    Charge:   -0.028779     Volume:    81.834 Bohr^3
 56 (H )    Charge:    0.051740     Volume:    47.380 Bohr^3
 57 (C )    Charge:   -0.025491     Volume:    82.189 Bohr^3
 58 (H )    Charge:    0.052465     Volume:    47.349 Bohr^3
 59 (C )    Charge:   -0.022226     Volume:    76.321 Bohr^3
 60 (H )    Charge:    0.060871     Volume:    45.977 Bohr^3
 61 (C )    Charge:   -0.605127     Volume:    74.600 Bohr^3
 62 (C )    Charge:   -0.031467     Volume:    79.599 Bohr^3
 63 (H )    Charge:    0.055767     Volume:    43.350 Bohr^3
 64 (C )    Charge:   -0.023737     Volume:    83.632 Bohr^3
 65 (H )    Charge:    0.050153     Volume:    47.365 Bohr^3
 66 (C )    Charge:   -0.022150     Volume:    83.210 Bohr^3
 67 (H )    Charge:    0.053770     Volume:    47.145 Bohr^3
 68 (C )    Charge:   -0.022634     Volume:    83.417 Bohr^3
 69 (H )    Charge:    0.050413     Volume:    47.368 Bohr^3
 70 (C )    Charge:   -0.029805     Volume:    76.288 Bohr^3
 71 (H )    Charge:    0.042267     Volume:    47.782 Bohr^3
 72 (C )    Charge:   -0.618036     Volume:    73.581 Bohr^3
 73 (C )    Charge:   -0.025101     Volume:    75.061 Bohr^3
 74 (H )    Charge:    0.062097     Volume:    46.160 Bohr^3
 75 (C )    Charge:   -0.028652     Volume:    82.299 Bohr^3
 76 (H )    Charge:    0.051936     Volume:    47.605 Bohr^3
 77 (C )    Charge:   -0.030183     Volume:    81.158 Bohr^3
 78 (H )    Charge:    0.054466     Volume:    47.211 Bohr^3
 79 (C )    Charge:   -0.028397     Volume:    79.613 Bohr^3
 80 (H )    Charge:    0.062115     Volume:    46.044 Bohr^3
 81 (C )    Charge:   -0.031181     Volume:    74.280 Bohr^3
 82 (H )    Charge:    0.062284     Volume:    42.654 Bohr^3
 83 (C )    Charge:   -0.620699     Volume:    75.161 Bohr^3
 84 (C )    Charge:   -0.022848     Volume:    77.135 Bohr^3
 85 (H )    Charge:    0.065059     Volume:    36.766 Bohr^3
 86 (C )    Charge:   -0.023075     Volume:    83.937 Bohr^3
 87 (H )    Charge:    0.057128     Volume:    47.554 Bohr^3
 88 (C )    Charge:   -0.028703     Volume:    84.071 Bohr^3
 89 (H )    Charge:    0.048105     Volume:    47.651 Bohr^3
 90 (C )    Charge:   -0.026579     Volume:    80.520 Bohr^3
 91 (H )    Charge:    0.048584     Volume:    47.880 Bohr^3
 92 (C )    Charge:   -0.040501     Volume:    71.858 Bohr^3
 93 (H )    Charge:    0.045857     Volume:    46.190 Bohr^3
 94 (C )    Charge:   -0.611223     Volume:    76.806 Bohr^3
 95 (C )    Charge:   -0.029914     Volume:    81.690 Bohr^3
 96 (H )    Charge:    0.051843     Volume:    43.066 Bohr^3
 97 (C )    Charge:   -0.024127     Volume:    83.351 Bohr^3
 98 (H )    Charge:    0.051919     Volume:    47.321 Bohr^3
 99 (C )    Charge:   -0.022178     Volume:    83.163 Bohr^3
100 (H )    Charge:    0.054270     Volume:    47.137 Bohr^3
101 (C )    Charge:   -0.021476     Volume:    83.517 Bohr^3
102 (H )    Charge:    0.049828     Volume:    47.412 Bohr^3
103 (C )    Charge:   -0.023727     Volume:    75.648 Bohr^3
104 (H )    Charge:    0.044805     Volume:    45.937 Bohr^3
105 (C )    Charge:    0.043702     Volume:    54.061 Bohr^3
106 (H )    Charge:    0.012445     Volume:    47.086 Bohr^3
107 (C )    Charge:   -0.116173     Volume:    61.257 Bohr^3
108 (H )    Charge:    0.058257     Volume:    45.853 Bohr^3
109 (C )    Charge:   -0.115135     Volume:    60.509 Bohr^3
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110 (H )    Charge:    0.055700     Volume:    44.343 Bohr^3
111 (C )    Charge:    0.036954     Volume:    53.507 Bohr^3
112 (H )    Charge:    0.016187     Volume:    47.401 Bohr^3
113 (C )    Charge:    0.010448     Volume:    60.655 Bohr^3
114 (H )    Charge:    0.006407     Volume:    49.219 Bohr^3
115 (H )    Charge:    0.006566     Volume:    49.131 Bohr^3
116 (C )    Charge:    0.009041     Volume:    60.718 Bohr^3
117 (H )    Charge:    0.005837     Volume:    49.209 Bohr^3
118 (H )    Charge:    0.006801     Volume:    49.151 Bohr^3
119 (C )    Charge:   -0.001685     Volume:    59.594 Bohr^3
120 (H )    Charge:    0.003950     Volume:    49.181 Bohr^3
121 (H )    Charge:   -0.005742     Volume:    43.949 Bohr^3
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$[(Ph_3P)AuPt(nbe)(PPh_3)_2]^+$ (6') (trigonal pyramidal form)

ZPE(BP86/def2-SVP) = 0.9568919 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3635.6597167 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3634.60448981573 Hartree (single point)

Cartesian coordinates in Å:

Au	-0.95661	-1.86241	0.53219
Pt	-2.71003	-0.05645	-0.05877
P	0.51870	-3.57235	0.67893
C	-4.97196	0.41364	-2.21476
H	-4.49581	0.90058	-3.08544
C	-4.15984	-0.69634	-1.54502
H	-3.81840	-1.55345	-2.14751
C	-4.71544	-0.84331	-0.21672
H	-4.82269	-1.81909	0.28383
C	-5.85098	0.17635	-0.12936
H	-6.18105	0.43401	0.89515
C	-6.97906	-0.38135	-1.05630
H	-7.23214	-1.43119	-0.80942
H	-7.90538	0.21579	-0.93657
C	-6.37524	-0.21597	-2.49008
H	-6.29739	-1.17413	-3.04080
H	-6.98813	0.46894	-3.10999
C	-5.30514	1.32265	-1.01100
H	-6.05783	2.10190	-1.24483
H	-4.40561	1.81426	-0.58529
C	0.54873	-4.36457	2.31857
C	1.07820	-5.66065	2.49094
H	1.44358	-6.23102	1.62371
C	1.12600	-6.22321	3.77460
H	1.53321	-7.23584	3.91216
C	0.65059	-5.49728	4.88179
H	0.68782	-5.94487	5.88621
C	0.12225	-4.20757	4.70728
H	-0.25398	-3.63778	5.56924
C	0.06495	-3.63859	3.42637
H	-0.35372	-2.63077	3.28210
C	0.14438	-4.84507	-0.57681
C	-1.20372	-5.04484	-0.94305
H	-1.98991	-4.43280	-0.47279
C	-1.53241	-6.00077	-1.91440
H	-2.58415	-6.15229	-2.19908
C	-0.51784	-6.75482	-2.53050
H	-0.77546	-7.49798	-3.29974
C	0.82487	-6.55837	-2.16650
H	1.61917	-7.14817	-2.64763
C	1.16010	-5.60752	-1.18960
H	2.21373	-5.44662	-0.91787
C	2.22396	-3.01974	0.33681
C	3.15395	-2.85680	1.38246
H	2.87661	-3.12727	2.41181

C	4.43517	-2.35495	1.10056
H	5.16478	-2.23644	1.91547
C	4.78735	-2.01263	-0.21596
H	5.79350	-1.62412	-0.43289
C	3.85346	-2.16548	-1.25680
H	4.11929	-1.88933	-2.28769
C	2.57178	-2.66252	-0.98528
H	1.84010	-2.76798	-1.80036
P	-0.93821	0.69867	-1.41905
C	-1.72624	2.04064	-2.38794
C	-2.38174	3.06793	-1.67073
H	-2.36466	3.07409	-0.57032
C	-3.08194	4.06894	-2.35676
H	-3.58553	4.86399	-1.78712
C	-3.15416	4.04286	-3.76021
H	-3.71361	4.82232	-4.29848
C	-2.51624	3.01515	-4.47445
H	-2.57597	2.98818	-5.57279
C	-1.80125	2.01565	-3.79419
H	-1.31202	1.20857	-4.35843
C	-0.23211	-0.49002	-2.63636
C	-0.77414	-1.78718	-2.74526
H	-1.65372	-2.05403	-2.14188
C	-0.18320	-2.73882	-3.59167
H	-0.60028	-3.75522	-3.64351
C	0.94793	-2.39404	-4.34980
H	1.41736	-3.13976	-5.00859
C	1.48111	-1.09483	-4.26467
H	2.36219	-0.81966	-4.86366
C	0.89821	-0.14675	-3.40973
H	1.33512	0.85960	-3.32695
C	0.58459	1.45840	-0.71063
C	1.67022	0.61406	-0.39080
H	1.62492	-0.45556	-0.63475
C	2.81065	1.12580	0.24259
H	3.64865	0.44981	0.46590
C	2.87396	2.48730	0.58599
H	3.76396	2.89099	1.09101
C	1.79814	3.33214	0.26945
H	1.84594	4.40265	0.51968
C	0.66123	2.82639	-0.38280
H	-0.16171	3.50632	-0.63909
P	-2.44852	0.48392	2.20231
C	-3.80944	-0.13541	3.25491
C	-4.14167	-1.50146	3.13367
H	-3.60573	-2.12200	2.39768
C	-5.14365	-2.05638	3.94135
H	-5.39732	-3.12266	3.84540
C	-5.83132	-1.24732	4.86352
H	-6.62766	-1.67929	5.48781
C	-5.50242	0.11268	4.98718
H	-6.03618	0.74546	5.71200
C	-4.48707	0.66996	4.19217
H	-4.22080	1.73147	4.30311
C	-2.59584	2.31106	2.15140
C	-3.84391	2.88469	1.81585

H	-4.73700	2.24826	1.73801
C	-3.94382	4.26245	1.57580
H	-4.91994	4.70012	1.31896
C	-2.80138	5.07834	1.65797
H	-2.87943	6.15832	1.46376
C	-1.56145	4.51112	1.99666
H	-0.66597	5.14596	2.07106
C	-1.45457	3.13345	2.24409
H	-0.47826	2.69821	2.49935
C	-0.95404	0.12864	3.22259
C	0.31490	0.18348	2.60758
H	0.40135	0.48116	1.55485
C	1.47063	-0.14546	3.32927
H	2.44736	-0.10197	2.82616
C	1.37032	-0.53551	4.67547
H	2.27340	-0.80611	5.24252
C	0.11102	-0.57907	5.29709
H	0.02829	-0.87451	6.35389
C	-1.05049	-0.25103	4.57705
H	-2.03308	-0.30187	5.06739

[(Ph_3P)AuPt(nbe)(PPh_3)$_2$]$^+$ (6'') (square planar form)
(The nbe ligand is bound in the position *cis* to the Au atom.)

ZPE(BP86/def2-SVP) = 0.9571154 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3635.6504779 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3634.59740614012 Hartree (single point)

Cartesian coordinates in Å:

Au	0.29619	-0.06326	-0.30139
Pt	-1.88311	1.43083	-0.84912
P	2.18620	-1.04306	0.71567
P	-1.46247	2.15717	1.31949
P	-3.41213	2.93112	-1.70671
C	3.40158	-1.45986	-0.58501
C	4.09063	-2.68834	-0.59594
H	3.89361	-3.43737	0.18533
C	5.02142	-2.95442	-1.61275
H	5.55417	-3.91690	-1.62526
C	5.27242	-1.99778	-2.61067
H	6.00217	-2.21193	-3.40565
C	4.58834	-0.76956	-2.59820
H	4.78137	-0.02074	-3.38073
C	3.64775	-0.50180	-1.59299
H	3.09633	0.45239	-1.58574
C	1.69668	-2.61894	1.50502
C	0.61417	-3.33186	0.94666
H	0.09647	-2.92688	0.06270
C	0.19103	-4.53722	1.52388
H	-0.65378	-5.08800	1.08434
C	0.83899	-5.03290	2.66906
H	0.50038	-5.97311	3.12928
C	1.91956	-4.32789	3.22500
H	2.43144	-4.71708	4.11770
C	2.35409	-3.12582	2.64421
H	3.19862	-2.57617	3.08444
C	3.13454	-0.13485	1.98565
C	4.40783	0.40543	1.71768
H	4.88846	0.23297	0.74387
C	5.06505	1.16072	2.70321
H	6.06202	1.57620	2.49343
C	4.45801	1.38121	3.95068
H	4.97652	1.97475	4.71814
C	3.18903	0.83773	4.21766
H	2.70566	1.00405	5.19162
C	2.52640	0.08414	3.24046
H	1.53363	-0.33542	3.45220
C	-1.06440	0.93609	2.65225
C	-0.68266	1.38871	3.93345
H	-0.56920	2.46583	4.12562
C	-0.45365	0.46887	4.96676
H	-0.15874	0.83015	5.96339
C	-0.59890	-0.91118	4.73092

H	-0.41010	-1.63163	5.54051
C	-0.98959	-1.36739	3.46201
H	-1.10286	-2.44402	3.26930
C	-1.23490	-0.44486	2.43065
H	-1.57054	-0.79442	1.44097
C	-0.01716	3.28030	1.22470
C	1.26689	2.84027	1.59725
H	1.39379	1.86757	2.08695
C	2.39051	3.64360	1.34797
H	3.38490	3.28185	1.64722
C	2.23849	4.89427	0.72673
H	3.11864	5.52530	0.53248
C	0.95732	5.34015	0.35637
H	0.82866	6.31719	-0.13259
C	-0.16528	4.53561	0.59786
H	-1.16049	4.88030	0.28391
C	-2.77138	3.09092	2.20524
C	-2.50196	4.23056	2.98668
H	-1.49422	4.67196	2.99181
C	-3.52408	4.80114	3.76268
H	-3.31301	5.69278	4.37207
C	-4.80801	4.23365	3.76606
H	-5.60557	4.68151	4.37727
C	-5.07947	3.10064	2.97940
H	-6.08894	2.66510	2.96781
C	-4.06692	2.53418	2.19572
H	-4.27284	1.65293	1.56798
C	-4.63826	3.84104	-0.67556
C	-4.19908	4.97046	0.04892
H	-3.14682	5.28308	-0.00536
C	-5.10168	5.71548	0.81621
H	-4.74626	6.59557	1.37093
C	-6.45371	5.33720	0.87784
H	-7.16348	5.92447	1.47906
C	-6.89471	4.21013	0.16871
H	-7.95345	3.91295	0.20541
C	-5.99350	3.46400	-0.60830
H	-6.35958	2.60244	-1.18321
C	-4.44669	2.15606	-3.01143
C	-5.15099	0.98002	-2.66558
H	-5.07492	0.58144	-1.64090
C	-5.91546	0.30330	-3.62635
H	-6.46627	-0.60680	-3.34544
C	-5.96159	0.77769	-4.94916
H	-6.55205	0.24137	-5.70676
C	-5.24334	1.93057	-5.30258
H	-5.26714	2.29925	-6.33893
C	-4.49013	2.62201	-4.33857
H	-3.92734	3.52080	-4.62764
C	-2.52131	4.32253	-2.50812
C	-1.11419	4.30796	-2.55706
H	-0.57704	3.46047	-2.10448
C	-0.41574	5.37168	-3.14874
H	0.68384	5.35365	-3.17414
C	-1.12115	6.45546	-3.69535
H	-0.57591	7.29062	-4.16018

C	-2.52694	6.48046	-3.64011
H	-3.08009	7.33458	-4.05845
C	-3.22779	5.42268	-3.04355
H	-4.32579	5.45654	-2.97967
C	0.33121	-0.38041	-3.25581
H	1.30332	-0.79453	-2.93334
C	-0.82949	-0.49875	-2.25377
H	-1.15934	-1.50527	-1.93821
C	-1.85349	0.43180	-2.73984
H	-2.87583	0.03664	-2.87585
C	-1.22484	1.11164	-3.96425
H	-1.67330	2.07776	-4.25663
C	-1.25107	0.03105	-5.08282
H	-2.26737	-0.38522	-5.22483
H	-0.93533	0.47037	-6.05052
C	-0.21739	-1.02002	-4.57350
H	-0.65968	-2.01998	-4.39441
H	0.61692	-1.15792	-5.29005
C	0.27754	1.12143	-3.59883
H	0.92922	1.39899	-4.45085
H	0.51887	1.76159	-2.72574

$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (7) (trigonal pyramidal form)

ZPE(BP86/def2-SVP) = 0.8384757 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2872.3353458 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2871.44878067104 Hartree (single point)

Cartesian coordinates in Å:

Au	0.70390	-0.29484	0.28782
Pt	-1.87138	-0.01190	0.51619
P	2.92589	-0.36701	-0.19132
C	-3.48380	-1.80108	-1.60066
H	-3.39358	-1.32590	-2.59389
C	-2.22194	-1.79754	-0.73891
H	-1.28818	-2.23139	-1.13110
C	-2.65518	-2.04281	0.60569
H	-2.08460	-2.65362	1.32210
C	-4.17936	-2.15346	0.53369
H	-4.72290	-2.00512	1.48449
C	-4.43505	-3.53361	-0.15720
H	-3.89393	-4.35678	0.34923
H	-5.51482	-3.78088	-0.12215
C	-3.95158	-3.29181	-1.62444
H	-3.13543	-3.97631	-1.92958
H	-4.77839	-3.42328	-2.35076
C	-4.51995	-1.19360	-0.63117
H	-5.56383	-1.29537	-0.98692
H	-4.32871	-0.12359	-0.40789
C	-3.40830	0.39113	3.28209
H	-4.01917	-0.51413	3.45114
C	-2.01549	0.16095	2.70127
H	-1.32456	-0.55593	3.17199
C	-1.59754	1.41881	2.16079
H	-0.56035	1.78317	2.21053
C	-2.74930	2.38847	2.42335
H	-2.74627	3.30999	1.81060
C	-2.71412	2.63961	3.96524
H	-1.70791	2.95220	4.30694
H	-3.41985	3.44946	4.23826
C	-3.16397	1.26455	4.55750
H	-2.40788	0.81263	5.22909
H	-4.10266	1.36042	5.13872
C	-3.97789	1.45495	2.31789
H	-4.91462	1.92057	2.68326
H	-4.15190	1.06234	1.29436
C	4.00461	-0.96144	1.14783
C	5.29793	-1.44674	0.86139
H	5.64561	-1.51709	-0.18033
C	6.13455	-1.84781	1.91297
H	7.14184	-2.23122	1.69294
C	5.68653	-1.76450	3.24322
H	6.34596	-2.08332	4.06409
C	4.39700	-1.28414	3.52714

H	4.04486	-1.22706	4.56763
C	3.55122	-0.88588	2.48079
H	2.53299	-0.52026	2.68907
C	3.23166	-1.41028	-1.65638
C	2.52041	-2.62451	-1.76544
H	1.79784	-2.90631	-0.98301
C	2.72814	-3.45965	-2.87175
H	2.17410	-4.40632	-2.95466
C	3.63779	-3.08256	-3.87644
H	3.79481	-3.73518	-4.74808
C	4.34466	-1.87346	-3.76877
H	5.05686	-1.57862	-4.55364
C	4.14744	-1.03542	-2.65954
H	4.69563	-0.08536	-2.58149
C	3.47796	1.32024	-0.60932
C	4.29794	2.05757	0.26791
H	4.69463	1.58825	1.18027
C	4.60783	3.39418	-0.03320
H	5.25294	3.96894	0.64786
C	4.10094	3.99352	-1.19827
H	4.34334	5.04185	-1.42676
C	3.28162	3.25565	-2.06991
H	2.87438	3.72042	-2.97935
C	2.96430	1.92399	-1.77809
H	2.31527	1.35297	-2.45474
P	-1.40344	1.57174	-1.19550
C	-3.06418	1.91699	-1.88645
C	-4.02914	2.55943	-1.07852
H	-3.74455	2.95824	-0.09507
C	-5.34949	2.69141	-1.52963
H	-6.09330	3.19750	-0.89653
C	-5.72202	2.17385	-2.78244
H	-6.76045	2.27117	-3.13214
C	-4.76440	1.53820	-3.58957
H	-5.05004	1.13952	-4.57440
C	-3.43844	1.40981	-3.14719
H	-2.69188	0.91247	-3.78321
C	-0.37966	1.19503	-2.68102
C	0.04999	-0.12036	-2.94383
H	-0.25167	-0.93198	-2.26902
C	0.87177	-0.39098	-4.04970
H	1.22280	-1.41724	-4.22892
C	1.25569	0.65040	-4.90925
H	1.90620	0.44071	-5.77120
C	0.80869	1.96223	-4.66644
H	1.10234	2.77898	-5.34279
C	-0.00088	2.23722	-3.55425
H	-0.32404	3.26885	-3.35205
C	-0.72939	3.19399	-0.66045
C	0.44301	3.20178	0.12398
H	0.90370	2.24514	0.42096
C	1.02654	4.41204	0.51909
H	1.94414	4.39898	1.12452
C	0.44006	5.63131	0.13943
H	0.89199	6.58339	0.45525
C	-0.72696	5.63208	-0.64211

H	-1.18878	6.58409	-0.94374
C	-1.31095	4.41986	-1.04606
H	-2.22038	4.43041	-1.66418

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	-0.04627	3.35148	6.06785	9.61143	0.01522	0.00029
2pt	-0.33769	2.77886	6.73943	8.77822	0.04030	0.00088
3p	0.30542	5.53310	8.65760	0.46009	0.04379	
4c	0.14211	3.00434	2.70594	0.13958	0.00803	
5h	0.08124	0.87736	0.03939	0.00201		
6c	-0.17388	3.15495	2.89286	0.11834	0.00773	
7h	0.12794	0.82834	0.04173	0.00199		
8c	-0.14172	3.18506	2.82605	0.12271	0.00790	
9h	0.12817	0.83106	0.03890	0.00187		
10c	0.10440	3.03551	2.71443	0.13767	0.00799	
11h	0.08443	0.87556	0.03804	0.00197		
12c	-0.20642	3.21193	2.89076	0.09826	0.00547	
13h	0.08463	0.87590	0.03760	0.00187		
14h	0.09654	0.86429	0.03728	0.00188		
15c	-0.19786	3.20858	2.88574	0.09806	0.00548	
16h	0.07954	0.88109	0.03750	0.00188		
17h	0.09592	0.86504	0.03715	0.00189		
18c	-0.18359	3.17144	2.90184	0.10432	0.00598	
19h	0.08893	0.87172	0.03745	0.00190		
20h	0.04438	0.90630	0.04729	0.00203		
21c	0.10366	3.03746	2.71360	0.13728	0.00800	
22h	0.08689	0.87325	0.03789	0.00197		
23c	-0.15066	3.16823	2.85151	0.12308	0.00784	
24h	0.13132	0.82823	0.03860	0.00185		
25c	-0.13592	3.12505	2.88071	0.12231	0.00785	
26h	0.12916	0.82615	0.04269	0.00200		
27c	0.11245	3.02854	2.71298	0.13800	0.00802	
28h	0.08872	0.87036	0.03891	0.00201		
29c	-0.20428	3.21633	2.88500	0.09747	0.00548	
30h	0.08367	0.87719	0.03727	0.00187		
31h	0.09714	0.86388	0.03709	0.00189		
32c	-0.20505	3.21022	2.89148	0.09789	0.00546	
33h	0.08451	0.87601	0.03760	0.00187		
34h	0.09675	0.86399	0.03738	0.00189		
35c	-0.21795	3.19530	2.91164	0.10501	0.00601	
36h	0.09536	0.86570	0.03706	0.00188		
37h	0.07069	0.88275	0.04455	0.00201		
38c	-0.00640	3.23915	2.62407	0.13524	0.00795	
39c	-0.12563	3.17565	2.83063	0.11203	0.00732	
40h	0.13162	0.82731	0.03921	0.00186		
41c	-0.13150	3.17743	2.83714	0.10976	0.00717	
42h	0.14391	0.81921	0.03510	0.00178		
43c	-0.08777	3.16361	2.80695	0.11004	0.00717	
44h	0.14540	0.81805	0.03480	0.00176		
45c	-0.14357	3.18004	2.84689	0.10948	0.00717	
46h	0.14213	0.82102	0.03507	0.00178		
47c	-0.12155	3.18036	2.82182	0.11199	0.00738	

48h	0.11082	0.84704	0.04025	0.00188	
49c	0.04337	3.21790	2.59749	0.13333	0.00791
50c	-0.15790	3.20153	2.83717	0.11177	0.00743
51h	0.12782	0.83065	0.03964	0.00190	
52c	-0.14360	3.18810	2.83844	0.10992	0.00714
53h	0.14294	0.82036	0.03492	0.00178	
54c	-0.11203	3.17568	2.81912	0.11009	0.00714
55h	0.14690	0.81664	0.03470	0.00176	
56c	-0.14218	3.18845	2.83567	0.11088	0.00719
57h	0.14530	0.81803	0.03488	0.00178	
58c	-0.11757	3.16865	2.83029	0.11133	0.00730
59h	0.14749	0.81104	0.03959	0.00189	
60c	-0.00109	3.24409	2.61489	0.13430	0.00781
61c	-0.10240	3.15018	2.83438	0.11051	0.00733
62h	0.14399	0.81382	0.04031	0.00188	
63c	-0.18469	3.21590	2.85111	0.11049	0.00719
64h	0.14479	0.81881	0.03463	0.00178	
65c	-0.09679	3.17114	2.80809	0.11038	0.00716
66h	0.14123	0.82249	0.03452	0.00176	
67c	-0.11699	3.18483	2.81542	0.10951	0.00723
68h	0.12960	0.83340	0.03521	0.00180	
69c	-0.05567	3.22783	2.70814	0.11225	0.00744
70h	0.09243	0.85857	0.04708	0.00193	
71p	0.31481	5.49094	8.70897	0.44532	0.03996
72c	0.07972	3.22245	2.55482	0.13519	0.00782
73c	-0.23232	3.25720	2.85119	0.11654	0.00739
74h	0.13962	0.81896	0.03958	0.00184	
75c	-0.11754	3.16624	2.83334	0.11078	0.00717
76h	0.14081	0.82254	0.03487	0.00178	
77c	-0.11551	3.17491	2.82382	0.10963	0.00715
78h	0.14244	0.82104	0.03476	0.00176	
79c	-0.13588	3.18034	2.83796	0.11039	0.00719
80h	0.14092	0.82254	0.03476	0.00178	
81c	-0.16514	3.19018	2.85582	0.11175	0.00739
82h	0.14006	0.81735	0.04069	0.00191	
83c	0.05994	3.22594	2.57346	0.13286	0.00780
84c	-0.11349	3.20715	2.78203	0.11687	0.00743
85h	0.07577	0.87913	0.04311	0.00199	
86c	-0.12512	3.19422	2.81168	0.11207	0.00715
87h	0.12930	0.83084	0.03802	0.00184	
88c	-0.10815	3.16901	2.82160	0.11042	0.00712
89h	0.13919	0.82409	0.03493	0.00178	
90c	-0.13141	3.17539	2.83939	0.10953	0.00709
91h	0.14447	0.81889	0.03485	0.00179	
92c	-0.17938	3.22485	2.83335	0.11386	0.00732
93h	0.13053	0.82691	0.04062	0.00193	
94c	0.07283	3.23175	2.55122	0.13629	0.00791
95c	-0.14639	3.28183	2.73871	0.11826	0.00759
96h	0.02692	0.92480	0.04635	0.00194	
97c	-0.14813	3.19620	2.83510	0.10966	0.00718
98h	0.12846	0.83369	0.03606	0.00180	
99c	-0.11141	3.16660	2.82774	0.10990	0.00716
100h	0.13987	0.82363	0.03474	0.00176	
101c	-0.14079	3.17778	2.84452	0.11129	0.00720
102h	0.14207	0.82143	0.03472	0.00177	
103c	-0.14561	3.16784	2.85836	0.11213	0.00728

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  104h      0.15341   0.80447   0.04024   0.00189
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NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.33511	2.88050	6.00384	9.77892	0.00155	0.00008
2 pt	0.38753	2.53571	6.01041	9.06304	0.00320	0.00010
3 p	1.01814	5.17226	8.76477	0.04325	0.00158	0.00000
4 c	-0.26095	3.01348	3.24118	0.00538	0.00090	0.00000
5 h	0.23050	0.76852	0.00080	0.00018	0.00000	0.00000
6 c	-0.35035	3.03678	3.30340	0.00883	0.00134	0.00000
7 h	0.22361	0.77528	0.00096	0.00014	0.00000	0.00000
8 c	-0.33811	3.04190	3.28550	0.00941	0.00130	0.00000
9 h	0.24132	0.75761	0.00093	0.00014	0.00000	0.00000
10 c	-0.25860	3.01722	3.23512	0.00537	0.00090	0.00000
11 h	0.22997	0.76905	0.00080	0.00019	0.00000	0.00000
12 c	-0.41143	3.07666	3.32785	0.00597	0.00095	0.00000
13 h	0.21560	0.78350	0.00075	0.00015	0.00000	0.00000
14 h	0.22319	0.77588	0.00078	0.00015	0.00000	0.00000
15 c	-0.41300	3.07546	3.33064	0.00595	0.00095	0.00000
16 h	0.21220	0.78691	0.00074	0.00015	0.00000	0.00000
17 h	0.22188	0.77719	0.00079	0.00015	0.00000	0.00000
18 c	-0.41057	3.06536	3.33775	0.00644	0.00101	0.00000
19 h	0.22715	0.77201	0.00070	0.00014	0.00000	0.00000
20 h	0.21230	0.78631	0.00123	0.00016	0.00000	0.00000
21 c	-0.25871	3.01557	3.23686	0.00539	0.00090	0.00000
22 h	0.23035	0.76868	0.00078	0.00019	0.00000	0.00000
23 c	-0.32520	3.03950	3.27495	0.00940	0.00135	0.00000
24 h	0.23954	0.75942	0.00090	0.00014	0.00000	0.00000
25 c	-0.34296	3.03743	3.29497	0.00922	0.00134	0.00000
26 h	0.23912	0.75972	0.00103	0.00014	0.00000	0.00000
27 c	-0.26290	3.01401	3.24277	0.00522	0.00090	0.00000
28 h	0.22743	0.77160	0.00080	0.00017	0.00000	0.00000
29 c	-0.41184	3.07503	3.32993	0.00594	0.00095	0.00000
30 h	0.21528	0.78383	0.00075	0.00015	0.00000	0.00000
31 h	0.22213	0.77695	0.00078	0.00015	0.00000	0.00000
32 c	-0.41162	3.07697	3.32772	0.00598	0.00095	0.00000
33 h	0.21556	0.78355	0.00074	0.00015	0.00000	0.00000
34 h	0.22335	0.77572	0.00078	0.00015	0.00000	0.00000
35 c	-0.41391	3.06631	3.34007	0.00651	0.00102	0.00000
36 h	0.22603	0.77311	0.00071	0.00015	0.00000	0.00000
37 h	0.21047	0.78825	0.00112	0.00016	0.00000	0.00000
38 c	-0.39092	3.01011	3.37062	0.00758	0.00260	0.00000
39 c	-0.18884	2.98373	3.19769	0.00529	0.00212	0.00000
40 h	0.23352	0.76568	0.00072	0.00008	0.00000	0.00000
41 c	-0.20200	2.99323	3.20166	0.00509	0.00202	0.00000
42 h	0.23361	0.76570	0.00060	0.00008	0.00000	0.00000
43 c	-0.18232	2.99834	3.17682	0.00515	0.00202	0.00000
44 h	0.23319	0.76613	0.00059	0.00008	0.00000	0.00000
45 c	-0.20753	2.99264	3.20778	0.00509	0.00202	0.00000
46 h	0.23246	0.76685	0.00061	0.00008	0.00000	0.00000
47 c	-0.19112	2.98410	3.19966	0.00522	0.00213	0.00000
48 h	0.23126	0.76800	0.00066	0.00008	0.00000	0.00000

49	c	-0.37586	3.00940	3.35637	0.00755	0.00255	0.00000
50	c	-0.19442	2.98222	3.20483	0.00526	0.00210	0.00000
51	h	0.23230	0.76696	0.00066	0.00007	0.00000	0.00000
52	c	-0.21290	2.99251	3.21326	0.00515	0.00198	0.00000
53	h	0.23391	0.76540	0.00061	0.00008	0.00000	0.00000
54	c	-0.19279	2.99788	3.18771	0.00522	0.00199	0.00000
55	h	0.23403	0.76529	0.00060	0.00008	0.00000	0.00000
56	c	-0.20770	2.99228	3.20831	0.00511	0.00198	0.00000
57	h	0.23346	0.76586	0.00061	0.00008	0.00000	0.00000
58	c	-0.19826	2.98413	3.20664	0.00540	0.00209	0.00000
59	h	0.23958	0.75960	0.00074	0.00008	0.00000	0.00000
60	c	-0.38832	3.01035	3.36791	0.00756	0.00250	0.00000
61	c	-0.20173	2.98312	3.21135	0.00519	0.00207	0.00000
62	h	0.23786	0.76132	0.00074	0.00008	0.00000	0.00000
63	c	-0.21126	2.99207	3.21213	0.00509	0.00197	0.00000
64	h	0.23205	0.76726	0.00061	0.00008	0.00000	0.00000
65	c	-0.18861	2.99558	3.18588	0.00519	0.00196	0.00000
66	h	0.23099	0.76832	0.00061	0.00008	0.00000	0.00000
67	c	-0.20361	2.98878	3.20777	0.00514	0.00192	0.00000
68	h	0.23043	0.76884	0.00065	0.00008	0.00000	0.00000
69	c	-0.20119	2.97922	3.21442	0.00551	0.00204	0.00000
70	h	0.24602	0.75289	0.00099	0.00009	0.00000	0.00000
71	p	1.00707	5.20288	8.75334	0.03556	0.00114	0.00000
72	c	-0.37675	3.01022	3.35637	0.00769	0.00247	0.00000
73	c	-0.21829	2.97865	3.23220	0.00540	0.00204	0.00000
74	h	0.23403	0.76508	0.00081	0.00009	0.00000	0.00000
75	c	-0.20865	2.98985	3.21177	0.00505	0.00198	0.00000
76	h	0.23049	0.76881	0.00062	0.00008	0.00000	0.00000
77	c	-0.19306	2.99596	3.19000	0.00511	0.00199	0.00000
78	h	0.23122	0.76811	0.00059	0.00008	0.00000	0.00000
79	c	-0.20462	2.99077	3.20682	0.00505	0.00198	0.00000
80	h	0.23046	0.76884	0.00061	0.00008	0.00000	0.00000
81	c	-0.20525	2.98107	3.21678	0.00534	0.00207	0.00000
82	h	0.23497	0.76419	0.00077	0.00008	0.00000	0.00000
83	c	-0.36768	3.01222	3.34551	0.00753	0.00242	0.00000
84	c	-0.21292	2.98083	3.22469	0.00538	0.00202	0.00000
85	h	0.23640	0.76277	0.00075	0.00009	0.00000	0.00000
86	c	-0.21727	2.98991	3.22010	0.00538	0.00188	0.00000
87	h	0.23724	0.76196	0.00073	0.00008	0.00000	0.00000
88	c	-0.19782	2.99537	3.19527	0.00523	0.00195	0.00000
89	h	0.23132	0.76800	0.00060	0.00008	0.00000	0.00000
90	c	-0.21667	2.99159	3.21799	0.00515	0.00194	0.00000
91	h	0.23171	0.76759	0.00062	0.00008	0.00000	0.00000
92	c	-0.20409	2.98357	3.21302	0.00546	0.00204	0.00000
93	h	0.23749	0.76169	0.00074	0.00008	0.00000	0.00000
94	c	-0.37203	3.01019	3.35157	0.00777	0.00251	0.00000
95	c	-0.20046	2.97794	3.21512	0.00534	0.00206	0.00000
96	h	0.22303	0.77599	0.00089	0.00009	0.00000	0.00000
97	c	-0.20745	2.98820	3.21211	0.00519	0.00194	0.00000
98	h	0.23021	0.76903	0.00069	0.00007	0.00000	0.00000
99	c	-0.19617	2.99477	3.19433	0.00508	0.00199	0.00000
100	h	0.22879	0.77053	0.00060	0.00008	0.00000	0.00000
101	c	-0.20834	2.99095	3.21040	0.00500	0.00198	0.00000
102	h	0.23030	0.76902	0.00060	0.00008	0.00000	0.00000
103	c	-0.21651	2.98344	3.22567	0.00532	0.00207	0.00000
104	h	0.23643	0.76276	0.00073	0.00008	0.00000	0.00000

QTAIM Charges:

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  1 (Au)    Charge:   -0.059054     Volume:   206.372 Bohr^3
  2 (Pt)    Charge:    0.039084     Volume:   132.963 Bohr^3
  3 (P )    Charge:    1.988976     Volume:    66.210 Bohr^3
  4 (C )    Charge:    0.043890     Volume:    53.630 Bohr^3
  5 (H )    Charge:    0.010462     Volume:    48.862 Bohr^3
  6 (C )    Charge:   -0.125760     Volume:    61.432 Bohr^3
  7 (H )    Charge:    0.016739     Volume:    46.867 Bohr^3
  8 (C )    Charge:   -0.113812     Volume:    62.426 Bohr^3
  9 (H )    Charge:    0.047774     Volume:    48.406 Bohr^3
 10 (C )    Charge:    0.040978     Volume:    54.166 Bohr^3
 11 (H )    Charge:    0.013688     Volume:    49.770 Bohr^3
 12 (C )    Charge:    0.008944     Volume:    60.606 Bohr^3
 13 (H )    Charge:    0.004678     Volume:    49.240 Bohr^3
 14 (H )    Charge:    0.011206     Volume:    48.858 Bohr^3
 15 (C )    Charge:    0.010510     Volume:    60.626 Bohr^3
 16 (H )    Charge:   -0.001029     Volume:    49.619 Bohr^3
 17 (H )    Charge:    0.007504     Volume:    49.047 Bohr^3
 18 (C )    Charge:    0.002823     Volume:    59.676 Bohr^3
 19 (H )    Charge:    0.012180     Volume:    49.250 Bohr^3
 20 (H )    Charge:   -0.004803     Volume:    38.721 Bohr^3
 21 (C )    Charge:    0.044952     Volume:    54.078 Bohr^3
 22 (H )    Charge:    0.014929     Volume:    49.571 Bohr^3
 23 (C )    Charge:   -0.109234     Volume:    62.464 Bohr^3
 24 (H )    Charge:    0.045047     Volume:    48.905 Bohr^3
 25 (C )    Charge:   -0.120304     Volume:    60.239 Bohr^3
 26 (H )    Charge:    0.040887     Volume:    45.078 Bohr^3
 27 (C )    Charge:    0.036776     Volume:    53.132 Bohr^3
 28 (H )    Charge:    0.005634     Volume:    48.603 Bohr^3
 29 (C )    Charge:    0.011245     Volume:    60.591 Bohr^3
 30 (H )    Charge:    0.004041     Volume:    49.284 Bohr^3
 31 (H )    Charge:    0.008628     Volume:    48.985 Bohr^3
 32 (C )    Charge:    0.009613     Volume:    60.672 Bohr^3
 33 (H )    Charge:    0.004100     Volume:    49.281 Bohr^3
 34 (H )    Charge:    0.011007     Volume:    48.860 Bohr^3
 35 (C )    Charge:    0.000033     Volume:    58.952 Bohr^3
 36 (H )    Charge:    0.010311     Volume:    48.813 Bohr^3
 37 (H )    Charge:   -0.007207     Volume:    39.777 Bohr^3
 38 (C )    Charge:   -0.658365     Volume:    81.166 Bohr^3
 39 (C )    Charge:   -0.016840     Volume:    81.419 Bohr^3
 40 (H )    Charge:    0.059407     Volume:    46.236 Bohr^3
 41 (C )    Charge:   -0.015719     Volume:    82.895 Bohr^3
 42 (H )    Charge:    0.061195     Volume:    46.676 Bohr^3
 43 (C )    Charge:   -0.015131     Volume:    82.464 Bohr^3
 44 (H )    Charge:    0.062438     Volume:    46.552 Bohr^3
 45 (C )    Charge:   -0.017683     Volume:    83.123 Bohr^3
 46 (H )    Charge:    0.058041     Volume:    46.866 Bohr^3
 47 (C )    Charge:   -0.022125     Volume:    81.545 Bohr^3
 48 (H )    Charge:    0.052400     Volume:    46.576 Bohr^3
 49 (C )    Charge:   -0.644895     Volume:    77.899 Bohr^3
 50 (C )    Charge:   -0.019550     Volume:    78.895 Bohr^3
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51	(H)	Charge:	0.051200	Volume:	47.462 Bohr^3
52	(C)	Charge:	-0.023948	Volume:	81.953 Bohr^3
53	(H)	Charge:	0.058879	Volume:	46.858 Bohr^3
54	(C)	Charge:	-0.022590	Volume:	82.124 Bohr^3
55	(H)	Charge:	0.061547	Volume:	46.655 Bohr^3
56	(C)	Charge:	-0.020516	Volume:	83.290 Bohr^3
57	(H)	Charge:	0.058946	Volume:	46.847 Bohr^3
58	(C)	Charge:	-0.019856	Volume:	78.942 Bohr^3
59	(H)	Charge:	0.065156	Volume:	44.615 Bohr^3
60	(C)	Charge:	-0.661817	Volume:	79.781 Bohr^3
61	(C)	Charge:	-0.023336	Volume:	82.206 Bohr^3
62	(H)	Charge:	0.063234	Volume:	45.060 Bohr^3
63	(C)	Charge:	-0.023211	Volume:	82.703 Bohr^3
64	(H)	Charge:	0.055260	Volume:	47.064 Bohr^3
65	(C)	Charge:	-0.017945	Volume:	81.723 Bohr^3
66	(H)	Charge:	0.056233	Volume:	47.066 Bohr^3
67	(C)	Charge:	-0.013032	Volume:	81.575 Bohr^3
68	(H)	Charge:	0.051348	Volume:	48.737 Bohr^3
69	(C)	Charge:	-0.026068	Volume:	74.453 Bohr^3
70	(H)	Charge:	0.072427	Volume:	36.059 Bohr^3
71	(P)	Charge:	1.835897	Volume:	67.641 Bohr^3
72	(C)	Charge:	-0.633068	Volume:	76.303 Bohr^3
73	(C)	Charge:	-0.035116	Volume:	74.202 Bohr^3
74	(H)	Charge:	0.055293	Volume:	41.153 Bohr^3
75	(C)	Charge:	-0.021020	Volume:	83.462 Bohr^3
76	(H)	Charge:	0.053205	Volume:	47.208 Bohr^3
77	(C)	Charge:	-0.020182	Volume:	83.574 Bohr^3
78	(H)	Charge:	0.057706	Volume:	46.901 Bohr^3
79	(C)	Charge:	-0.019600	Volume:	83.831 Bohr^3
80	(H)	Charge:	0.053708	Volume:	47.153 Bohr^3
81	(C)	Charge:	-0.020170	Volume:	77.553 Bohr^3
82	(H)	Charge:	0.056604	Volume:	44.966 Bohr^3
83	(C)	Charge:	-0.612376	Volume:	73.922 Bohr^3
84	(C)	Charge:	-0.035597	Volume:	75.266 Bohr^3
85	(H)	Charge:	0.057387	Volume:	38.770 Bohr^3
86	(C)	Charge:	-0.026899	Volume:	78.770 Bohr^3
87	(H)	Charge:	0.060285	Volume:	45.317 Bohr^3
88	(C)	Charge:	-0.027718	Volume:	82.660 Bohr^3
89	(H)	Charge:	0.054922	Volume:	47.465 Bohr^3
90	(C)	Charge:	-0.029164	Volume:	81.574 Bohr^3
91	(H)	Charge:	0.052476	Volume:	47.536 Bohr^3
92	(C)	Charge:	-0.022831	Volume:	77.453 Bohr^3
93	(H)	Charge:	0.061661	Volume:	45.141 Bohr^3
94	(C)	Charge:	-0.622687	Volume:	76.846 Bohr^3
95	(C)	Charge:	-0.025069	Volume:	75.071 Bohr^3
96	(H)	Charge:	0.045316	Volume:	37.433 Bohr^3
97	(C)	Charge:	-0.017569	Volume:	81.740 Bohr^3
98	(H)	Charge:	0.049649	Volume:	48.128 Bohr^3
99	(C)	Charge:	-0.018935	Volume:	83.371 Bohr^3
100	(H)	Charge:	0.052826	Volume:	47.221 Bohr^3
101	(C)	Charge:	-0.028431	Volume:	83.551 Bohr^3
102	(H)	Charge:	0.053083	Volume:	47.172 Bohr^3
103	(C)	Charge:	-0.032118	Volume:	80.020 Bohr^3
104	(H)	Charge:	0.058011	Volume:	44.018 Bohr^3

$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (7') (square planar form)
(The PPh_3 ligand is bound in the position *cis* to the Au atom.)

ZPE(BP86/def2-SVP) = 0.8388882 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2872.3330021 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2871.44759305621 Hartree (single point)

Cartesian coordinates in Å:

Au	0.37455	0.39444	-0.51087
Pt	-2.00382	1.60558	-0.96392
P	1.86382	-0.94811	0.64413
P	-1.22691	2.31032	1.16684
C	3.20459	-1.49787	-0.47117
C	3.86872	-2.72452	-0.26663
H	3.56208	-3.38930	0.55456
C	4.91470	-3.09988	-1.12277
H	5.42861	-4.06008	-0.96745
C	5.30319	-2.25519	-2.17737
H	6.12280	-2.55529	-2.84708
C	4.64234	-1.03221	-2.38193
H	4.94314	-0.37265	-3.20938
C	3.58975	-0.65440	-1.53434
H	3.05853	0.29848	-1.69096
C	1.01368	-2.46394	1.21596
C	-0.07146	-2.94224	0.45055
H	-0.38477	-2.39142	-0.45089
C	-0.75591	-4.09940	0.84721
H	-1.60273	-4.46632	0.24855
C	-0.36479	-4.78282	2.01253
H	-0.90708	-5.68645	2.32845
C	0.71825	-4.31158	2.77324
H	1.02778	-4.84704	3.68307
C	1.41106	-3.15625	2.37749
H	2.25213	-2.78592	2.98149
C	2.70368	-0.25608	2.10972
C	4.05056	0.15158	2.04432
H	4.62213	0.02374	1.11365
C	4.66361	0.71367	3.17515
H	5.71713	1.02608	3.12318
C	3.94045	0.86806	4.36979
H	4.42798	1.29976	5.25662
C	2.59485	0.46577	4.43124
H	2.02084	0.58261	5.36250
C	1.97265	-0.08829	3.30446
H	0.92191	-0.40103	3.35724
C	-1.31281	1.08919	2.53215
C	-1.17119	1.46708	3.88631
H	-1.04049	2.52575	4.15399
C	-1.21588	0.49336	4.89581
H	-1.10403	0.79415	5.94822
C	-1.40569	-0.86107	4.56566
H	-1.43470	-1.62179	5.35979

C	-1.56733	-1.24038	3.22305
H	-1.71619	-2.29635	2.95516
C	-1.52913	-0.26726	2.21307
H	-1.66268	-0.55458	1.15958
C	0.50468	2.94811	1.10512
C	1.36147	2.93848	2.22080
H	1.01799	2.54091	3.18347
C	2.67818	3.40926	2.09954
H	3.34372	3.37837	2.97338
C	3.14408	3.90552	0.87219
H	4.17848	4.26894	0.78164
C	2.28385	3.94593	-0.23890
H	2.63724	4.34948	-1.19945
C	0.97063	3.46789	-0.12562
H	0.29355	3.48367	-0.99479
C	-2.15500	3.76533	1.80723
C	-1.83744	5.04819	1.31433
H	-0.98162	5.18284	0.63666
C	-2.60700	6.15918	1.69152
H	-2.34814	7.15632	1.30546
C	-3.69816	6.00115	2.56226
H	-4.29894	6.87376	2.85846
C	-4.01657	4.72567	3.05705
H	-4.86684	4.59499	3.74297
C	-3.25219	3.61063	2.68029
H	-3.51245	2.61702	3.07136
C	-4.71444	1.17979	0.58612
H	-4.45162	1.15925	1.65867
C	-3.97067	2.20406	-0.27164
H	-3.96390	3.26815	0.00995
C	-4.10175	1.75692	-1.62012
H	-4.18864	2.44571	-2.47445
C	-4.93736	0.47829	-1.55961
H	-4.89309	-0.18156	-2.44410
C	-6.37518	0.98019	-1.19754
H	-6.71881	1.78269	-1.87924
H	-7.09944	0.14585	-1.28245
C	-6.22160	1.45878	0.28308
H	-6.47997	2.52656	0.42398
H	-6.86405	0.87171	0.96904
C	-4.49900	-0.12690	-0.20927
H	-5.15496	-0.95241	0.13083
H	-3.44248	-0.46498	-0.21152
C	-2.28977	0.13467	-3.82364
H	-3.38935	0.13038	-3.91950
C	-1.70211	1.31794	-3.05919
H	-1.85656	2.32513	-3.48735
C	-0.35272	0.91120	-2.66650
H	0.46842	1.63327	-2.82819
C	-0.20091	-0.51871	-3.23940
H	0.61428	-1.13369	-2.81544
C	-0.09245	-0.32172	-4.78325
H	0.68170	0.42430	-5.05054
H	0.19784	-1.27849	-5.26109
C	-1.53369	0.11096	-5.18740
H	-1.56836	1.09427	-5.69604

H	-2.00167	-0.62741	-5.86852
C	-1.63842	-1.06151	-3.09689
H	-1.79006	-2.02725	-3.61766
H	-1.96429	-1.15211	-2.04007

$[(Ph_3P)AuPt(nbe)_2(PPh_3)]^+$ (7'') (square planar form)
(The PPh_3 ligand is bound in the position *trans* to the Au atom.)

ZPE(BP86/def2-SVP) = 0.8388371 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2872.3185755 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2871.44012536051 Hartree (single point)

Cartesian coordinates in Å:

Au	0.08978	-0.48868	-0.59925
Pt	-1.67522	1.57158	-1.04896
P	1.73187	-1.27996	0.88278
P	-3.36276	3.02503	-1.70119
C	3.41687	-0.91961	0.27317
C	4.53244	-1.63028	0.76389
H	4.39233	-2.44090	1.49485
C	5.81934	-1.30782	0.30843
H	6.68834	-1.86455	0.68939
C	5.99822	-0.28186	-0.63630
H	7.00925	-0.03488	-0.99299
C	4.88768	0.41994	-1.13386
H	5.02530	1.21464	-1.88193
C	3.59724	0.10035	-0.68483
H	2.71991	0.63492	-1.08290
C	1.68224	-3.08153	1.18181
C	1.36027	-3.92863	0.10045
H	1.10239	-3.49179	-0.87768
C	1.36637	-5.31951	0.27589
H	1.11552	-5.97878	-0.56825
C	1.68337	-5.86879	1.53067
H	1.68110	-6.96026	1.66861
C	1.99529	-5.02625	2.61057
H	2.23813	-5.45597	3.59379
C	1.99704	-3.63255	2.44118
H	2.23554	-2.97267	3.28862
C	1.61840	-0.51315	2.53968
C	2.67550	0.23132	3.09635
H	3.62178	0.34022	2.54695
C	2.51470	0.83877	4.35286
H	3.34167	1.42166	4.78466
C	1.30591	0.70476	5.05395
H	1.18429	1.18207	6.03756
C	0.24906	-0.03949	4.49837
H	-0.69879	-0.14732	5.04625
C	0.40021	-0.64313	3.24264
H	-0.42798	-1.22285	2.80452
C	-4.23201	3.89220	-0.32592
C	-3.80621	5.17861	0.07127
H	-3.01984	5.69817	-0.49294
C	-4.38538	5.80482	1.18515
H	-4.04635	6.80926	1.47939
C	-5.39381	5.15658	1.91630
H	-5.84876	5.64942	2.78821

C	-5.82361	3.87830	1.52396
H	-6.61997	3.36651	2.08445
C	-5.24627	3.24714	0.41171
H	-5.60174	2.25115	0.11718
C	-4.69965	2.20173	-2.65525
C	-5.29950	1.04695	-2.10121
H	-4.95447	0.66286	-1.12847
C	-6.29653	0.35787	-2.80499
H	-6.76075	-0.53473	-2.36001
C	-6.68440	0.79410	-4.08386
H	-7.46010	0.24829	-4.64103
C	-6.06622	1.91746	-4.65385
H	-6.35204	2.25320	-5.66177
C	-5.07767	2.62109	-3.94526
H	-4.59574	3.49317	-4.40819
C	-2.76570	4.40068	-2.75003
C	-1.42294	4.42310	-3.17254
H	-0.75322	3.60996	-2.86043
C	-0.95132	5.47530	-3.97274
H	0.09994	5.48671	-4.29644
C	-1.81956	6.51053	-4.35415
H	-1.45059	7.33628	-4.98062
C	-3.16063	6.49691	-3.93001
H	-3.84039	7.31101	-4.22228
C	-3.63529	5.44922	-3.12823
H	-4.68059	5.45155	-2.78451
C	-0.08718	-0.48087	-3.58959
H	0.90721	-0.91768	-3.38195
C	-1.11101	-0.53016	-2.43184
H	-1.51797	-1.52601	-2.15551
C	-2.12989	0.47497	-2.79174
H	-3.18316	0.15115	-2.75216
C	-1.66154	1.05898	-4.12980
H	-2.10995	2.03040	-4.40638
C	-1.89722	-0.06553	-5.17887
H	-2.93403	-0.45264	-5.13517
H	-1.73495	0.32618	-6.20287
C	-0.82277	-1.13186	-4.80151
H	-1.25661	-2.11755	-4.54150
H	-0.10490	-1.29966	-5.62904
C	-0.12475	1.01180	-3.97400
H	0.41873	1.23393	-4.91348
H	0.25659	1.66661	-3.16321
C	-0.43903	4.17769	0.33818
H	-0.87556	5.01552	-0.23385
C	-1.36238	2.99438	0.62157
H	-2.32938	3.14875	1.12204
C	-0.52127	1.89420	0.91385
H	-0.80332	1.12004	1.64296
C	0.90890	2.43125	0.85064
H	1.71550	1.68471	0.76052
C	1.03059	3.35041	2.10925
H	0.72096	2.82150	3.03090
H	2.08472	3.66204	2.24975
C	0.11357	4.56260	1.74967
H	-0.70306	4.72381	2.48039

H	0.69173	5.50606	1.68745
C	0.79683	3.47998	-0.27244
H	1.68001	4.14506	-0.34113
H	0.59550	3.02045	-1.26173

$[(Ph_3P)AuPt(CO)_3]^+$ (8) (square planar form)

ZPE(BP86/def2-SVP) = 0.2916213 Hartree (optimized geometry)
E(BP86/def2-SVP) = −1630.9783626 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −1630.43512057231 Hartree (single point)

Cartesian coordinates in Å:

C	-1.80817	2.23661	-0.50957
C	-0.07020	4.82500	-0.01907
C	1.79328	2.34017	0.51929
O	-2.88033	1.95318	-0.81542
O	-0.10139	5.96945	-0.02932
O	2.87115	2.08856	0.82733
Au	-0.02505	0.13916	0.00395
Pt	-0.02287	2.83690	-0.00094
P	0.01035	-2.18073	0.00283
C	1.69818	-2.82239	-0.23115
C	2.17413	-3.90613	0.53398
H	1.54029	-4.35507	1.31277
C	3.46417	-4.40650	0.29525
H	3.83897	-5.25104	0.89207
C	4.27241	-3.83198	-0.69933
H	5.28299	-4.22684	-0.88083
C	3.79600	-2.74963	-1.46093
H	4.43093	-2.29858	-2.23765
C	2.51198	-2.23954	-1.22692
H	2.13656	-1.39025	-1.82010
C	-0.61399	-2.87014	1.56745
C	-0.18764	-2.29087	2.78229
H	0.47721	-1.41239	2.77213
C	-0.61078	-2.84036	4.00002
H	-0.27883	-2.39156	4.94775
C	-1.46378	-3.95873	4.00825
H	-1.79950	-4.38455	4.96537
C	-1.89294	-4.52959	2.79878
H	-2.56276	-5.40201	2.80668
C	-1.47050	-3.98966	1.57351
H	-1.80590	-4.43550	0.62561
C	-1.01566	-2.86889	-1.33445
C	-0.56673	-3.96441	-2.09937
H	0.43179	-4.39091	-1.92333
C	-1.40344	-4.50544	-3.08858
H	-1.05513	-5.35918	-3.68832
C	-2.67799	-3.95940	-3.31244
H	-3.32849	-4.38581	-4.09035
C	-3.12339	-2.86511	-2.54927
H	-4.12019	-2.43582	-2.72795
C	-2.29382	-2.31474	-1.56308
H	-2.63911	-1.45539	-0.96643

$[(Ph_3P)AuPt(CO)_3]^+$ (8') (trigonal pyramidal form)
(Note that this structure has an imaginary frequency of −8.4 cm^{-1}, which could not be eliminated even after several attempts.)

ZPE(BP86/def2-SVP) = 0.2907341 Hartree (optimized geometry)
E(BP86/def2-SVP) = −1630.9609423 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −1630.41209083565 Hartree (single point)

Cartesian coordinates in Å:

C	-0.69669	0.29000	-1.93489
C	-1.61931	-0.15241	1.32427
C	1.62064	-0.68044	0.38418
O	-0.97853	0.51536	-3.02702
O	-2.43900	-0.18411	2.13045
O	2.68798	-1.02021	0.64550
Au	-0.78673	-2.72240	-0.58820
Pt	-0.22253	-0.14189	-0.06907
P	-1.25625	-4.90117	-1.03935
C	-1.52213	-5.83497	0.49346
C	-2.60023	-6.73777	0.60436
H	-3.31592	-6.85218	-0.22269
C	-2.74835	-7.49148	1.77917
H	-3.58688	-8.19737	1.87003
C	-1.83173	-7.34459	2.83337
H	-1.95528	-7.93530	3.75309
C	-0.75918	-6.44071	2.72095
H	-0.04552	-6.32422	3.54961
C	-0.60256	-5.68083	1.55476
H	0.23218	-4.96782	1.46504
C	-2.75495	-5.03877	-2.05312
C	-3.90329	-4.30841	-1.67396
H	-3.86814	-3.63303	-0.80455
C	-5.08638	-4.44925	-2.41030
H	-5.98292	-3.88308	-2.11829
C	-5.12389	-5.30739	-3.52484
H	-6.05296	-5.41086	-4.10469
C	-3.97902	-6.02765	-3.90353
H	-4.01026	-6.69655	-4.77607
C	-2.78842	-5.89752	-3.17153
H	-1.89148	-6.46183	-3.46537
C	0.11294	-5.67478	-1.94463
C	0.58990	-6.94907	-1.57320
H	0.16280	-7.47011	-0.70405
C	1.61254	-7.54712	-2.32612
H	1.98738	-8.54101	-2.04088
C	2.15490	-6.88020	-3.43696
H	2.95852	-7.35262	-4.02101
C	1.67909	-5.60754	-3.80301
H	2.10844	-5.08545	-4.67058
C	0.66148	-4.99895	-3.05749
H	0.29061	-4.00013	-3.33697

$[(Ph_3P)AuPt(PF_3)_3]^+$ (9) (square planar form)

ZPE(BP86/def2-SVP) = 0.2992929 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3213.3195364 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3212.93169192826 Hartree (single point)

Cartesian coordinates in Å:

P	0.52373	1.84810	0.14406
P	3.33241	4.10567	0.90757
P	4.64711	0.74165	0.94479
F	-0.43182	1.03245	1.12972
F	-0.25841	3.23765	0.16805
F	0.03455	1.32910	-1.28109
F	3.78808	4.53800	2.36972
F	2.27756	5.25414	0.59034
F	4.56944	4.62305	0.04914
F	5.91423	1.58786	1.42092
F	4.68356	-0.37555	2.08351
F	5.31792	-0.02442	-0.28044
Au	2.14844	-0.65956	0.12871
Pt	2.74412	1.91978	0.60344
P	1.53981	-2.83527	-0.39708
C	1.55241	-3.92654	1.05593
C	0.54206	-4.89162	1.24349
H	-0.29305	-4.96449	0.53105
C	0.60963	-5.75504	2.34829
H	-0.17738	-6.50848	2.49938
C	1.67568	-5.65620	3.25778
H	1.72222	-6.33355	4.12335
C	2.67997	-4.68942	3.07064
H	3.51012	-4.60908	3.78770
C	2.62005	-3.81973	1.97347
H	3.39944	-3.05489	1.82921
C	-0.14208	-2.85548	-1.09125
C	-1.14827	-2.11090	-0.43713
H	-0.90547	-1.51688	0.45758
C	-2.45841	-2.13026	-0.93302
H	-3.24411	-1.55242	-0.42437
C	-2.76462	-2.88071	-2.08270
H	-3.79271	-2.88857	-2.47390
C	-1.76104	-3.61467	-2.73601
H	-2.00137	-4.19816	-3.63687
C	-0.44570	-3.60621	-2.24446
H	0.34253	-4.17772	-2.75630
C	2.65780	-3.55343	-1.63766
C	3.05586	-4.90334	-1.55912
H	2.72263	-5.53101	-0.71941
C	3.88392	-5.43743	-2.55910
H	4.19845	-6.48979	-2.50059
C	4.31100	-4.63199	-3.62791
H	4.96239	-5.05505	-4.40689

C	3.91530	-3.28429	-3.70219
H	4.25553	-2.65337	-4.53642
C	3.09252	-2.74027	-2.70686
H	2.78575	-1.68299	-2.75497

$[(Ph_3P)AuPt(PF_3)_3]^+$ (9') (trigonal pyramidal form)

ZPE(BP86/def2-SVP) = 0.2983926 Hartree (optimized geometry)
E(BP86/def2-SVP) = −3213.3094985 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −3212.91163797098 Hartree (single point)

Cartesian coordinates in Å:

P	-2.31561	-0.35128	0.91883
P	-0.22690	0.04371	-2.38182
P	1.61173	-0.70524	1.01067
F	-2.46621	-1.34968	2.16411
F	-2.93473	0.97513	1.55189
F	-3.57088	-0.86603	0.06747
F	-0.03367	1.51136	-2.97498
F	-1.48963	-0.43802	-3.24681
F	0.90764	-0.74292	-3.19180
F	2.48320	0.49480	1.59553
F	1.50179	-1.63686	2.30660
F	2.74455	-1.52752	0.23427
Au	-0.62377	-2.79796	-0.60636
Pt	-0.29238	-0.20189	-0.11994
P	-1.15669	-4.95168	-1.10132
C	0.06140	-6.11870	-0.44028
C	-0.34834	-7.25013	0.29520
H	-1.41430	-7.41827	0.50731
C	0.61833	-8.16146	0.74843
H	0.30491	-9.04741	1.31988
C	1.97855	-7.94310	0.47425
H	2.73157	-8.65950	0.83461
C	2.38397	-6.80917	-0.25418
H	3.45025	-6.63818	-0.46238
C	1.42969	-5.89149	-0.71041
H	1.74286	-4.99898	-1.27497
C	-2.77984	-5.34038	-0.39182
C	-3.07246	-4.91404	0.92271
H	-2.34406	-4.30973	1.48589
C	-4.30138	-5.25600	1.50147
H	-4.53440	-4.92474	2.52397
C	-5.23714	-6.01181	0.77185
H	-6.20361	-6.27336	1.22753
C	-4.94709	-6.42618	-0.53881
H	-5.68296	-7.01200	-1.10890
C	-3.71873	-6.09147	-1.12933
H	-3.49015	-6.41113	-2.15668
C	-1.24180	-5.16899	-2.89937
C	-0.78503	-6.36360	-3.49521
H	-0.32666	-7.15142	-2.87943
C	-0.92175	-6.53619	-4.88129
H	-0.56822	-7.46565	-5.35122
C	-1.50319	-5.52549	-5.66509
H	-1.60256	-5.66438	-6.75180
C	-1.95067	-4.33266	-5.06832

H	-2.39657	-3.53869	-5.68499
C	-1.82005	-4.14821	-3.68594
H	-2.15536	-3.20927	-3.21860

$AuPt^+$ (10)

ZPE(BP86/def2-SVP) = 0.0003119 Hartree (optimized geometry)
E(BP86/def2-SVP) = −255.0000882 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −254.70008303611 Hartree (single point)

Cartesian coordinates in Å:

```
Au        -1.19121       -1.40815       -0.01843
Pt         1.45687       -1.40815       -0.01843
```

MULLIKEN Charges:

```
atom      charge    n(s)      n(p)      n(d)      n(f)      n(g)
     1au     0.60241   2.45961   6.02225   9.91027   0.00538   0.00009
     2pt     0.39759   2.36265   6.08329   9.14942   0.00691   0.00014
```

NPA Charges:

```
atom          charge    n(s)      n(p)      n(d)      n(f)      n(g)
  1 au         0.47910   2.55763   6.00928   9.95313   0.00083   0.00003
  2 pt         0.52090   2.28217   6.01535   9.18045   0.00111   0.00003
```

QTAIM Charges:

```
1 (Au)    Charge:    0.423112     Volume:   247.824 Bohr^3
2 (Pt)    Charge:    0.576888     Volume:   239.864 Bohr^3
```

[(Ph$_3$P)Au]$^+$ (11)

ZPE(BP86/def2-SVP) = 0.2684934 Hartree (optimized geometry)
E(BP86/def2-SVP) = −1171.5601041 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −1171.19035677378 Hartree (single point)

Cartesian coordinates in Å:

Au	0.53210	0.40205	0.03283
P	2.15571	1.69714	0.94211
C	2.80525	0.89441	2.42627
C	4.19939	0.77774	2.61413
H	4.89779	1.13018	1.84157
C	4.68481	0.21255	3.80342
H	5.76985	0.12000	3.95698
C	3.79081	-0.23388	4.79043
H	4.17811	-0.68113	5.71779
C	2.40122	-0.11871	4.59709
H	1.70401	-0.47445	5.36954
C	1.90231	0.44120	3.41495
H	0.81546	0.52512	3.25752
C	3.49115	1.91964	-0.25635
C	4.03907	0.78436	-0.89587
H	3.61928	-0.21678	-0.70997
C	5.12019	0.94301	-1.77104
H	5.55004	0.06400	-2.27297
C	5.64779	2.22527	-2.01389
H	6.49281	2.34586	-2.70775
C	5.09705	3.35165	-1.38093
H	5.51069	4.35224	-1.57377
C	4.01432	3.20791	-0.49975
H	3.58385	4.08824	-0.00115
C	1.46597	3.30959	1.38179
C	1.72390	3.86527	2.65349
H	2.30278	3.30374	3.40079
C	1.23876	5.14807	2.95093
H	1.43748	5.58784	3.93917
C	0.50272	5.86518	1.99350
H	0.12071	6.86798	2.23541
C	0.24485	5.30537	0.72796
H	-0.33681	5.86726	-0.01721
C	0.72088	4.02596	0.41760
H	0.51407	3.58231	-0.56907

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	0.37712	2.92838	6.02317	9.66606	0.00501	0.00027
2p	-0.03917	5.55300	8.94867	0.49203	0.04547	
3c	0.09622	3.14383	2.61663	0.13538	0.00795	
4c	-0.11536	3.17116	2.82850	0.10839	0.00731	
5h	0.14592	0.81191	0.04030	0.00187		

6c	-0.13612	3.18555	2.83399	0.10938	0.00719
7h	0.15297	0.81005	0.03520	0.00178	
8c	-0.08266	3.17155	2.79378	0.11019	0.00714
9h	0.15592	0.80759	0.03474	0.00176	
10c	-0.12823	3.18192	2.83002	0.10912	0.00717
11h	0.15340	0.80955	0.03528	0.00178	
12c	-0.15629	3.19046	2.84784	0.11060	0.00739
13h	0.13497	0.82480	0.03839	0.00185	
14c	0.09838	3.14162	2.61681	0.13525	0.00794
15c	-0.15807	3.19097	2.84929	0.11042	0.00739
16h	0.13515	0.82460	0.03841	0.00185	
17c	-0.12858	3.18217	2.83024	0.10899	0.00717
18h	0.15361	0.80935	0.03526	0.00178	
19c	-0.08244	3.17174	2.79346	0.11009	0.00714
20h	0.15583	0.80766	0.03475	0.00176	
21c	-0.13611	3.18517	2.83452	0.10923	0.00719
22h	0.15316	0.80985	0.03520	0.00178	
23c	-0.11670	3.17198	2.82899	0.10841	0.00732
24h	0.14673	0.81121	0.04019	0.00187	
25c	0.09709	3.14160	2.61839	0.13498	0.00794
26c	-0.11681	3.17226	2.82917	0.10806	0.00731
27h	0.14655	0.81132	0.04026	0.00187	
28c	-0.13646	3.18549	2.83462	0.10915	0.00719
29h	0.15327	0.80975	0.03519	0.00178	
30c	-0.08382	3.17243	2.79422	0.11001	0.00715
31h	0.15612	0.80742	0.03470	0.00175	
32c	-0.12682	3.18066	2.83022	0.10877	0.00716
33h	0.15351	0.80939	0.03532	0.00178	
34c	-0.15680	3.19151	2.84758	0.11031	0.00739
35h	0.13451	0.82513	0.03851	0.00185	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.29274	2.90798	5.99551	9.80290	0.00075	0.00012
2 p	1.19035	5.13409	8.62462	0.04912	0.00182	0.00000
3 c	-0.42278	3.00891	3.40299	0.00815	0.00273	0.00000
4 c	-0.18326	2.98608	3.18972	0.00532	0.00213	0.00000
5 h	0.24204	0.75711	0.00077	0.00008	0.00000	0.00000
6 c	-0.19912	2.99490	3.19703	0.00517	0.00202	0.00000
7 h	0.24073	0.75859	0.00059	0.00008	0.00000	0.00000
8 c	-0.16638	3.00177	3.15737	0.00523	0.00201	0.00000
9 h	0.24018	0.75915	0.00058	0.00008	0.00000	0.00000
10 c	-0.19922	2.99495	3.19706	0.00518	0.00203	0.00000
11 h	0.24082	0.75851	0.00059	0.00008	0.00000	0.00000
12 c	-0.18784	2.98222	3.19817	0.00529	0.00217	0.00000
13 h	0.23375	0.76551	0.00066	0.00008	0.00000	0.00000
14 c	-0.42268	3.00888	3.40291	0.00816	0.00273	0.00000
15 c	-0.18784	2.98223	3.19815	0.00529	0.00217	0.00000
16 h	0.23371	0.76555	0.00066	0.00008	0.00000	0.00000
17 c	-0.19923	2.99496	3.19707	0.00518	0.00203	0.00000
18 h	0.24082	0.75851	0.00059	0.00008	0.00000	0.00000
19 c	-0.16638	3.00177	3.15738	0.00523	0.00201	0.00000
20 h	0.24019	0.75915	0.00058	0.00008	0.00000	0.00000

21 c	-0.19909	2.99490	3.19700	0.00517	0.00202	0.00000
22 h	0.24074	0.75859	0.00059	0.00008	0.00000	0.00000
23 c	-0.18331	2.98609	3.18977	0.00532	0.00213	0.00000
24 h	0.24205	0.75709	0.00077	0.00008	0.00000	0.00000
25 c	-0.42269	3.00888	3.40292	0.00816	0.00273	0.00000
26 c	-0.18336	2.98610	3.18981	0.00532	0.00213	0.00000
27 h	0.24206	0.75708	0.00077	0.00008	0.00000	0.00000
28 c	-0.19915	2.99490	3.19707	0.00517	0.00202	0.00000
29 h	0.24074	0.75858	0.00059	0.00008	0.00000	0.00000
30 c	-0.16642	3.00177	3.15741	0.00523	0.00201	0.00000
31 h	0.24019	0.75915	0.00058	0.00008	0.00000	0.00000
32 c	-0.19911	2.99495	3.19696	0.00518	0.00203	0.00000
33 h	0.24080	0.75853	0.00059	0.00008	0.00000	0.00000
34 c	-0.18776	2.98222	3.19808	0.00529	0.00217	0.00000
35 h	0.23373	0.76553	0.00066	0.00008	0.00000	0.00000

QTAIM Charges:

1 (Au)	Charge:	0.019943	Volume:	258.463	Bohr^3
2 (P)	Charge:	2.150701	Volume:	61.448	Bohr^3
3 (C)	Charge:	-0.692219	Volume:	81.986	Bohr^3
4 (C)	Charge:	-0.013231	Volume:	81.221	Bohr^3
5 (H)	Charge:	0.074079	Volume:	44.018	Bohr^3
6 (C)	Charge:	-0.007230	Volume:	82.538	Bohr^3
7 (H)	Charge:	0.073192	Volume:	45.886	Bohr^3
8 (C)	Charge:	-0.007698	Volume:	81.915	Bohr^3
9 (H)	Charge:	0.076610	Volume:	45.673	Bohr^3
10 (C)	Charge:	-0.007623	Volume:	82.550	Bohr^3
11 (H)	Charge:	0.073363	Volume:	45.885	Bohr^3
12 (C)	Charge:	-0.016198	Volume:	80.034	Bohr^3
13 (H)	Charge:	0.056594	Volume:	47.252	Bohr^3
14 (C)	Charge:	-0.692315	Volume:	81.985	Bohr^3
15 (C)	Charge:	-0.017065	Volume:	80.050	Bohr^3
16 (H)	Charge:	0.057292	Volume:	47.249	Bohr^3
17 (C)	Charge:	-0.007592	Volume:	82.544	Bohr^3
18 (H)	Charge:	0.073567	Volume:	45.879	Bohr^3
19 (C)	Charge:	-0.007066	Volume:	81.912	Bohr^3
20 (H)	Charge:	0.076248	Volume:	45.672	Bohr^3
21 (C)	Charge:	-0.007249	Volume:	82.549	Bohr^3
22 (H)	Charge:	0.073300	Volume:	45.876	Bohr^3
23 (C)	Charge:	-0.013670	Volume:	81.226	Bohr^3
24 (H)	Charge:	0.074240	Volume:	44.039	Bohr^3
25 (C)	Charge:	-0.692378	Volume:	81.952	Bohr^3
26 (C)	Charge:	-0.013520	Volume:	81.240	Bohr^3
27 (H)	Charge:	0.074338	Volume:	44.032	Bohr^3
28 (C)	Charge:	-0.007406	Volume:	82.537	Bohr^3
29 (H)	Charge:	0.073298	Volume:	45.889	Bohr^3
30 (C)	Charge:	-0.007595	Volume:	81.934	Bohr^3
31 (H)	Charge:	0.076594	Volume:	45.664	Bohr^3
32 (C)	Charge:	-0.007436	Volume:	82.533	Bohr^3
33 (H)	Charge:	0.073733	Volume:	45.878	Bohr^3
34 (C)	Charge:	-0.016699	Volume:	80.054	Bohr^3
35 (H)	Charge:	0.057099	Volume:	47.269	Bohr^3

[(Cy$_3$P)Au]$^+$ (12)

ZPE(BP86/def2-SVP) = 0.4709260 Hartree (optimized geometry)
E(BP86/def2-SVP) = −1182.4419203 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −1182.07622201866 Hartree (single point)

Cartesian coordinates in Å:

Au	0.78447	-1.21841	-2.06398
P	1.12453	-2.66712	-3.78201
C	1.11085	-4.39625	-3.12256
H	0.02348	-4.60534	-3.01915
C	1.70162	-5.38372	-4.15692
H	1.22276	-5.25558	-5.15069
H	2.78368	-5.16893	-4.29102
C	1.52931	-6.83000	-3.66118
H	0.44482	-7.07556	-3.62793
H	1.98470	-7.52311	-4.39762
C	2.14776	-7.02559	-2.27081
H	3.25033	-6.88957	-2.33618
H	1.98385	-8.06527	-1.92260
C	1.57088	-6.02848	-1.25534
H	2.05367	-6.15305	-0.26505
H	0.48814	-6.23566	-1.10389
C	1.74274	-4.57594	-1.72742
H	2.82234	-4.32145	-1.76094
H	1.27344	-3.87186	-1.00735
C	2.74892	-2.27276	-4.57935
H	2.84655	-3.07441	-5.34921
C	3.92189	-2.38682	-3.58479
H	3.95353	-3.39774	-3.13286
H	3.74997	-1.67052	-2.74950
C	5.26381	-2.07495	-4.26653
H	6.07545	-2.13007	-3.51314
H	5.48156	-2.86559	-5.01842
C	5.24545	-0.70438	-4.95370
H	5.13494	0.09345	-4.18585
H	6.21201	-0.51530	-5.46247
C	4.08882	-0.61178	-5.95618
H	4.25284	-1.33916	-6.78189
H	4.05205	0.39107	-6.42786
C	2.73328	-0.90485	-5.29190
H	1.92889	-0.86848	-6.05318
H	2.50646	-0.11294	-4.54257
C	-0.22632	-2.47083	-5.05049
H	0.30221	-2.67950	-6.01059
C	-0.77381	-1.02493	-5.09198
H	-1.25198	-0.81075	-4.10926
H	0.04691	-0.29038	-5.20710
C	-1.80982	-0.85943	-6.21370
H	-2.19584	0.18000	-6.20298
H	-1.30906	-0.99615	-7.19789
C	-2.95497	-1.86945	-6.06873

H	-3.67128	-1.76565	-6.90846
H	-3.52685	-1.64581	-5.14086
C	-2.41958	-3.30514	-6.00329
H	-1.95160	-3.57269	-6.97669
H	-3.24578	-4.02804	-5.84704
C	-1.37645	-3.48463	-4.88575
H	-1.85995	-3.32915	-3.89542
H	-0.99573	-4.52500	-4.90228

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1au	0.37855	2.92242	6.01867	9.67466	0.00544	0.00026
2p	-0.22745	5.66203	9.07845	0.44328	0.04369	
3c	0.10340	3.04406	2.71528	0.13132	0.00595	
4h	0.10832	0.84501	0.04438	0.00229		
5c	-0.22079	3.19810	2.90629	0.11092	0.00548	
6h	0.11194	0.84790	0.03831	0.00185		
7h	0.09611	0.86364	0.03835	0.00190		
8c	-0.16059	3.17457	2.87458	0.10611	0.00532	
9h	0.08257	0.87797	0.03760	0.00187		
10h	0.10390	0.85699	0.03728	0.00183		
11c	-0.12892	3.14921	2.86868	0.10573	0.00530	
12h	0.07538	0.88540	0.03736	0.00186		
13h	0.10260	0.85818	0.03738	0.00184		
14c	-0.15493	3.16865	2.87554	0.10545	0.00528	
15h	0.10172	0.85904	0.03741	0.00184		
16h	0.08243	0.87821	0.03749	0.00187		
17c	-0.18537	3.17262	2.89343	0.11378	0.00554	
18h	0.09619	0.86194	0.03998	0.00189		
19h	0.08221	0.87525	0.04059	0.00195		
20c	0.06503	3.03926	2.75545	0.13437	0.00590	
21h	0.11569	0.84007	0.04204	0.00220		
22c	-0.19728	3.17522	2.90313	0.11340	0.00553	
23h	0.09429	0.86131	0.04250	0.00190		
24h	0.08944	0.87078	0.03788	0.00190		
25c	-0.15342	3.16975	2.87271	0.10566	0.00531	
26h	0.10134	0.85955	0.03728	0.00183		
27h	0.08220	0.87871	0.03723	0.00186		
28c	-0.12844	3.14712	2.86994	0.10605	0.00532	
29h	0.07377	0.88712	0.03725	0.00186		
30h	0.10275	0.85815	0.03726	0.00183		
31c	-0.15757	3.17303	2.87322	0.10601	0.00531	
32h	0.08224	0.87866	0.03724	0.00186		
33h	0.10232	0.85848	0.03737	0.00184		
34c	-0.19014	3.18147	2.89222	0.11095	0.00550	
35h	0.09728	0.85951	0.04126	0.00195		
36h	0.09192	0.86878	0.03742	0.00189		
37c	0.12560	3.01917	2.71701	0.13226	0.00596	
38h	0.10719	0.84943	0.04121	0.00217		
39c	-0.22700	3.20154	2.90714	0.11276	0.00555	
40h	0.08275	0.87560	0.03965	0.00199		
41h	0.11526	0.84301	0.03985	0.00189		
42c	-0.15264	3.17068	2.87132	0.10533	0.00530	

43h	0.10207	0.85871	0.03740	0.00183	
44h	0.07893	0.88147	0.03774	0.00187	
45c	-0.13003	3.14844	2.87002	0.10625	0.00531
46h	0.10266	0.85816	0.03734	0.00183	
47h	0.07478	0.88593	0.03743	0.00187	
48c	-0.15827	3.17203	2.87527	0.10566	0.00531
49h	0.08063	0.88007	0.03744	0.00186	
50h	0.10152	0.85939	0.03726	0.00184	
51c	-0.21548	3.19161	2.90590	0.11246	0.00551
52h	0.09731	0.86367	0.03716	0.00186	
53h	0.09605	0.86144	0.04060	0.00192	

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 au	0.30067	2.88515	5.99618	9.81699	0.00090	0.00011
2 p	1.20846	5.18615	8.56581	0.03772	0.00185	0.00000
3 c	-0.54928	3.08491	3.45292	0.01032	0.00113	0.00000
4 h	0.25493	0.74337	0.00150	0.00021	0.00000	0.00000
5 c	-0.42003	3.05684	3.35570	0.00648	0.00101	0.00000
6 h	0.21832	0.78076	0.00077	0.00015	0.00000	0.00000
7 h	0.21102	0.78791	0.00093	0.00015	0.00000	0.00000
8 c	-0.40321	3.05878	3.33722	0.00626	0.00096	0.00000
9 h	0.20586	0.79325	0.00076	0.00014	0.00000	0.00000
10 h	0.23226	0.76697	0.00062	0.00015	0.00000	0.00000
11 c	-0.41001	3.06061	3.34209	0.00633	0.00098	0.00000
12 h	0.20424	0.79491	0.00070	0.00015	0.00000	0.00000
13 h	0.23291	0.76631	0.00063	0.00015	0.00000	0.00000
14 c	-0.40531	3.05905	3.33907	0.00623	0.00096	0.00000
15 h	0.23204	0.76718	0.00063	0.00015	0.00000	0.00000
16 h	0.20580	0.79332	0.00073	0.00014	0.00000	0.00000
17 c	-0.40954	3.05352	3.34848	0.00653	0.00102	0.00000
18 h	0.21019	0.78879	0.00087	0.00016	0.00000	0.00000
19 h	0.22115	0.77802	0.00068	0.00015	0.00000	0.00000
20 c	-0.54388	3.08573	3.44590	0.01111	0.00114	0.00000
21 h	0.24877	0.74948	0.00154	0.00020	0.00000	0.00000
22 c	-0.41697	3.05365	3.35580	0.00647	0.00104	0.00000
23 h	0.21860	0.78040	0.00084	0.00016	0.00000	0.00000
24 h	0.21108	0.78802	0.00076	0.00015	0.00000	0.00000
25 c	-0.40444	3.05791	3.33933	0.00623	0.00096	0.00000
26 h	0.23112	0.76811	0.00062	0.00015	0.00000	0.00000
27 h	0.20629	0.79283	0.00073	0.00014	0.00000	0.00000
28 c	-0.40973	3.05971	3.34268	0.00636	0.00098	0.00000
29 h	0.20375	0.79542	0.00069	0.00015	0.00000	0.00000
30 h	0.23204	0.76718	0.00062	0.00015	0.00000	0.00000
31 c	-0.40367	3.05802	3.33846	0.00622	0.00096	0.00000
32 h	0.20674	0.79239	0.00073	0.00014	0.00000	0.00000
33 h	0.23122	0.76801	0.00063	0.00015	0.00000	0.00000
34 c	-0.41604	3.05397	3.35462	0.00641	0.00103	0.00000
35 h	0.22017	0.77887	0.00081	0.00015	0.00000	0.00000
36 h	0.21035	0.78873	0.00078	0.00014	0.00000	0.00000
37 c	-0.53958	3.08577	3.44243	0.01026	0.00112	0.00000
38 h	0.24574	0.75255	0.00151	0.00020	0.00000	0.00000

39 c	-0.41373	3.05660	3.34953	0.00655	0.00104	0.00000
40 h	0.20930	0.78974	0.00082	0.00014	0.00000	0.00000
41 h	0.22602	0.77304	0.00078	0.00016	0.00000	0.00000
42 c	-0.40742	3.05788	3.34234	0.00624	0.00097	0.00000
43 h	0.23168	0.76755	0.00062	0.00015	0.00000	0.00000
44 h	0.20618	0.79294	0.00074	0.00014	0.00000	0.00000
45 c	-0.40976	3.05983	3.34258	0.00637	0.00098	0.00000
46 h	0.23201	0.76721	0.00062	0.00015	0.00000	0.00000
47 h	0.20456	0.79461	0.00069	0.00015	0.00000	0.00000
48 c	-0.40225	3.05840	3.33667	0.00622	0.00096	0.00000
49 h	0.20605	0.79308	0.00073	0.00014	0.00000	0.00000
50 h	0.23172	0.76751	0.00063	0.00015	0.00000	0.00000
51 c	-0.41635	3.05435	3.35453	0.00644	0.00102	0.00000
52 h	0.21095	0.78815	0.00076	0.00014	0.00000	0.00000
53 h	0.21904	0.77998	0.00082	0.00015	0.00000	0.00000

QTAIM Charges:

1 (Au)	Charge:	0.006347	Volume:	249.809 Bohr^3
2 (P)	Charge:	1.663968	Volume:	69.141 Bohr^3
3 (C)	Charge:	-0.509771	Volume:	58.692 Bohr^3
4 (H)	Charge:	0.042596	Volume:	41.562 Bohr^3
5 (C)	Charge:	0.023215	Volume:	55.962 Bohr^3
6 (H)	Charge:	0.001403	Volume:	47.781 Bohr^3
7 (H)	Charge:	0.004379	Volume:	45.977 Bohr^3
8 (C)	Charge:	0.032424	Volume:	58.463 Bohr^3
9 (H)	Charge:	0.000670	Volume:	49.576 Bohr^3
10 (H)	Charge:	0.022417	Volume:	47.889 Bohr^3
11 (C)	Charge:	0.032664	Volume:	58.556 Bohr^3
12 (H)	Charge:	-0.002545	Volume:	49.626 Bohr^3
13 (H)	Charge:	0.022401	Volume:	47.860 Bohr^3
14 (C)	Charge:	0.032637	Volume:	58.436 Bohr^3
15 (H)	Charge:	0.022016	Volume:	47.920 Bohr^3
16 (H)	Charge:	-0.000710	Volume:	49.321 Bohr^3
17 (C)	Charge:	0.032698	Volume:	56.631 Bohr^3
18 (H)	Charge:	0.003799	Volume:	45.083 Bohr^3
19 (H)	Charge:	0.003745	Volume:	46.826 Bohr^3
20 (C)	Charge:	-0.504382	Volume:	58.593 Bohr^3
21 (H)	Charge:	0.036903	Volume:	44.896 Bohr^3
22 (C)	Charge:	0.026197	Volume:	56.383 Bohr^3
23 (H)	Charge:	0.004187	Volume:	43.430 Bohr^3
24 (H)	Charge:	0.001122	Volume:	48.395 Bohr^3
25 (C)	Charge:	0.031774	Volume:	58.457 Bohr^3
26 (H)	Charge:	0.021369	Volume:	47.964 Bohr^3
27 (H)	Charge:	-0.000483	Volume:	49.439 Bohr^3
28 (C)	Charge:	0.035052	Volume:	58.540 Bohr^3
29 (H)	Charge:	-0.003174	Volume:	49.696 Bohr^3
30 (H)	Charge:	0.021381	Volume:	47.927 Bohr^3
31 (C)	Charge:	0.034068	Volume:	58.432 Bohr^3
32 (H)	Charge:	0.000642	Volume:	49.320 Bohr^3
33 (H)	Charge:	0.021078	Volume:	47.951 Bohr^3
34 (C)	Charge:	0.027016	Volume:	55.749 Bohr^3
35 (H)	Charge:	0.005857	Volume:	44.376 Bohr^3

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36 (H )    Charge:   -0.000277     Volume:    48.721 Bohr^3
37 (C )    Charge:   -0.459265     Volume:    58.672 Bohr^3
38 (H )    Charge:    0.033736     Volume:    45.915 Bohr^3
39 (C )    Charge:    0.026392     Volume:    55.626 Bohr^3
40 (H )    Charge:   -0.000728     Volume:    47.205 Bohr^3
41 (H )    Charge:    0.010163     Volume:    44.543 Bohr^3
42 (C )    Charge:    0.032331     Volume:    58.511 Bohr^3
43 (H )    Charge:    0.021402     Volume:    47.948 Bohr^3
44 (H )    Charge:   -0.000317     Volume:    49.512 Bohr^3
45 (C )    Charge:    0.033818     Volume:    58.558 Bohr^3
46 (H )    Charge:    0.021583     Volume:    47.924 Bohr^3
47 (H )    Charge:   -0.002725     Volume:    49.561 Bohr^3
48 (C )    Charge:    0.034112     Volume:    58.392 Bohr^3
49 (H )    Charge:   -0.000281     Volume:    49.329 Bohr^3
50 (H )    Charge:    0.021008     Volume:    47.916 Bohr^3
51 (C )    Charge:    0.028610     Volume:    55.580 Bohr^3
52 (H )    Charge:    0.001738     Volume:    49.481 Bohr^3
53 (H )    Charge:    0.005742     Volume:    44.587 Bohr^3
```

[Pt(PCy$_3$)$_2$] (13)

ZPE(BP86/def2-SVP) = 0.9393237 Hartree (optimized geometry)
E(BP86/def2-SVP) = −2213.0814383 Hartree (optimized geometry)
E(PBE0/def2-TZVPP) = −2212.49281546489 Hartree (single point)

Cartesian coordinates in Å:

Pt	11.90832	6.29346	7.18960
P	12.87146	8.09996	6.21373
P	10.40525	4.84784	8.08086
C	14.68360	8.05244	5.71467
H	14.64618	7.66829	4.66835
C	15.44143	7.00619	6.55740
H	15.44103	7.32817	7.62246
H	14.88499	6.04568	6.53724
C	16.88712	6.83519	6.07061
H	17.42278	6.10319	6.71137
H	16.87519	6.40226	5.04440
C	17.63606	8.17614	6.04239
H	18.66707	8.04053	5.65240
H	17.74277	8.55499	7.08426
C	16.87963	9.21931	5.20670
H	16.86190	8.89350	4.14187
H	17.41096	10.19462	5.22608
C	15.43368	9.39697	5.70017
H	15.45556	9.81445	6.73031
H	14.90378	10.14146	5.07311
C	12.66015	9.60613	7.30785
H	13.13909	10.48748	6.82615
C	13.34332	9.32707	8.66337
H	12.95369	8.35321	9.03947
H	14.43534	9.18658	8.52457
C	13.07777	10.43287	9.69382
H	13.56141	10.17104	10.65872
H	13.55174	11.38180	9.35327
C	11.57306	10.66160	9.88692
H	11.39038	11.47282	10.62304
H	11.11581	9.73977	10.31139
C	10.89829	10.98575	8.54774
H	9.80444	11.12320	8.68373
H	11.29018	11.95706	8.16830
C	11.15627	9.88894	7.50461
H	10.68666	10.17109	6.53966
H	10.67289	8.93562	7.82236
C	11.95557	8.51215	4.63478
H	10.91737	8.67749	5.00140
C	11.90806	7.27761	3.71445
H	12.93754	7.03196	3.36711
H	11.56040	6.40369	4.30664
C	11.00766	7.52932	2.49689
H	11.01108	6.64320	1.82747
H	9.95756	7.65269	2.84647

C	11.43677	8.78854	1.72780
H	10.75145	8.97803	0.87473
H	12.44513	8.61791	1.28654
C	11.49599	10.01615	2.64990
H	10.46938	10.25396	3.00960
H	11.84529	10.90850	2.08831
C	12.40403	9.76502	3.86651
H	12.41089	10.65449	4.53117
H	13.44934	9.62456	3.51280
C	9.35603	5.74823	9.34193
H	8.91078	6.56878	8.73536
C	8.21512	4.95861	10.00229
H	7.55575	4.50119	9.23479
H	8.64319	4.11974	10.59447
C	7.39472	5.86170	10.93984
H	6.88595	6.64411	10.33247
H	6.58995	5.27432	11.43077
C	8.28581	6.53913	11.99232
H	8.70950	5.75892	12.66485
H	7.68057	7.21096	12.63701
C	9.43942	7.31367	11.33605
H	10.09834	7.76182	12.10958
H	9.02378	8.16392	10.74912
C	10.25793	6.41750	10.39633
H	10.77747	5.63392	10.99375
H	11.05349	6.99128	9.87364
C	9.20249	4.27944	6.76173
H	8.47261	3.56601	7.20490
C	8.44340	5.49962	6.20017
H	7.80674	5.95431	6.98718
H	9.20047	6.27016	5.92390
C	7.58336	5.14235	4.97939
H	7.09077	6.05758	4.58745
H	6.76348	4.45622	5.29250
C	8.41396	4.46359	3.88233
H	7.77304	4.19743	3.01535
H	9.17540	5.18238	3.50468
C	9.12568	3.22070	4.43257
H	9.74889	2.74539	3.64564
H	8.36391	2.46377	4.72868
C	9.99890	3.57207	5.64461
H	10.82229	4.25674	5.33614
H	10.49186	2.65983	6.03982
C	10.99248	3.29894	8.97078
H	11.09506	3.63980	10.02770
C	12.40047	2.90288	8.48126
H	13.06557	3.79105	8.51876
H	12.34486	2.61756	7.40730
C	12.96853	1.73343	9.29749
H	13.96703	1.44354	8.90733
H	13.12868	2.06843	10.34769
C	12.01747	0.52692	9.29363
H	11.94419	0.12491	8.25753
H	12.42559	-0.29501	9.91920
C	10.61404	0.92207	9.77643
H	10.66638	1.22567	10.84665

H	9.92638	0.05082	9.73207
C	10.04150	2.08807	8.95272
H	9.89988	1.74980	7.90314
H	9.03678	2.36587	9.32900

MULLIKEN Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1pt	-0.59476	3.26556	6.18951	9.12156	0.01733	0.00079
2p	0.05892	5.61588	8.83792	0.44458	0.04270	
3p	0.06506	5.61541	8.83216	0.44468	0.04268	
4c	0.02043	3.06529	2.78056	0.12774	0.00599	
5h	0.06784	0.88771	0.04225	0.00220		
6c	-0.15557	3.15863	2.88036	0.11104	0.00554	
7h	0.07217	0.88825	0.03769	0.00189		
8h	0.09062	0.86655	0.04089	0.00195		
9c	-0.14052	3.15055	2.87689	0.10774	0.00534	
10h	0.07393	0.88712	0.03710	0.00185		
11h	0.05779	0.90345	0.03688	0.00188		
12c	-0.10977	3.12890	2.86730	0.10821	0.00535	
13h	0.07343	0.88752	0.03718	0.00186		
14h	0.05529	0.90620	0.03665	0.00187		
15c	-0.14100	3.15467	2.87280	0.10818	0.00535	
16h	0.05968	0.90164	0.03681	0.00187		
17h	0.07273	0.88805	0.03736	0.00186		
18c	-0.19257	3.18237	2.89101	0.11367	0.00551	
19h	0.06842	0.89050	0.03915	0.00193		
20h	0.07886	0.87895	0.04026	0.00192		
21c	0.08808	3.02611	2.75132	0.12856	0.00593	
22h	0.07172	0.88238	0.04368	0.00221		
23c	-0.21440	3.18668	2.91091	0.11125	0.00556	
24h	0.11071	0.84576	0.04159	0.00194		
25h	0.07052	0.88716	0.04041	0.00191		
26c	-0.14236	3.15560	2.87380	0.10760	0.00536	
27h	0.07327	0.88773	0.03715	0.00185		
28h	0.05666	0.90467	0.03680	0.00187		
29c	-0.07732	3.09757	2.86687	0.10748	0.00541	
30h	0.07388	0.88750	0.03676	0.00186		
31h	0.03007	0.92938	0.03866	0.00188		
32c	-0.13895	3.15362	2.87249	0.10747	0.00536	
33h	0.07035	0.89060	0.03719	0.00186		
34h	0.05576	0.90558	0.03679	0.00188		
35c	-0.18191	3.17020	2.89612	0.11004	0.00555	
36h	0.07102	0.88802	0.03903	0.00192		
37h	0.08973	0.86720	0.04115	0.00193		
38c	0.05000	3.06023	2.75306	0.13073	0.00599	
39h	0.08750	0.86746	0.04278	0.00227		
40c	-0.12554	3.12737	2.88084	0.11173	0.00560	
41h	0.07008	0.89029	0.03775	0.00188		
42h	0.05526	0.89891	0.04391	0.00192		
43c	-0.15086	3.16273	2.87512	0.10767	0.00535	
44h	0.07482	0.88645	0.03689	0.00184		
45h	0.05892	0.90207	0.03713	0.00188		
46c	-0.11876	3.13692	2.86847	0.10803	0.00534	
47h	0.07438	0.88673	0.03704	0.00186		

48h	0.05789	0.90373	0.03652	0.00186	
49c	-0.14328	3.15648	2.87298	0.10847	0.00535
50h	0.06242	0.89885	0.03686	0.00187	
51h	0.07415	0.88681	0.03719	0.00185	
52c	-0.18856	3.17742	2.89276	0.11288	0.00551
53h	0.07982	0.88003	0.03824	0.00190	
54h	0.06168	0.89738	0.03898	0.00195	
55c	0.04491	3.06324	2.75533	0.13053	0.00599
56h	0.09052	0.86474	0.04249	0.00225	
57c	-0.18354	3.17320	2.89193	0.11291	0.00551
58h	0.07966	0.88006	0.03838	0.00191	
59h	0.06158	0.89746	0.03902	0.00195	
60c	-0.14572	3.15840	2.87375	0.10823	0.00535
61h	0.06145	0.89966	0.03702	0.00188	
62h	0.07381	0.88716	0.03717	0.00186	
63c	-0.11487	3.13486	2.86663	0.10803	0.00534
64h	0.05669	0.90486	0.03659	0.00186	
65h	0.07410	0.88692	0.03712	0.00186	
66c	-0.15237	3.16337	2.87572	0.10793	0.00535
67h	0.07439	0.88670	0.03707	0.00185	
68h	0.05937	0.90156	0.03719	0.00188	
69c	-0.12013	3.12730	2.87629	0.11096	0.00559
70h	0.06826	0.89198	0.03786	0.00189	
71h	0.05108	0.90294	0.04404	0.00194	
72c	0.08713	3.02837	2.75007	0.12849	0.00594
73h	0.06946	0.88413	0.04419	0.00222	
74c	-0.17489	3.16525	2.89390	0.11019	0.00555
75h	0.07090	0.88801	0.03916	0.00193	
76h	0.08767	0.86944	0.04097	0.00192	
77c	-0.14354	3.15610	2.87435	0.10774	0.00536
78h	0.07003	0.89091	0.03719	0.00186	
79h	0.05582	0.90530	0.03700	0.00188	
80c	-0.07342	3.09682	2.86365	0.10754	0.00541
81h	0.07316	0.88832	0.03665	0.00186	
82h	0.02793	0.93148	0.03871	0.00188	
83c	-0.13964	3.15369	2.87291	0.10768	0.00536
84h	0.07293	0.88800	0.03720	0.00186	
85h	0.05488	0.90626	0.03698	0.00188	
86c	-0.21228	3.18764	2.90783	0.11125	0.00555
87h	0.10864	0.84765	0.04176	0.00195	
88h	0.07114	0.88650	0.04045	0.00191	
89c	0.00790	3.07145	2.78678	0.12787	0.00599
90h	0.06917	0.88628	0.04235	0.00221	
91c	-0.15065	3.15561	2.87811	0.11138	0.00554
92h	0.08954	0.86765	0.04086	0.00195	
93h	0.07139	0.88888	0.03784	0.00190	
94c	-0.13880	3.15080	2.87473	0.10793	0.00534
95h	0.07343	0.88762	0.03710	0.00185	
96h	0.05760	0.90347	0.03705	0.00188	
97c	-0.11359	3.13090	2.86886	0.10848	0.00536
98h	0.05651	0.90497	0.03665	0.00186	
99h	0.07392	0.88708	0.03714	0.00186	
100c	-0.14073	3.15371	2.87328	0.10838	0.00535
101h	0.05944	0.90186	0.03683	0.00187	
102h	0.07366	0.88724	0.03723	0.00186	
103c	-0.18752	3.18113	2.88711	0.11378	0.00551

104h	0.06808	0.89053	0.03946	0.00194
105h	0.07782	0.87987	0.04038	0.00193

NPA Charges:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 pt	-0.46695	2.90314	5.99854	9.56361	0.00139	0.00027
2 p	1.03216	5.24239	8.69110	0.03278	0.00157	0.00000
3 p	1.03226	5.24247	8.69094	0.03277	0.00157	0.00000
4 c	-0.52641	3.08108	3.43517	0.00909	0.00107	0.00000
5 h	0.22467	0.77387	0.00126	0.00020	0.00000	0.00000
6 c	-0.41407	3.05367	3.35291	0.00645	0.00103	0.00000
7 h	0.20243	0.79660	0.00082	0.00015	0.00000	0.00000
8 h	0.23705	0.76211	0.00071	0.00014	0.00000	0.00000
9 c	-0.40380	3.05654	3.34023	0.00606	0.00097	0.00000
10 h	0.21246	0.78676	0.00063	0.00016	0.00000	0.00000
11 h	0.19478	0.80436	0.00071	0.00015	0.00000	0.00000
12 c	-0.40405	3.05890	3.33802	0.00614	0.00099	0.00000
13 h	0.21042	0.78878	0.00064	0.00016	0.00000	0.00000
14 h	0.19536	0.80378	0.00070	0.00015	0.00000	0.00000
15 c	-0.40058	3.05657	3.33705	0.00600	0.00096	0.00000
16 h	0.19471	0.80442	0.00073	0.00015	0.00000	0.00000
17 h	0.21068	0.78854	0.00063	0.00015	0.00000	0.00000
18 c	-0.41609	3.05007	3.35867	0.00632	0.00102	0.00000
19 h	0.20152	0.79746	0.00087	0.00015	0.00000	0.00000
20 h	0.21482	0.78430	0.00074	0.00015	0.00000	0.00000
21 c	-0.52046	3.07931	3.43046	0.00966	0.00103	0.00000
22 h	0.21992	0.77858	0.00129	0.00021	0.00000	0.00000
23 c	-0.42372	3.05163	3.36472	0.00633	0.00104	0.00000
24 h	0.22770	0.77136	0.00081	0.00014	0.00000	0.00000
25 h	0.20908	0.78999	0.00077	0.00016	0.00000	0.00000
26 c	-0.40234	3.05489	3.34049	0.00601	0.00096	0.00000
27 h	0.21149	0.78772	0.00064	0.00015	0.00000	0.00000
28 h	0.19345	0.80568	0.00072	0.00015	0.00000	0.00000
29 c	-0.40532	3.05753	3.34062	0.00618	0.00098	0.00000
30 h	0.20894	0.79028	0.00062	0.00016	0.00000	0.00000
31 h	0.20106	0.79804	0.00076	0.00014	0.00000	0.00000
32 c	-0.40056	3.05498	3.33862	0.00600	0.00096	0.00000
33 h	0.21032	0.78889	0.00064	0.00015	0.00000	0.00000
34 h	0.19358	0.80557	0.00071	0.00015	0.00000	0.00000
35 c	-0.42330	3.05122	3.36473	0.00632	0.00103	0.00000
36 h	0.20853	0.79061	0.00071	0.00015	0.00000	0.00000
37 h	0.22676	0.77233	0.00078	0.00013	0.00000	0.00000
38 c	-0.52265	3.07921	3.43314	0.00921	0.00109	0.00000
39 h	0.23389	0.76471	0.00119	0.00020	0.00000	0.00000
40 c	-0.42041	3.05173	3.36130	0.00635	0.00103	0.00000
41 h	0.19460	0.80449	0.00077	0.00015	0.00000	0.00000
42 h	0.24076	0.75837	0.00073	0.00014	0.00000	0.00000
43 c	-0.40466	3.05640	3.34135	0.00594	0.00097	0.00000
44 h	0.21263	0.78659	0.00063	0.00015	0.00000	0.00000
45 h	0.19665	0.80247	0.00074	0.00014	0.00000	0.00000
46 c	-0.40414	3.05884	3.33818	0.00613	0.00098	0.00000
47 h	0.21114	0.78806	0.00064	0.00016	0.00000	0.00000
48 h	0.19526	0.80389	0.00070	0.00015	0.00000	0.00000
49 c	-0.40028	3.05694	3.33638	0.00601	0.00096	0.00000
50 h	0.19589	0.80323	0.00073	0.00015	0.00000	0.00000

51	h	0.21093	0.78828	0.00063	0.00016	0.00000	0.00000
52	c	-0.41879	3.05055	3.36091	0.00630	0.00103	0.00000
53	h	0.21184	0.78727	0.00074	0.00015	0.00000	0.00000
54	h	0.19965	0.79933	0.00088	0.00014	0.00000	0.00000
55	c	-0.52273	3.07921	3.43322	0.00921	0.00109	0.00000
56	h	0.23404	0.76457	0.00119	0.00020	0.00000	0.00000
57	c	-0.41893	3.05056	3.36103	0.00631	0.00103	0.00000
58	h	0.21184	0.78727	0.00074	0.00015	0.00000	0.00000
59	h	0.19968	0.79930	0.00088	0.00014	0.00000	0.00000
60	c	-0.40010	3.05691	3.33622	0.00601	0.00096	0.00000
61	h	0.19583	0.80329	0.00073	0.00015	0.00000	0.00000
62	h	0.21089	0.78832	0.00063	0.00016	0.00000	0.00000
63	c	-0.40409	3.05882	3.33816	0.00613	0.00098	0.00000
64	h	0.19524	0.80391	0.00070	0.00015	0.00000	0.00000
65	h	0.21109	0.78811	0.00064	0.00016	0.00000	0.00000
66	c	-0.40479	3.05639	3.34149	0.00594	0.00097	0.00000
67	h	0.21264	0.78659	0.00063	0.00015	0.00000	0.00000
68	h	0.19669	0.80243	0.00074	0.00014	0.00000	0.00000
69	c	-0.42041	3.05166	3.36137	0.00635	0.00103	0.00000
70	h	0.19454	0.80454	0.00077	0.00015	0.00000	0.00000
71	h	0.24080	0.75833	0.00073	0.00014	0.00000	0.00000
72	c	-0.52058	3.07938	3.43051	0.00965	0.00103	0.00000
73	h	0.21993	0.77857	0.00128	0.00021	0.00000	0.00000
74	c	-0.42310	3.05120	3.36455	0.00633	0.00103	0.00000
75	h	0.20843	0.79070	0.00071	0.00015	0.00000	0.00000
76	h	0.22666	0.77243	0.00078	0.00013	0.00000	0.00000
77	c	-0.40046	3.05501	3.33848	0.00601	0.00096	0.00000
78	h	0.21032	0.78888	0.00064	0.00015	0.00000	0.00000
79	h	0.19354	0.80560	0.00071	0.00015	0.00000	0.00000
80	c	-0.40534	3.05762	3.34056	0.00618	0.00098	0.00000
81	h	0.20892	0.79030	0.00062	0.00016	0.00000	0.00000
82	h	0.20103	0.79808	0.00075	0.00014	0.00000	0.00000
83	c	-0.40218	3.05489	3.34031	0.00601	0.00096	0.00000
84	h	0.21142	0.78779	0.00064	0.00015	0.00000	0.00000
85	h	0.19341	0.80573	0.00072	0.00015	0.00000	0.00000
86	c	-0.42363	3.05168	3.36458	0.00633	0.00104	0.00000
87	h	0.22762	0.77143	0.00081	0.00014	0.00000	0.00000
88	h	0.20907	0.79000	0.00077	0.00016	0.00000	0.00000
89	c	-0.52637	3.08107	3.43515	0.00909	0.00107	0.00000
90	h	0.22471	0.77383	0.00126	0.00020	0.00000	0.00000
91	c	-0.41404	3.05366	3.35289	0.00646	0.00103	0.00000
92	h	0.23692	0.76223	0.00071	0.00014	0.00000	0.00000
93	h	0.20251	0.79652	0.00082	0.00015	0.00000	0.00000
94	c	-0.40385	3.05659	3.34023	0.00606	0.00097	0.00000
95	h	0.21250	0.78671	0.00063	0.00016	0.00000	0.00000
96	h	0.19474	0.80440	0.00071	0.00015	0.00000	0.00000
97	c	-0.40414	3.05892	3.33809	0.00614	0.00099	0.00000
98	h	0.19538	0.80376	0.00070	0.00015	0.00000	0.00000
99	h	0.21048	0.78873	0.00064	0.00016	0.00000	0.00000
100	c	-0.40066	3.05655	3.33715	0.00601	0.00096	0.00000
101	h	0.19473	0.80440	0.00073	0.00015	0.00000	0.00000
102	h	0.21071	0.78850	0.00063	0.00015	0.00000	0.00000
103	c	-0.41600	3.05007	3.35858	0.00633	0.00102	0.00000
104	h	0.20147	0.79751	0.00087	0.00015	0.00000	0.00000
105	h	0.21479	0.78433	0.00074	0.00015	0.00000	0.00000

QTAIM Charges:

1	(Pt)	Charge:	-0.530440	Volume:	237.829 Bohr^3
2	(P)	Charge:	1.588593	Volume:	72.412 Bohr^3
3	(P)	Charge:	1.589133	Volume:	72.415 Bohr^3
4	(C)	Charge:	-0.490506	Volume:	59.400 Bohr^3
5	(H)	Charge:	0.000861	Volume:	45.848 Bohr^3
6	(C)	Charge:	0.027583	Volume:	56.433 Bohr^3
7	(H)	Charge:	-0.011956	Volume:	48.695 Bohr^3
8	(H)	Charge:	0.020157	Volume:	47.503 Bohr^3
9	(C)	Charge:	0.029694	Volume:	58.382 Bohr^3
10	(H)	Charge:	-0.007909	Volume:	50.020 Bohr^3
11	(H)	Charge:	-0.018687	Volume:	50.730 Bohr^3
12	(C)	Charge:	0.031666	Volume:	58.391 Bohr^3
13	(H)	Charge:	-0.010342	Volume:	50.179 Bohr^3
14	(H)	Charge:	-0.017324	Volume:	50.694 Bohr^3
15	(C)	Charge:	0.031189	Volume:	58.297 Bohr^3
16	(H)	Charge:	-0.018531	Volume:	50.776 Bohr^3
17	(H)	Charge:	-0.010389	Volume:	50.160 Bohr^3
18	(C)	Charge:	0.032505	Volume:	55.395 Bohr^3
19	(H)	Charge:	-0.011222	Volume:	45.624 Bohr^3
20	(H)	Charge:	-0.007464	Volume:	46.022 Bohr^3
21	(C)	Charge:	-0.496508	Volume:	58.418 Bohr^3
22	(H)	Charge:	-0.004750	Volume:	46.495 Bohr^3
23	(C)	Charge:	0.020242	Volume:	56.165 Bohr^3
24	(H)	Charge:	0.017565	Volume:	45.241 Bohr^3
25	(H)	Charge:	-0.015122	Volume:	45.735 Bohr^3
26	(C)	Charge:	0.032182	Volume:	58.345 Bohr^3
27	(H)	Charge:	-0.009186	Volume:	50.085 Bohr^3
28	(H)	Charge:	-0.021155	Volume:	51.102 Bohr^3
29	(C)	Charge:	0.031177	Volume:	58.389 Bohr^3
30	(H)	Charge:	-0.012462	Volume:	50.315 Bohr^3
31	(H)	Charge:	-0.009131	Volume:	51.673 Bohr^3
32	(C)	Charge:	0.033513	Volume:	58.268 Bohr^3
33	(H)	Charge:	-0.011192	Volume:	50.282 Bohr^3
34	(H)	Charge:	-0.020267	Volume:	51.029 Bohr^3
35	(C)	Charge:	0.018645	Volume:	56.192 Bohr^3
36	(H)	Charge:	-0.014490	Volume:	47.374 Bohr^3
37	(H)	Charge:	0.017278	Volume:	47.254 Bohr^3
38	(C)	Charge:	-0.501426	Volume:	58.138 Bohr^3
39	(H)	Charge:	0.009336	Volume:	45.528 Bohr^3
40	(C)	Charge:	0.020201	Volume:	56.784 Bohr^3
41	(H)	Charge:	-0.021873	Volume:	49.361 Bohr^3
42	(H)	Charge:	0.025484	Volume:	46.135 Bohr^3
43	(C)	Charge:	0.030416	Volume:	58.298 Bohr^3
44	(H)	Charge:	-0.008845	Volume:	50.831 Bohr^3
45	(H)	Charge:	-0.016862	Volume:	51.610 Bohr^3
46	(C)	Charge:	0.031173	Volume:	58.434 Bohr^3
47	(H)	Charge:	-0.009929	Volume:	50.123 Bohr^3
48	(H)	Charge:	-0.017408	Volume:	50.729 Bohr^3
49	(C)	Charge:	0.031328	Volume:	58.346 Bohr^3
50	(H)	Charge:	-0.016518	Volume:	50.595 Bohr^3
51	(H)	Charge:	-0.009712	Volume:	50.131 Bohr^3
52	(C)	Charge:	0.030783	Volume:	55.785 Bohr^3
53	(H)	Charge:	-0.010747	Volume:	48.645 Bohr^3

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 54 (H )    Charge:   -0.014278     Volume:    46.980 Bohr^3
 55 (C )    Charge:   -0.502091     Volume:    58.143 Bohr^3
 56 (H )    Charge:    0.010068     Volume:    45.482 Bohr^3
 57 (C )    Charge:    0.030237     Volume:    55.781 Bohr^3
 58 (H )    Charge:   -0.010766     Volume:    48.660 Bohr^3
 59 (H )    Charge:   -0.014221     Volume:    46.982 Bohr^3
 60 (C )    Charge:    0.031396     Volume:    58.322 Bohr^3
 61 (H )    Charge:   -0.016642     Volume:    50.615 Bohr^3
 62 (H )    Charge:   -0.009751     Volume:    50.142 Bohr^3
 63 (C )    Charge:    0.031205     Volume:    58.444 Bohr^3
 64 (H )    Charge:   -0.017583     Volume:    50.719 Bohr^3
 65 (H )    Charge:   -0.009365     Volume:    50.108 Bohr^3
 66 (C )    Charge:    0.030794     Volume:    58.212 Bohr^3
 67 (H )    Charge:   -0.009229     Volume:    50.855 Bohr^3
 68 (H )    Charge:   -0.017292     Volume:    51.573 Bohr^3
 69 (C )    Charge:    0.020973     Volume:    56.760 Bohr^3
 70 (H )    Charge:   -0.022060     Volume:    49.340 Bohr^3
 71 (H )    Charge:    0.024838     Volume:    45.944 Bohr^3
 72 (C )    Charge:   -0.497462     Volume:    58.424 Bohr^3
 73 (H )    Charge:   -0.004811     Volume:    46.458 Bohr^3
 74 (C )    Charge:    0.019788     Volume:    56.150 Bohr^3
 75 (H )    Charge:   -0.014363     Volume:    47.379 Bohr^3
 76 (H )    Charge:    0.016870     Volume:    47.353 Bohr^3
 77 (C )    Charge:    0.032622     Volume:    58.277 Bohr^3
 78 (H )    Charge:   -0.011315     Volume:    50.274 Bohr^3
 79 (H )    Charge:   -0.020401     Volume:    51.011 Bohr^3
 80 (C )    Charge:    0.031759     Volume:    58.407 Bohr^3
 81 (H )    Charge:   -0.012651     Volume:    50.315 Bohr^3
 82 (H )    Charge:   -0.009197     Volume:    51.870 Bohr^3
 83 (C )    Charge:    0.031815     Volume:    58.351 Bohr^3
 84 (H )    Charge:   -0.009524     Volume:    50.095 Bohr^3
 85 (H )    Charge:   -0.020609     Volume:    51.072 Bohr^3
 86 (C )    Charge:    0.019969     Volume:    56.181 Bohr^3
 87 (H )    Charge:    0.017541     Volume:    45.324 Bohr^3
 88 (H )    Charge:   -0.014920     Volume:    45.767 Bohr^3
 89 (C )    Charge:   -0.490093     Volume:    59.403 Bohr^3
 90 (H )    Charge:    0.001032     Volume:    45.778 Bohr^3
 91 (C )    Charge:    0.027813     Volume:    56.452 Bohr^3
 92 (H )    Charge:    0.019679     Volume:    47.524 Bohr^3
 93 (H )    Charge:   -0.012097     Volume:    48.732 Bohr^3
 94 (C )    Charge:    0.030534     Volume:    58.362 Bohr^3
 95 (H )    Charge:   -0.008398     Volume:    50.031 Bohr^3
 96 (H )    Charge:   -0.018421     Volume:    50.725 Bohr^3
 97 (C )    Charge:    0.031595     Volume:    58.400 Bohr^3
 98 (H )    Charge:   -0.017561     Volume:    50.707 Bohr^3
 99 (H )    Charge:   -0.010342     Volume:    50.176 Bohr^3
100 (C )    Charge:    0.031081     Volume:    58.300 Bohr^3
101 (H )    Charge:   -0.018657     Volume:    50.768 Bohr^3
102 (H )    Charge:   -0.009954     Volume:    50.153 Bohr^3
103 (C )    Charge:    0.032354     Volume:    55.376 Bohr^3
104 (H )    Charge:   -0.010840     Volume:    45.613 Bohr^3
105 (H )    Charge:   -0.007418     Volume:    46.019 Bohr^3
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