Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry. This journal is © The Royal Society of Chemistry 2017

SUPPORTING INFORMATION

Role of the gold-gold interaction in C-H activation of acetone

Mariarosa Anania, Lucie Jašíková, Juraj Jašík, and Jana Roithová^{*}

*Correspondence to: roithova@natur.cuni.cz

Contents

Preparation of reaction mixtures	S2
Reaction with cyclohexanone	S3
IRPD, IRMPD and theoretical IR spectra for [Au(PMe₃)(SbF₅)]	S4
Kinetic isotope effect (KIE)	S6
Formation of gold acetonyl complexes in time	S30
C-H activation	S 35
ESI-MS source and CID spectra	S41
IRPD spectrum for [Au(IPr)(BF₄)]	S44
Computational results	S45

Preparation of reaction mixtures

A) Solutions of gold complexes:

Gold chloride (L)AuCl (L= PMe₃, PPh₃) (5 μ mol) was dissolved in dry THF (1 ml) and mixed with the solution of AgX (X = SbF₆, PF₆, OTf, NTf₂) (1.2 eq) in dry THF (1 ml). The reaction mixture was sonicated for 10 minutes and filtered through a PTFE filter (pore size 0.2 μ m) to remove precipitated AgX.

Purchased gold complexes $[Au(L)(CH_3CN)]SbF_6$ (L = JohnPhos) and $[Au(L)(CH_3CN)]BF_4$ (L = IPr) were dissolved in THF (1 ml).

The stock solutions were stored for no longer than 2 days.

B) MS samples for labelling experiments:

The samples for measurements of labelling experiments were obtained by diluting a solution of (L)AuX or $[Au(JohnPhos)(CH_3CN)]SbF_6$ or $[Au(IPr)(CH_3CN)]BF_4$ (200 µL) with dry THF (600 µL). The solution was mixed with a 1:1 mixture of acetone and acetone-d₆. The specific percentage of water is then added. The obtained solutions were immediately monitored by ESI-MS.

C) Preparation of reaction mixtures:

- 1) (PMe₃)Au(SbF₆): The complex solution was prepared by dissolving 1.54 mg of (PMe₃)Au(Cl) (5 μmol) in 1 ml of dry THF and 2.06 mg of AgSbF₆ (6 μmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PMe₃)Au]⁺ [SbF₆]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 2) (PMe₃)Au(PF₆): The complex solution was prepared by dissolving 1.54 mg of [(PMe₃)Au(Cl) (5 µmol) in 1 ml of dry THF and 1.5 mg AgPF₆ (6 µmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PMe₃)Au]⁺[PF₆]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 3) (PMe₃)Au(OTf): The complex solution was prepared by dissolving 1.54 mg of [(PMe₃)Au(Cl) (5 μmol) in 1 ml of dry THF and 1.28 mg AgOTf (6 μmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PMe₃)Au]⁺[OTf]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 4) (PMe₃)Au(NTf₂): The complex solution was prepared by dissolving 1.54 mg of (PMe₃)Au(Cl) (5 μmol) in 1 ml of dry THF and 1.94 mg AgNTf₂ (6 μmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PMe₃)Au]⁺[NTf₂]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 5) (PPh₃)Au(SbF₆): The complex solution was prepared by dissolving 2.48 mg of [(PPh₃)Au(Cl)] (5 μmol) in 1 ml of dry THF and 2.06 mg of AgNTf₂ (6 μmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PPh₃)Au]⁺[SbF₆]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 6) (PPh₃)Au(NTf₂): The complex solution was prepared by dissolving 2.48 mg of [(PPh₃)Au(Cl)] (5 μmol) in 1 ml of dry THF and 1.94 mg of AgNTf₂ (6 μmol) in 1 ml of dry THF. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(PPh₃)Au]⁺[NTf₂]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- **7)** (JohnPhos)Au(CH₃CN)(SbF₆): The complex solution was prepared by dissolving 1.93 mg of $[(JohnPhos)Au(SbF_6) (5 \mu mol) in 1 ml of dry THF. The solution is ready to be used as a stock solution.$

- **8)** (IPr)Au(CH₃CN)(BF₄): The complex solution was prepared by dissolving 1.79 mg of [(IPr)Au(ACN)(BF₄) (5 μ mol) in 1 ml of dry THF. The solution is ready to be used as a stock solution.
- 9) (IPr)₂Au₂(OH)(BF₄): The complex solution was prepared by dissolving 3.158 mg of gold(I) complex [(IPr)₂ Au₂(OH)]⁺ BF₄⁻ (5 μmol) in 1 ml of dry THF.
- 10) (IPr)Au(OTf): The complex solution was prepared by dissolving 3.08 mg of [(IPr)Au(Cl) (5 μmol) in 1 ml of dry dioxane and 1.28 mg AgOTf (6 μmol) in 1 ml of dry dioxane. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(IPr)Au]⁺[OTf]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.
- 11) (IPr)Au(NTf₂): The complex solution was prepared by dissolving 3.08 mg of [(IPr)Au(Cl) (5 μmol) in 1 ml of dry dioxane and 1.94 mg AgOTf (6 μmol) in 1 ml of dry dioxane. This two solution are then mixed in the same vial and put in ultrasonic bath for ten minutes in order to get a 2.5 mM solution of gold complex [(IPr)Au]⁺[NTf₂]⁻ in 2 ml of THF. The white precipitate of AgCl which is obtained is then filtered away.

Reaction of [Au(IPr)(OTf)] with cyclohexanone in dioxane/water solution.

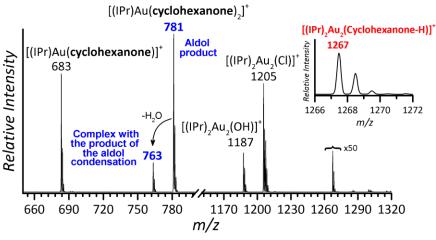
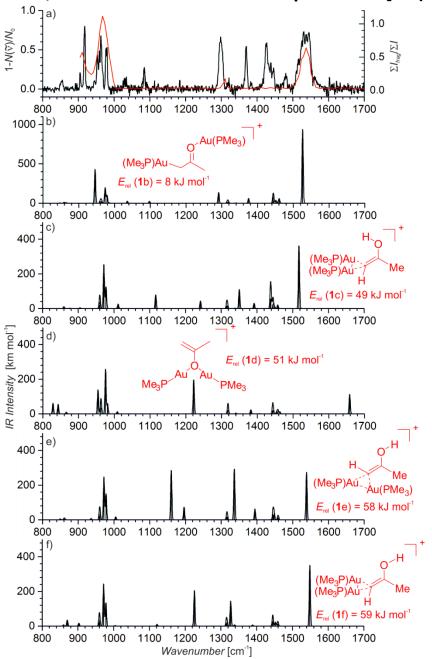


Figure S1: ESI-MS source spectrum of the [(IPr)Au(OTf)] (184 μ g) complex in dry dioxane (0.1 ml) after the addition of cyclohexanone (0.1 mL) and 0.1 mL of H₂O.

The spectrum clearly shows formation of the digold kenonyl complex (m/z 1267). More importantly, it reveals aldol reaction (m/z 781) and subsequent water elimination (m/z 763).



IRPD, IRMPD and theoretical IR spectra for [Au(PMe₃)(SbF₆)]

Figure S2: a) IRPD and IRMPD (an experiment from the CLIO facility in France) experimental spectra (black and red lines respectively) of the mass selected ion $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$ with m/z 603. Theoretical IR spectra (B3LYP-D3/6-311+G*(SDD:Au); scaling factor: 0.975) of different isomers of $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$ b) **1b**, c) **1c**, d) **1d**, e) **1e**, and f) **1f**.

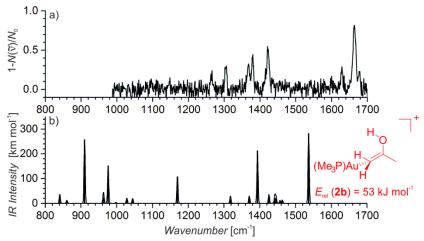


Figure S3: a) IRPD experimental spectrum of the mass selected ion $[(PMe_3)Au(CH_3COCH_3)]^+$ with m/z 331. b) Theoretical IR spectrum (B3LYP-D3/6-311+G*(SDD:Au); scaling factor: 0.975) of isomer **2b** of $[(PMe_3)Au(CH_3COCH_3)]^+$.

Kinetic Isotope Effect (KIE)

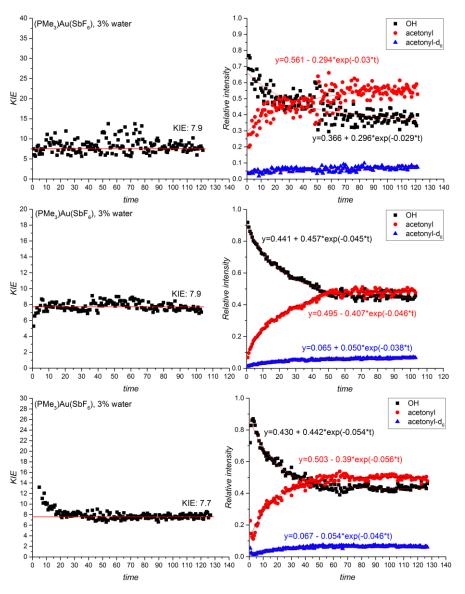


Figure S4: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 3% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

 $\mathsf{KIE:} (\mathsf{PMe_3})_2\mathsf{Au}_2(\mathsf{CH}_2\mathsf{COCH}_3)/(\mathsf{PMe}_3)_2\mathsf{Au}_2(\mathsf{CD}_2\mathsf{COCD}_3).$

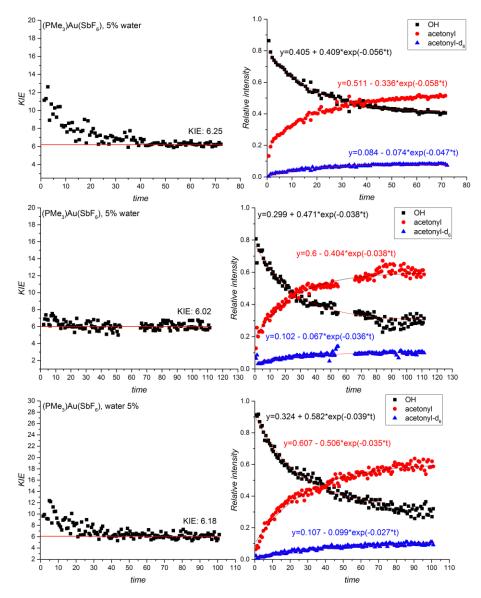


Figure S5: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 5% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= PMe₃)₂Au₂(CD₂COCD₃).

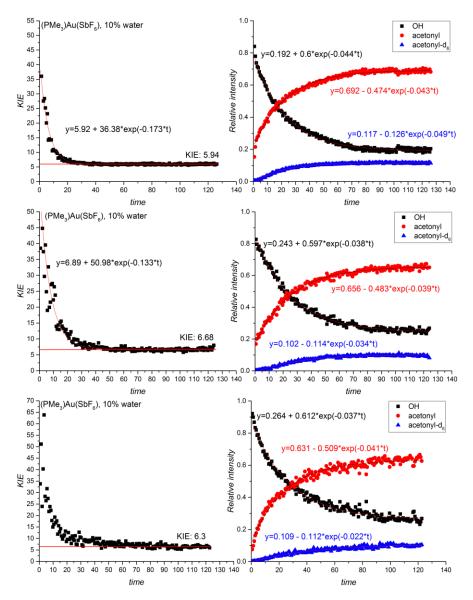


Figure S6: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 10% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

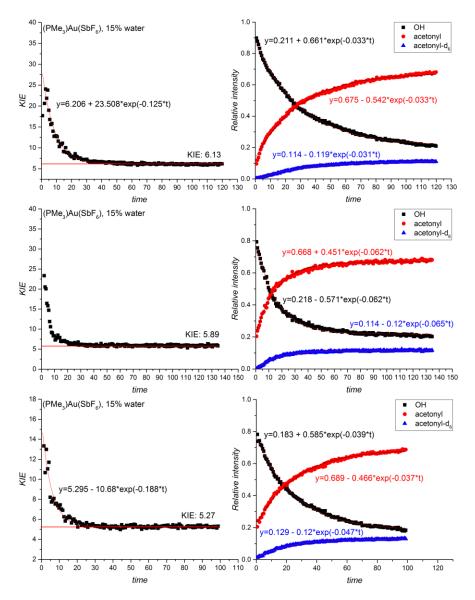


Figure S7: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 15% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

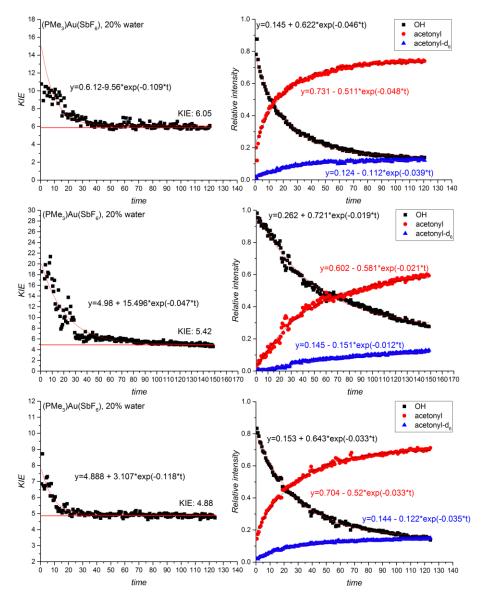


Figure S8: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 20% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

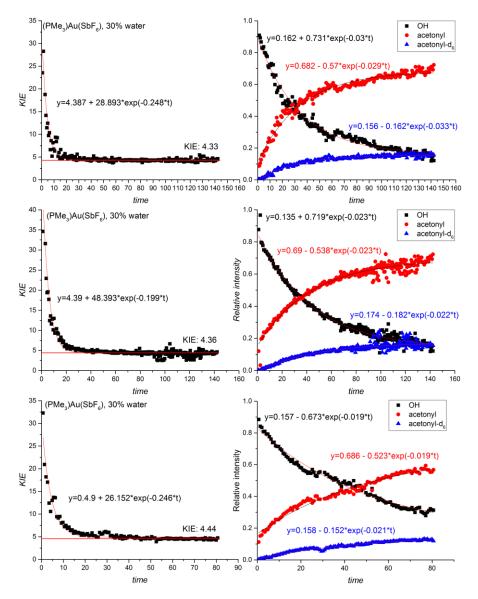


Figure S9: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 30% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

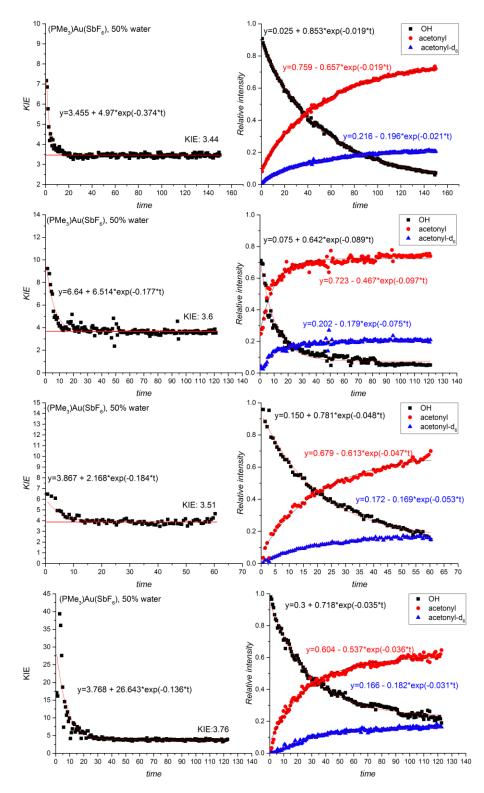


Figure S10: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 50% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

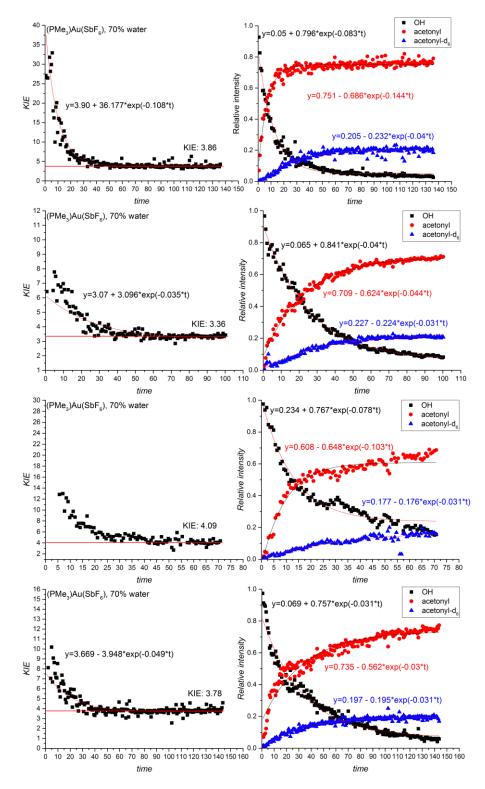


Figure S11: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 70% of water to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

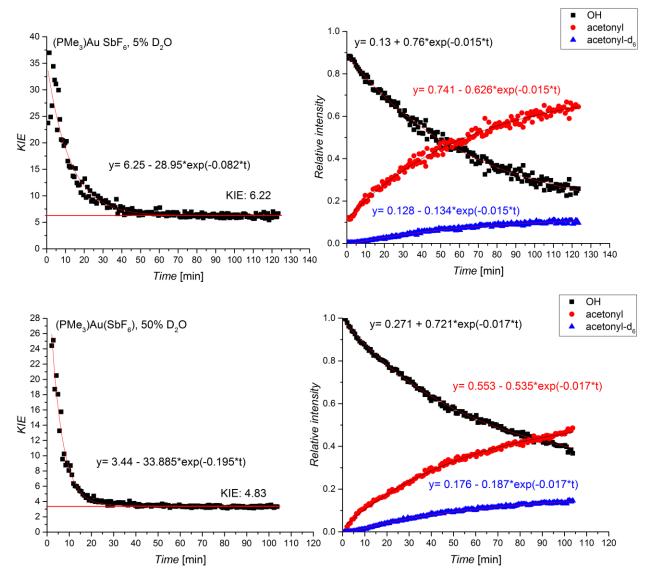


Figure S12: KIE as a function of time for the (PMe₃)Au(SbF₆) complex after addition of 5% and 50% of D₂O to the total volume of the solution. **OH**= (PMe₃)₂Au₂(OH), **acetonyl**= (PMe₃)₂Au₂(CH₂COCH₃), **acetonyl-d**₆= (PMe₃)₂Au₂(CD₂COCD₃).

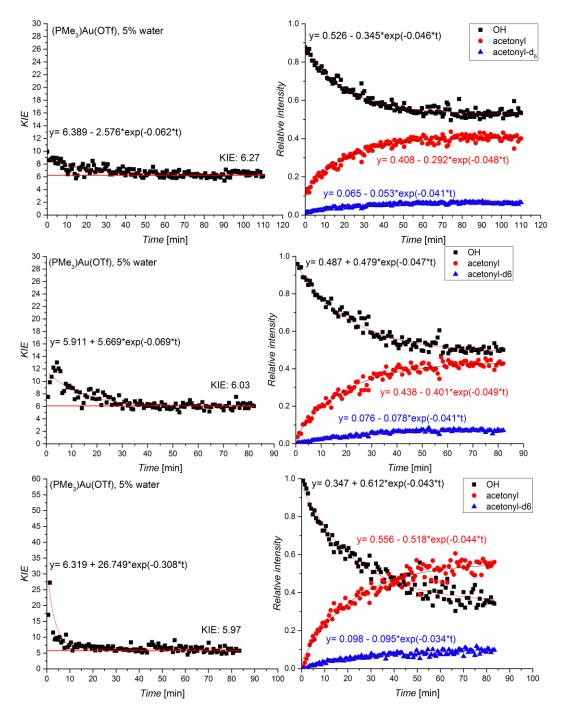


Figure S13. Relative intensity of selected ions $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$, $[(PMe_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PMe_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the (PMe_3)Au(OTf) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

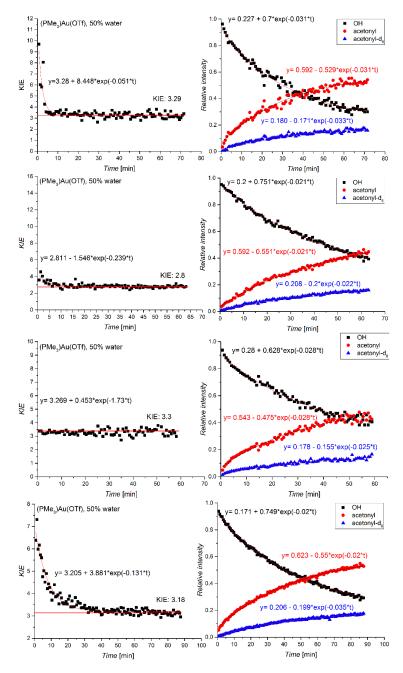


Figure S14. Relative intensity of selected ions $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$, $[(PMe_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PMe_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (PMe_3)Au(OTf) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

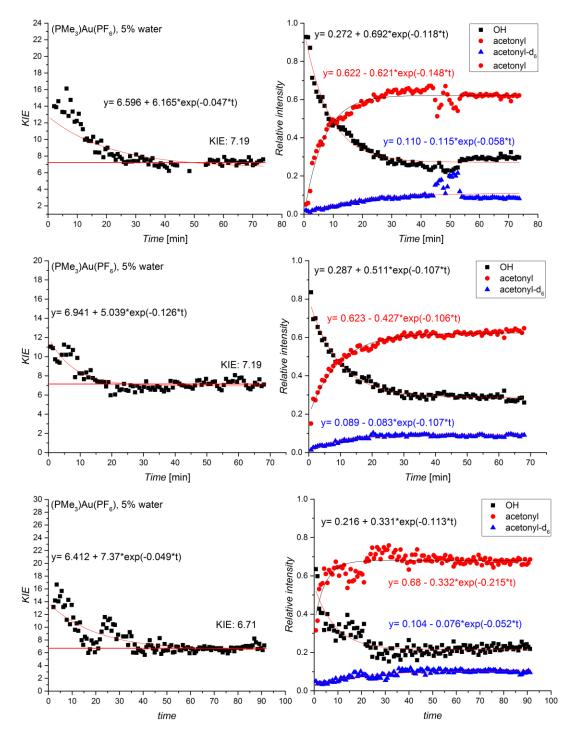


Figure S15. Relative intensity of selected ions $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$, $[(PMe_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PMe_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the $(PMe_3)Au(PF_6)$ complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

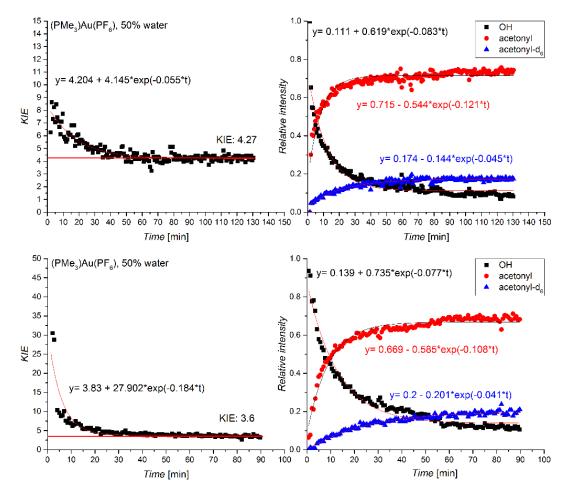


Figure S16. Relative intensity of selected ions $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$, $[(PMe_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PMe_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (PMe_3)Au(PF_6) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

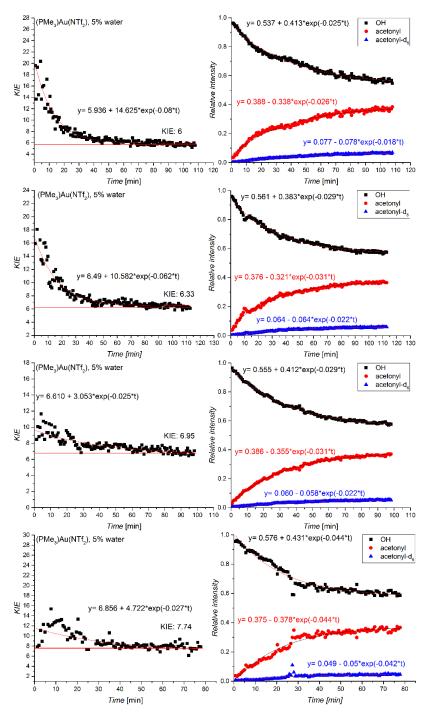


Figure S17. Relative intensity of selected ions $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$, $[(PMe_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PMe_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the (PMe_3)Au(NTf_2) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

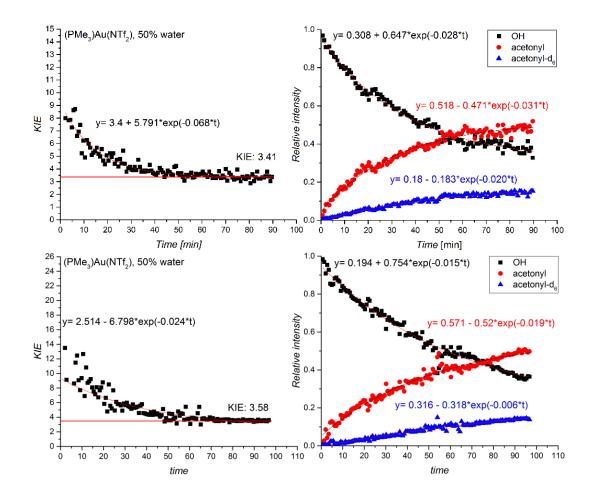


Figure S18. Relative intensity of selected ions ($(PMe_3)_2Au_2(CH_2COCH_3)$, $(PMe_3)_2Au_2(CD_2COCD_3)$ and $(PMe_3)_2Au_2(\mu$ -OH)) as a function of time for the addition of 50% of water to the reaction mixture of the (PMe_3)Au(NTf_2) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

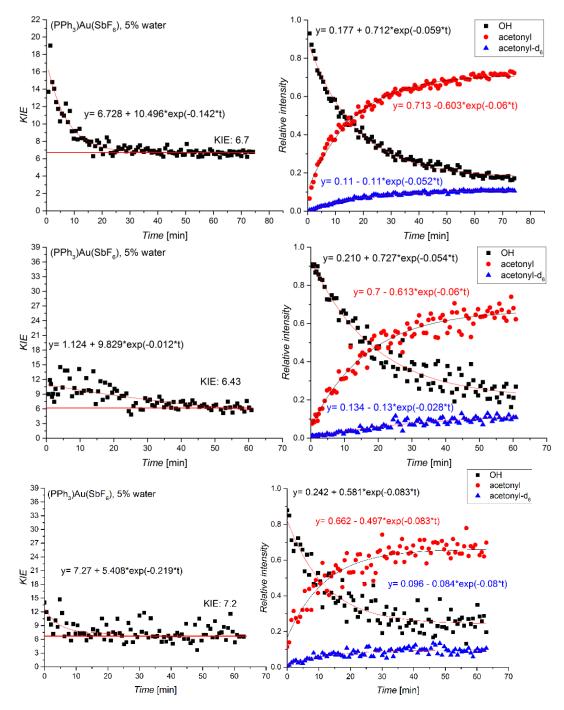


Figure S19. Relative intensity of selected ions $[(PPh_3)_2Au_2(CH_2COCH_3)]^+$, $[(PPh_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PPh_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the $(PPh_3)Au(SbF_6)$ complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

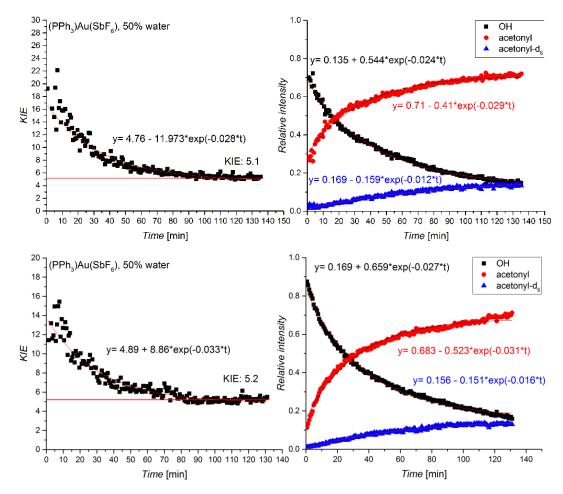


Figure S20. Relative intensity of selected ions $[(PPh_3)_2Au_2(CH_2COCH_3)]^+$, $[(PPh_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PPh_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (PPh_3)Au(SbF_6) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

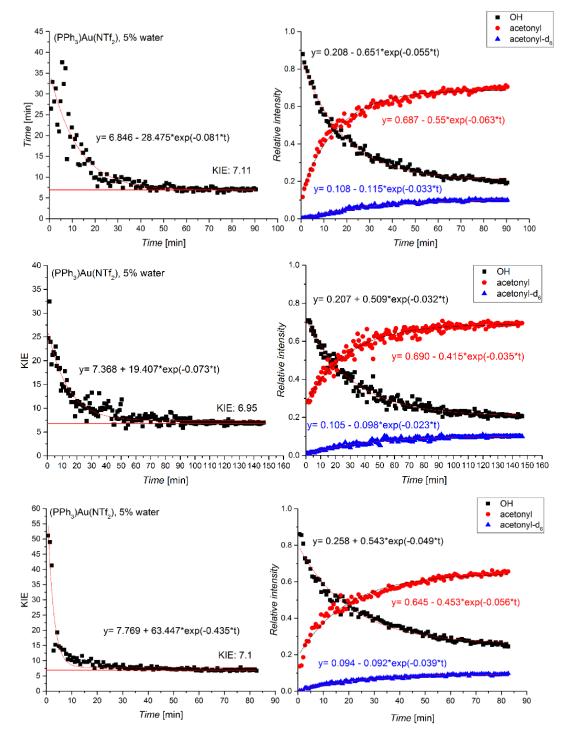


Figure S21. Relative intensity of selected ions $[(PPh_3)_2Au_2(CH_2COCH_3)]^+$, $[(PPh_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PPh_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the (PPh_3)Au(NTf_2) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

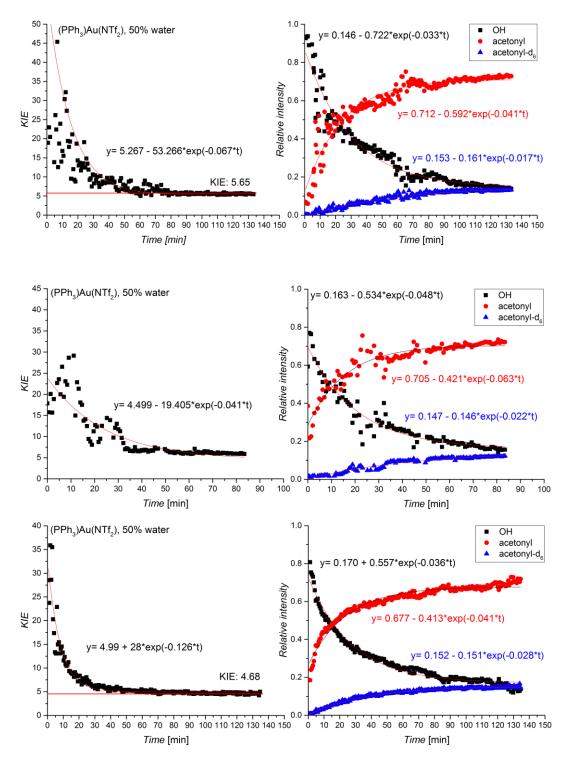


Figure S22. Relative intensity of selected ions $[(PPh_3)_2Au_2(CH_2COCH_3)]^+$, $[(PPh_3)_2Au_2(CD_2COCD_3)]^+$ and $[(PPh_3)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (PPh_3)Au(NTf₂) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

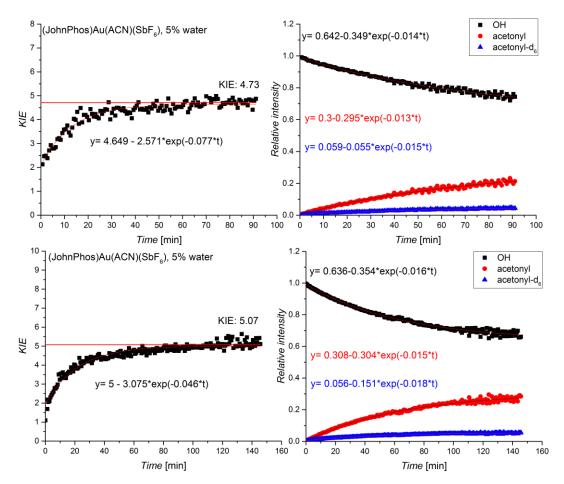


Figure S23. Relative intensity of selected ions $[(JohnPhos)_2Au_2(CH_2COCH_3)]^+$, $[(JohnPhos)_2Au_2(CD_2COCD_3)]^+$ and $[(JohnPhos)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the (JohnPhos)Au(ACN)(SbF₆) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

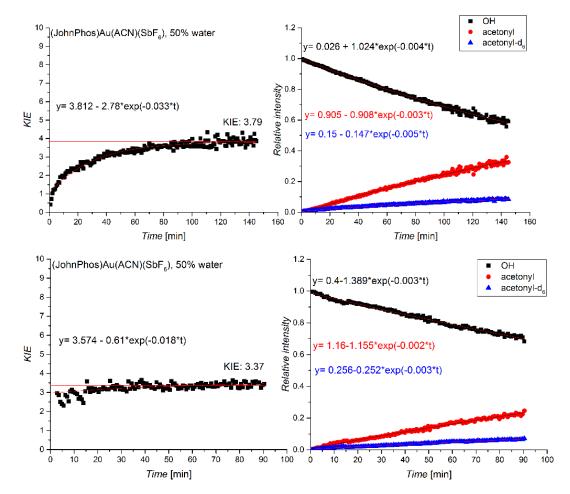


Figure S24. Relative intensity of selected ions $[(JohnPhos)_2Au_2(CH_2COCH_3)]^+$, $[(JohnPhos)_2Au_2(CD_2COCD_3)]^+$ and $[(JohnPhos)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (JohnPhos)Au(ACN)(SbF₆) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

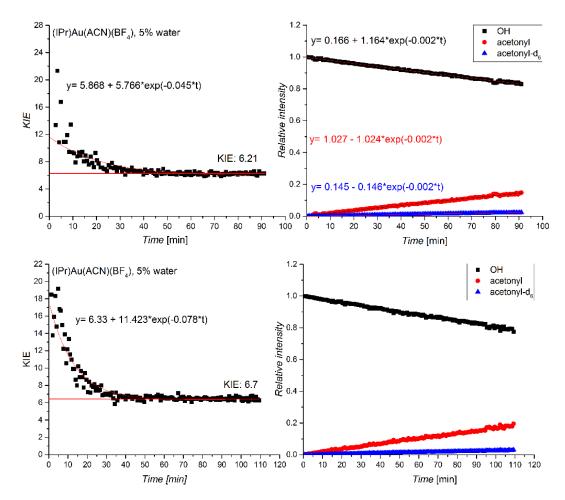


Figure S25. Relative intensity of selected ions $[(IPr)_2Au_2(CH_2COCH_3)]^+$, $[(IPr)_2Au_2(CD_2COCD_3)]^+$ and $[(IPr)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 5% of water to the reaction mixture of the (IPr)Au(ACN)(BF_4) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

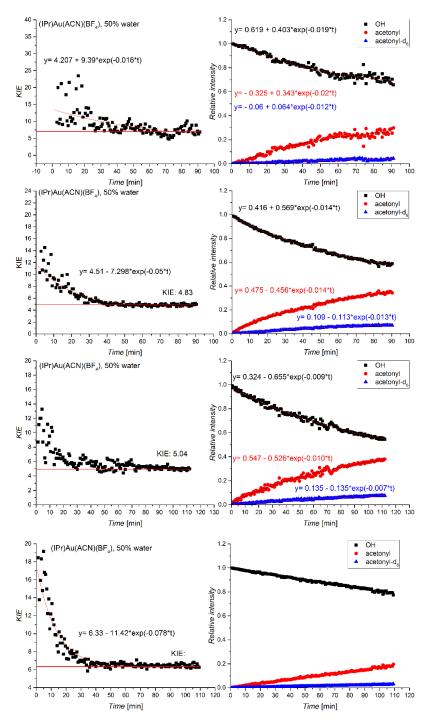


Figure S26. Relative intensity of selected ions $[(IPr)_2Au_2(CH_2COCH_3)]^+$, $[(IPr)_2Au_2(CD_2COCD_3)]^+$ and $[(IPr)_2Au_2(\mu-OH)]^+$ as a function of time for the addition of 50% of water to the reaction mixture of the (IPr)Au(ACN)(BF₄) complex. The sum of the signal intensities of the labelled and the unlabelled ions and the diaurated hydroxide was normalized to 1.

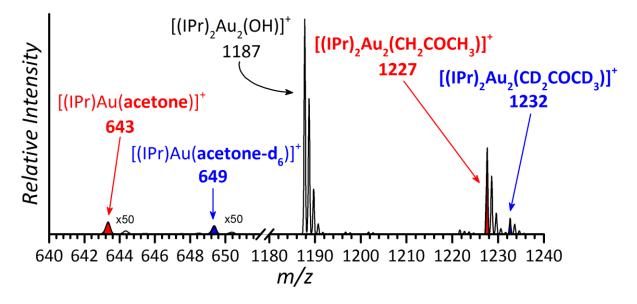
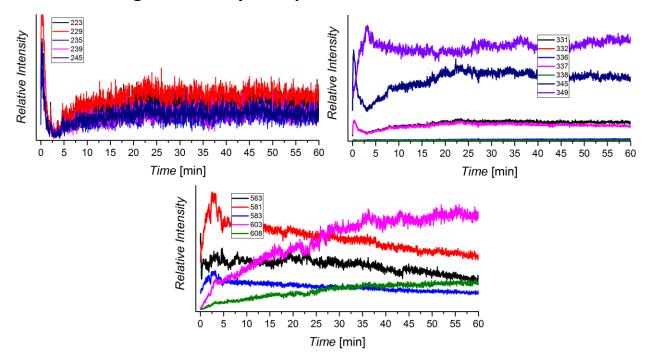


Figure S27. The ESI-MS source spectrum of the $[(IPr)_2Au_2(OH)BF_4]$ (637 µg) complex in dry dioxane (0.2 ml), dry acetone (0.7 ml) and dry acetone-d₆ (0.7 ml).



Formation of gold acetonyl complexes in time

Figure S28. Experiment: $[(PMe_3)AuSbF_6]$ (77 µg) was dissolved in THF (0.8 ml) and of H₂O (0.56 ml) and left to react overnight. Then, 0.8 ml of a 1:1 solution of CH₃COCH₃ and CD₃COCD₃ was added to the solution, and the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $[({}^{107}Ag(CH_3COCH_3)_2]^* (\textit{m/z 223}), [{}^{107}Ag(CH_3COCH_3)(CD_3COCD_3)]^* (\textit{m/z 229}), [{}^{107}Ag(CD_3COCD_3)_2]^* (\textit{m/z 235}), \\ [{}^{107}Ag(CH_3COCH_3)(THF)]^* (\textit{m/z 239}), [{}^{109}Ag(CD_3COCD_3)(THF)]^* (\textit{m/z 245}), [(PMe_3)Au(CH_3COCH_3)]^* (\textit{m/z 331}), \\ [(PMe_3)Au(CH_2COCH_3)]D^* (\textit{m/z 332}), [(PMe_3)Au(CD_2COCD_3)]H^* (\textit{m/z 336}), [(PMe_3)Au(CD_3COCD_3)]^* (\textit{m/z 337}), \\ [(PMe_3)Au(CD_2COCD_3)]D^* (\textit{m/z 338}), [(PMe_3)Au(THF)]^* (\textit{m/z 345}), [(PMe_3)_2Au]^* (\textit{m/z 349}), [(PMe_3)_2Au_2(OH)]^* (\textit{m/z 563}), [(PMe_3)_2Au_2(CI)]^* (\textit{m/z 581}), [(PMe_3)_2Au_2({}^{37}CI)]^* (\textit{m/z 583}), [(PMe_3)_2Au_2(CH_2COCH_3)]^* (\textit{m/z 603}), \\ [(PMe_3)_2Au_2(CD_2COCD_3)]^* (\textit{m/z 608}).$

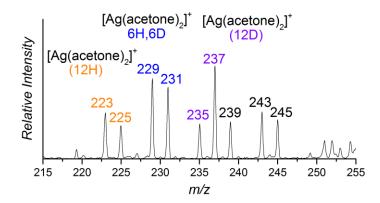


Figure S29. ESI-MS spectrum of the experiment, in which [(PMe₃)AuSbF₆] (77 μ g) was dissolved in THF (0.8 ml) and H₂O (0.56 ml) and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (0.8 ml) was added and the solution was immediately monitored by ESI-MS.

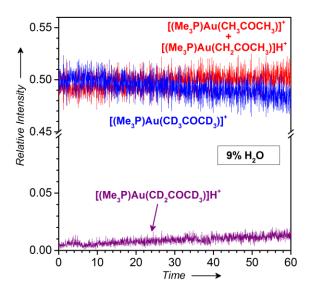


Figure S30. Results of the experiment, in which $[(PMe_3)AuSbF_6]$ (77 µg) was dissolved in THF (0.8 ml), of H₂O 0.08 ml (9% v/v) and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (0.8 ml) was added and the solution was immediately monitored by ESI-MS. The figure shows the time evolution of the relative concentration of $[(PMe_3)Au(CD_3COCD_3)]^+$ (m/z 337) with respect to the sum of both gold acetone complexes $[(PMe_3)Au(CH_3COCH_3)]^+$ and $[(PMe_3)Au(CD_2COCD_3)]D^+$. The purple lines show the evolution of the $[(PMe_3)Au(CD_2COCD_3)]H^+$ species (m/z 337).

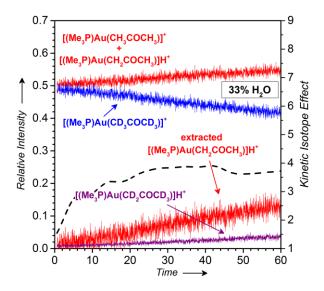


Figure S31. Results of the experiment, in which $[(PMe_3)AuSbF_6]$ (77 µg) was dissolved in THF (0.8 ml), 0.4 ml of H₂O (33% v/v) and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (0.8 ml) was added and the solution was immediately monitored by ESI-MS. The figure shows the time evolution of the relative concentration of $[(PMe_3)Au(CD_3COCD_3)]^+$ (m/z 337) with respect to the sum of both gold acetone complexes $[(PMe_3)Au(CH_3COCH_3)]^+$ and $[(PMe_3)Au(CD_2COCD_3)]D^+$. The purple lines show the evolution of the $[(PMe_3)Au(CD_2COCD_3)]H^+$ species (m/z 337).

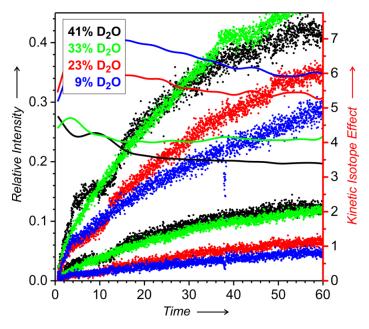


Figure S32. Time evolution of the relative concentrations $[(PMe_3)_2Au_2(CH_2COCH_3)]^*$ (*m/z* 603, the upper curves) and $[(PMe_3)_2Au_2(CD_2COCD_3)]^*$ (*m/z* 608, the lower curves) with respect to the sum of all diaurated complexes $([(PMe_3)_2Au_2OH]^*, [(PMe_3)_2Au_2CI]^*, [(PMe_3)_2Au_2(CH_2COCH_3)]^*$ and $[(PMe_3)_2Au_2(CD_2COCD_3)]^*$) in solution with D₂O. The right-hand axis refers to the kinetic isotope effect for the formation of digold acetonyls and the smoothed out ratio of $[(PMe_3)_2Au_2(CH_2COCH_3)]^*$ and $[(PMe_3)_2Au_2(CD_2COCD_3)]^*$ is shown as lines. Experiment: $[(PMe_3)AuSbF_6]$ (77 µg) was dissolved in THF (0.8 ml) and D₂O (80 – 9 % v/v in blue, 240 – 23% v/v in red, 400 – 33% v/v in green, and 560 – 41% v/v in black µL and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (0.8 ml) was added and the solution was immediately monitored by ESI-MS.

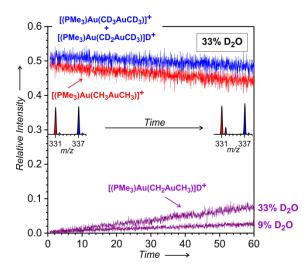


Figure S33: Results of the experiment, in which $[(PMe_3)AuSbF_6]$ (77 µg) was dissolved in THF (0.8 ml), 0.56 ml of D₂O (33% v/v) and left to react for 15 hours. Then, a 1:1 mixture of CD₃COCD₃ and CH₃COCH₃ (0.8 ml) was added and the solution was immediately monitored by ESI-MS. Time evolution of the relative concentration of $[(PMe_3)Au(CH_3COCH_3)]^+$ (m/z 331) with respect to the sum of both gold acetone complexes $[(PMe_3)Au(CD_3COCD_3)]^+$ and $[(PMe_3)Au(CD_2COCD_3)]D^+$. The purple lines show the evolution of the $[(PMe_3)Au(CH_3COCH_3)]^-$ species (m/z 332).

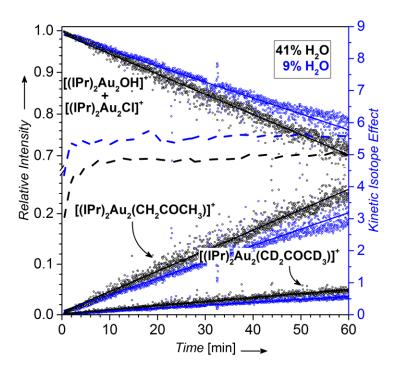


Figure S34. Results of the experiment, in which [(IPr)AuBF₄] (358 µg) was dissolved in dioxane (0.2 ml) and 0.14 ml or 0.02 ml of H₂O (41 % v/v or 9 % v/v, respectively) and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (1.4 ml) was added and the solution was immediately monitored by ESI-MS. Time evolution of the relative concentrations of [(IPr)₂Au₂OH]⁺ together with [(IPr)₂Au₂Cl]⁺ (*m/z* 1187 + *m/z* 1205 + *m/z* 1207), [(IPr)₂Au₂(CH₂COCH₃)]⁺ (*m/z* 1227) and [(IPr)₂Au₂(CD₂COCD₃)]⁺ (*m/z* 1232) with respect to the sum of all these diaurated complexes in solution with H₂O (41 % v/v in black and 9% v/v in blue; the lines serve to guide the eyes). The right-hand axis refers to the kinetic isotope effect for the formation of digold acetonyls and the smoothed out ratio of [(IPr)₂Au₂(CH₂COCH₃)]⁺ and [(IPr)₂Au₂(CD₂COCD₃)]⁺ is shown as dashed lines.

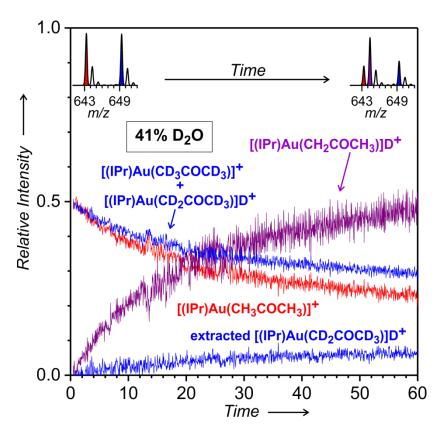


Figure S35: Results of the experiment, in which [(IPr)AuBF₄] (358 µg) was dissolved in dioxane (0.2 ml), 41% of D₂O (0.14 ml) and left to react for 15 hours. Then, a 1:1 mixture of CH₃COCH₃ and CD₃COCD₃ (1.4 ml) was added and the solution was immediately monitored by ESI-MS. Time evolution of the relative concentration of [(IPr)Au(CH₃COCH₃)]⁺ (m/z 643) with respect to the sum of both gold acetone complexes [(IPr)Au(CD₃COCD₃)]⁺ and [(IPr)Au(CD₂COCD₃)]D⁺. The purple lines show the evolution of the [(IPr)Au(CH₂COCH₃)]D⁺ species.

C-H activation

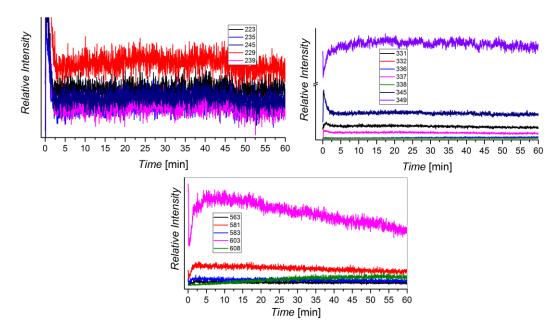


Figure S36. Results of the experiment, in which a final solution was prepared by addition of 0.4 ml of CD_3COCD_3 to an overnight reaction mixture of [(PMe₃)AuSbF₆] (77 µg) in THF (0.8 ml), H₂O (0.6 ml) and CH₃COCH₃ (0.4 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ion was normalized to TIC.

 $[({}^{107}Ag(CH_3COCH_3)_2]^+ (m/z 223), [{}^{107}Ag(CH_3COCH_3)(CD_3COCD_3)]^+ (m/z 229), [{}^{107}Ag(CD_3COCD_3)_2]^+ (m/z 235), \\ [{}^{107}Ag(CH_3COCH_3)(THF)]^+ (m/z 239), [{}^{109}Ag(CD_3COCD_3)(THF)]^+ (m/z 245), ([(PMe_3)Au(CH_3COCH_3)]^+ (m/z 331), \\ [(PMe_3)Au(CH_2COCH_3)]D^+ (m/z 332), [(PMe_3)Au(CD_2COCD_3)]H^+ (m/z 336), [(PMe_3)Au(CD_3COCD_3)]^+ (m/z 337), \\ [(PMe_3)Au(CD_2COCD_3)]D^+ (m/z 338), [(PMe_3)Au(THF)]^+ (m/z 345), [(PMe_3)_2Au]^+ (m/z 349), [(PMe_3)_2Au_2(OH)]^+ \\ (m/z 563), [(PMe_3)_2Au_2(CI)]^+ (m/z 581), [(PMe_3)_2Au_2({}^{37}CI)]^+ (m/z 583), [(PMe_3)_2Au_2(CH_2COCH_3)]^+ (m/z 603), \\ [(PMe_3)_2Au_2(CD_2COCD_3)]^+ (m/z 608).$

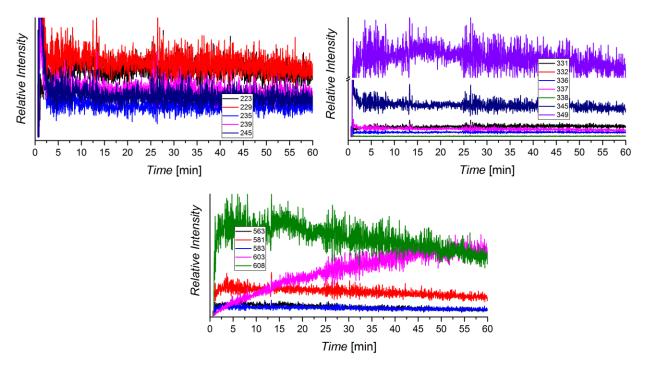


Figure S37. Results of the experiment, in which a final solution was prepared by addition of 0.4 ml of CH_3COCH_3 to an overnight reaction mixture of [(PMe₃)AuSbF₆] (77 µg) in THF (0.8 ml), H₂O (0.6 ml) and CD_3COCD_3 (0.4 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $\begin{bmatrix} (^{107}Ag(CH_3COCH_3)_2]^* (m/z 223), [^{107}Ag(CH_3COCH_3)(CD_3COCD_3)]^* (m/z 229), [^{107}Ag(CD_3COCD_3)_2]^* (m/z 235), \\ [^{107}Ag(CH_3COCH_3)(THF)]^* (m/z 239), [^{109}Ag(CD_3COCD_3)(THF)]^* (m/z 245), ([(PMe_3)Au(CH_3COCH_3)]^* (m/z 331), \\ [(PMe_3)Au(CH_2COCH_3)]D^* (m/z 332), [(PMe_3)Au(CD_2COCD_3)]H^* (m/z 336), [(PMe_3)Au(CD_3COCD_3)]^* (m/z 337), \\ [(PMe_3)Au(CD_2COCD_3)]D^* (m/z 338), [(PMe_3)Au(THF)]^* (m/z 345), [(PMe_3)_2Au]^* (m/z 349), [(PMe_3)_2Au_2(OH)]^* \\ (m/z 563), [(PMe_3)_2Au_2(CI)]^* (m/z 581), [(PMe_3)_2Au_2(^{37}CI)]^* (m/z 583), [(PMe_3)_2Au_2(CH_2COCH_3)]^* (m/z 603), \\ [(PMe_3)_2Au_2(CD_2COCD_3)]^* (m/z 608). \end{bmatrix}$

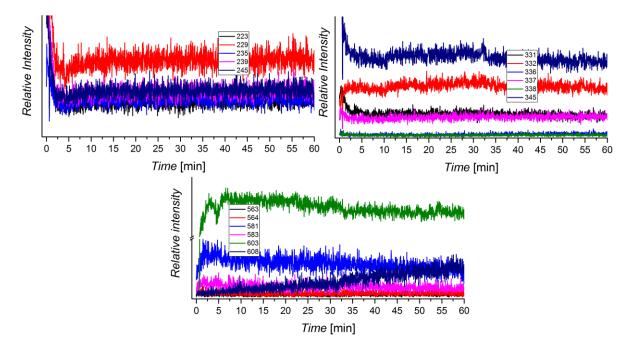


Figure S38. Results of the experiment, in which a final solution was prepared by addition of 0.4 ml of CH_3COCH_3 to an overnight reaction mixture of [(PMe_3)AuSbF₆] (77 µg) in THF (0.8 ml), D₂O (0.6 ml) and CD₃COCD₃ (0.4 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $[({}^{107}Ag(CH_3COCH_3)_2]^* (m/z 223), [{}^{107}Ag(CH_3COCH_3)(CD_3COCD_3)]^* (m/z 229), [{}^{107}Ag(CD_3COCD_3)_2]^* (m/z 235), [{}^{107}Ag(CH_3COCH_3)(THF)]^* (m/z 239), [{}^{109}Ag(CD_3COCD_3)(THF)]^* (m/z 245), ([(PMe_3)Au(CH_3COCH_3)]^* (m/z 331), [(PMe_3)Au(CH_2COCH_3)]D^* (m/z 332), [(PMe_3)Au(CD_2COCD_3)]H^* (m/z 336), [(PMe_3)Au(CD_3COCD_3)]^* (m/z 337), [(PMe_3)Au(CD_2COCD_3)]D^* (m/z 338), [(PMe_3)Au(CH_2)^* (m/z 345), [(PMe_3)_2Au]^* (m/z 349), [(PMe_3)_2Au_2(OH)]^* (m/z 563), [(PMe_3)_2Au_2(CI)]^* (m/z 581), [(PMe_3)_2Au_2({}^{37}CI)]^* (m/z 583), [(PMe_3)_2Au_2(CH_2COCH_3)]^* (m/z 603), [(PMe_3)_2Au_2(CD_2COCD_3)]^* (m/z 608).$

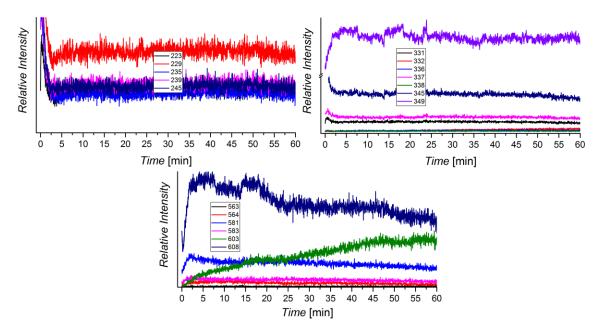


Figure S39. Results of the experiment, in which a final solution was prepared by addition of 0.4 ml of CD_3COCD_3 to an overnight reaction mixture of [(PMe₃)AuSbF₆] (77 µg) in THF (0.8 ml), D₂O (0.6 ml) and CH₃COCH₃ (0.4 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $[({}^{107}Ag(CH_3COCH_3)_2]^+ (m/z 223), [{}^{107}Ag(CH_3COCH_3)(CD_3COCD_3)]^+ (m/z 229), [{}^{107}Ag(CD_3COCD_3)_2]^+ (m/z 235), \\ [{}^{107}Ag(CH_3COCH_3)(THF)]^+ (m/z 239), [{}^{109}Ag(CD_3COCD_3)(THF)]^+ (m/z 245), ([(PMe_3)Au(CH_3COCH_3)]^+ (m/z 331), \\ [(PMe_3)Au(CH_2COCH_3)]D^+ (m/z 332), [(PMe_3)Au(CD_2COCD_3)]H^+ (m/z 336), [(PMe_3)Au(CD_3COCD_3)]^+ (m/z 337), \\ [(PMe_3)Au(CD_2COCD_3)]D^+ (m/z 338), [(PMe_3)Au(THF)]^+ (m/z 345), [(PMe_3)_2Au]^+ (m/z 349), [(PMe_3)_2Au_2(OH)]^+ \\ (m/z 563), [(PMe_3)_2Au_2(CI)]^+ (m/z 581), [(PMe_3)_2Au_2({}^{37}CI)]^+ (m/z 583), [(PMe_3)_2Au_2(CH_2COCH_3)]^+ (m/z 603), \\ [(PMe_3)_2Au_2(CD_2COCD_3)]^+ (m/z 608).$

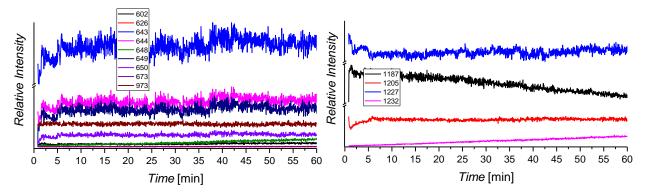


Figure S40. Results of the experiment, in which a final solution was prepared by addition of 0.7 ml of CD_3COCD_3 to an overnight reaction mixture of [(IPr)AuBF₄] (358 µg) in dioxane (0.2 ml), H₂O (0.45 ml) and CH₃COCH₃ (0.7 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $([(IPr)Au(H_2O)]^+ (m/z 602), [(IPr)Au(CH_3CN)]^+ (m/z 626), [(IPr)Au(CH_3COCH_3)]^+ (m/z 643), [(IPr)Au(CH_3COCH_3)]^+ (m/z 644), [(IPr)Au(CD_2COCH_3)]H^+ (m/z 648), [(IPr)Au(CD_3COCD_3)]^+ (m/z 649), [(IPr)Au(^{13}CH_3COCH_3)]^+ (m/z 650), [(IPr)_2Au(CH_3COCH_3)]^+ (m/z 973), [(IPr)_2Au_2(OH)]^+ (m/z 1187), [(IPr)_2Au_2(CI)]^+ (m/z 1205), [(IPr)_2Au_2(CH_2COCH_3)]^+ (m/z 1227), [(IPr)_2Au_2(CD_2COCD_3)]^+ (m/z 1232).$

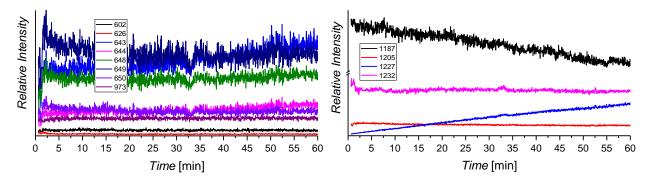


Figure S41. Results of the experiment, in which a final solution was prepared by addition of 0.7 ml of CH_3COCH_3 to an overnight reaction mixture of [(IPr)AuBF₄] (358 µg) in dioxane (0.2 ml), H₂O (0.45 ml) and CD_3COCD_3 (0.7 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

([(IPr)Au(H₂O)]⁺ (*m/z* 602), [(IPr)Au(CH₃CN)]⁺ (*m/z* 626), [(IPr)Au(CH₃COCH₃)]⁺ (*m/z* 643), [(IPr)Au(CH₃COCH₃)]⁺ (*m/z* 644), [(IPr)Au(CD₂COCH₃)]H⁺ (*m/z* 648), [(IPr)Au(CD₃COCD₃)]⁺ (*m/z* 649), [(IPr)Au(¹³CH₃COCH₃)]⁺ (*m/z* 650), [(IPr)₂Au(CH₃COCH₃)]⁺ (*m/z* 973), [(IPr)₂Au₂(OH)]⁺ (*m/z* 1187), [(IPr)₂Au₂(CI)]⁺ (*m/z* 1205), [(IPr)₂Au₂(CH₂COCH₃)]⁺ (*m/z* 1227), [(IPr)₂Au₂(CD₂COCD₃)]⁺ (*m/z* 1232).

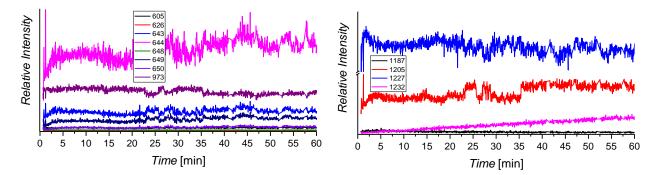


Figure S42. Results of the experiment, in which a final solution was prepared by addition of 0.7 ml of CD_3COCD_3 to an overnight reaction mixture of [(IPr)AuBF₄] (358 µg) in dioxane (0.2 ml), D₂O (0.45 ml) and CH₃COCH₃ (0.7 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

 $([(IPr)Au(H_2O)]^+ (m/z 602), [(IPr)Au(CH_3CN)]^+ (m/z 626), [(IPr)Au(CH_3COCH_3)]^+ (m/z 643), [(IPr)Au(CH_3COCH_3)]^+ (m/z 644), [(IPr)Au(CD_2COCH_3)]H^+ (m/z 648), [(IPr)Au(CD_3COCD_3)]^+ (m/z 649), [(IPr)Au(^{13}CH_3COCH_3)]^+ (m/z 650), [(IPr)_2Au(CH_3COCH_3)]^+ (m/z 973), [(IPr)_2Au_2(OH)]^+ (m/z 1187), [(IPr)_2Au_2(CI)]^+ (m/z 1205), [(IPr)_2Au_2(CH_2COCH_3)]^+ (m/z 1227), [(IPr)_2Au_2(CD_2COCD_3)]^+ (m/z 1232).$

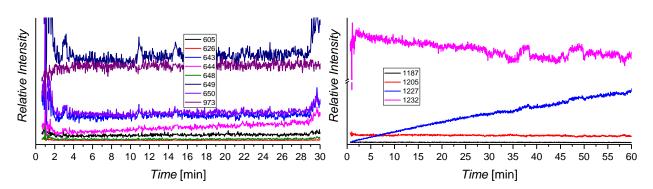


Figure S43. Results of the experiment, in which a final solution was prepared by addition of 0.7 ml of CH_3COCH_3 to an overnight reaction mixture of [(IPr)AuBF₄] (358 µg) in dioxane (0.2 ml), D₂O (0.45 ml) and CD₃COCD₃ (0.7 ml). Then the solution was immediately monitored by ESI-MS. The sum of the signal intensities of the ions was normalized to TIC.

([(IPr)Au(H₂O)]⁺ (*m/z* 602), [(IPr)Au(CH₃CN)]⁺ (*m/z* 626), [(IPr)Au(CH₃COCH₃)]⁺ (*m/z* 643), [(IPr)Au(CH₃COCH₃)]⁺ (*m/z* 644), [(IPr)Au(CD₂COCH₃)]H⁺ (*m/z* 648), [(IPr)Au(CD₃COCD₃)]⁺ (*m/z* 649), [(IPr)Au(¹³CH₃COCH₃)]⁺ (*m/z* 650), [(IPr)₂Au(CH₃COCH₃)]⁺ (*m/z* 973), [(IPr)₂Au₂(OH)]⁺ (*m/z* 1187), [(IPr)₂Au₂(CI)]⁺ (*m/z* 1205), [(IPr)₂Au₂(CH₂COCH₃)]⁺ (*m/z* 1227), [(IPr)₂Au₂(CD₂COCD₃)]⁺ (*m/z* 1232).

ESI-MS source and CID spectra

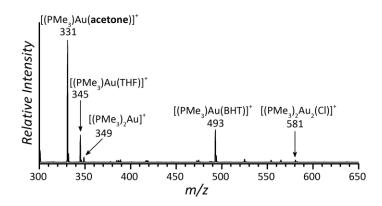


Figure S44. The ESI-MS source spectrum of $[(PMe_3)Au(SbF_6)]$ (77 µg) complex in dry THF (0.8 ml) and acetone (0.4 ml).

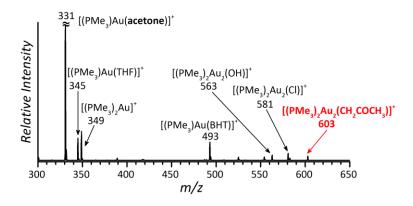


Figure S45. The ESI-MS source spectrum of $[(PMe_3)Au(SbF_6)]$ (77 µg) complex in dry THF (0.8 ml) and acetone (0.4 ml), upon water (0.4 ml) addition.

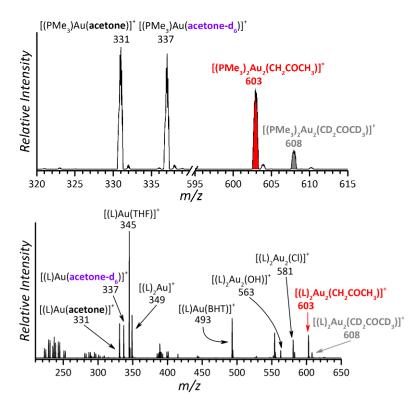


Figure S46. The ESI-MS source spectrum of $[(PMe_3)Au(SbF_6)]$ (77 µg) complex in THF (0.8 ml), acetone (0.4 ml) and acetone-d₆ (0.4 ml), upon water (0.8 ml) addition. (L= PMe₃)

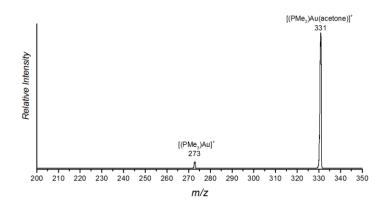


Figure S47: CID (Collision Induced Dissociation) experiment for the mass selected [(PMe₃)Au(acetone)]⁺ ion with m/z 331. The main fragmentation channel leads to the loss of acetone.

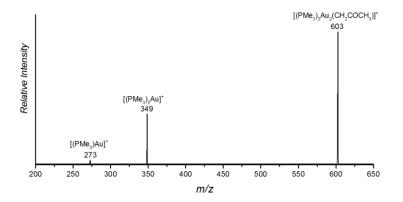
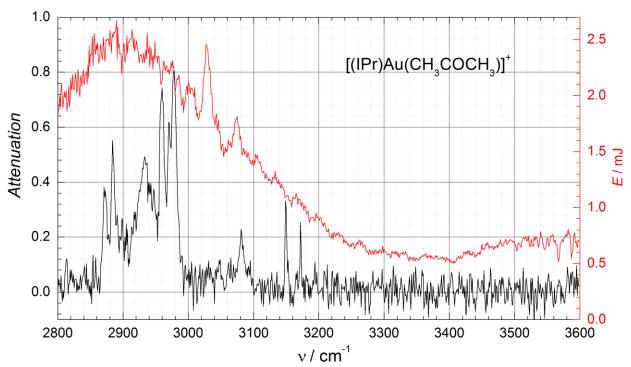


Figure S48: CID (Collision Induced Dissociation) experiment for the mass selected $[(PMe_3)_2Au_2(CH_2COCH_3)]^+$ ion with m/z 603. The main fragmentation channels is the loss of neutral Au(CH₂COCH₃).



IRPD spectrum for [Au(IPr)(BF₄)]

Figure 49: IRPD spectrum (in black) of the mass selected ion [(IPr)Au(CH₃COCH₃)]⁺ with m/z 643 and the power of the OPO/OPA is in red.

Computational results

Table S1. Geometries and energetics for the stationary points on the potential energy surface shown in Figure 9 ofthe main document. The structures were optimized at the M06-D3/6-311+G*(SDD:Au) + SMD (water) level oftheory.

А	TT1.log
	Low frequencies5.3789 -0.0012 -0.0012 -0.0011 10.2867 16.2408
	Low frequencies 29.3364 33.1439 40.8786
	Zero-point correction= 0.328056 (Hartree/Particle)
	Thermal correction to Energy= 0.354632
	Thermal correction to Enthalpy= 0.355576
	Thermal correction to Gibbs Free Energy= 0.268380
	Sum of electronic and zero-point Energies= -1462.117529
	Sum of electronic and thermal Energies= -1462.090952
	Sum of electronic and thermal Enthalpies= -1462.090008
	Sum of electronic and thermal Free Energies= -1462.177204
	C,0,1.5959369042,-2.5388430028,-0.4231908803
	P,0,2.4493859503,-0.9445709425,-0.5487412296
	Au,0,1.188515906,0.8014901682,0.2276594539
	Au,0,-1.8228314463,1.3458263612,0.1756722729
	0,0,-0.0902121776,2.4166902996,0.8667680309
	C,0,4.0351261932,-1.2016322643,0.2891050707
	C,0,2.8676005037,-0.7990772574,-2.3066095783
	0,0,5.0352429967,1.8187130612,-1.0159037748
	C,0,4.1786053506,2.5319767112,-0.5157638673
	C,0,3.2328130581,3.327821082,-1.3500034999
	C,0,4.0403341232,2.6660554376,0.9652690657
	P,0,-3.6003170127,0.1633550691,-0.6462378873
	C,0,-4.7487617532,-0.4532498776,0.6123333155
	C,0,-3.0769275183,-1.3173373493,-1.5516137192
	C,0,-4.6506536438,1.0681156501,-1.8132790991
	H,0,2.2248205555,-3.3314126204,-0.8448847585
	H,0,1.3798447463,-2.7689764682,0.623931465
	H,0,0.6518498255,-2.4963509438,-0.9746637017
	H,0,-5.542076971,-1.0369850118,0.1312635261
	H,0,-4.2165951072,-1.089500836,1.3251259774
	H,0,-5.1963618021,0.3840271041,1.1550295742
	H,0,3.5284756803,3.330623818,-2.4016069626 H,0,2.2310314412,2.8829937532,-1.2582959126
	H,0,3.1499738494,4.3538986851,-0.9742349517
	H,0,4.4850538394,1.813586352,1.4859933842
	H,0,4.5737295348,3.575554069,1.2742838004
	H,0,3.4066943432,0.1346298284,-2.4905810309
	H,0,3.494922896,-1.6451014426,-2.6111394165
	H,0,1.9505252929,-0.7962729976,-2.9030552574
	H,0,4.6998050884,-0.3528051848,0.1019233712
	H,0,3.8811043318,-1.3017923109,1.3672690161
	H,0,4.5052534758,-2.1153253029,-0.0931391809
	H,0,-2.4116152725,-1.0379770621,-2.3738197409
	H,0,-2.5354918237,-1.9898140038,-0.8793594459
	H,0,-3.9522748098,-1.8389254565,-1.9557659651
	H,0,-4.0604956576,1.3936875764,-2.6744768868
	H,0,-5.4620246411,0.4164382668,-2.1574540915

	H,0,-5.0782743664,1.949468359,-1.3273387451
	H,0,-0.1106932248,2.3874515716,1.8306631691
	H,0,2.993875948,2.7917291114,1.2636210905
В	TT 2.log
-	_ 0
	Low frequencies9.3718 -0.0009 -0.0007 0.0004 9.6969 18.1289
	Low frequencies 37.5633 46.7835 50.6424
	Zero-point correction= 0.327880 (Hartree/Particle)
	Thermal correction to Energy= 0.354346
	Thermal correction to Enthalpy= 0.355290
	Thermal correction to Gibbs Free Energy= 0.270158
	Sum of electronic and zero-point Energies= -1462.114649
	Sum of electronic and thermal Energies= -1462.088183
	Sum of electronic and thermal Enthalpies= -1462.087238
	Sum of electronic and thermal Free Energies= -1462.172370
	C,0,3.2984904349,-0.9404771502,1.6196457699
	P,0,2.7005347035,-1.0239975125,-0.0878083911
	Au,0,1.2364545528,0.6636918073,-0.6134138394
	0,0,-0.1034431844,2.306960957,-1.2413568186
	C,0,-0.8161402844,2.9873944706,-0.4971092001
	C,0,-0.6990422206,2.9391055796,0.9773302713
	C,0,4.1995560917,-1.0629381796,-1.1032701833
	C,0,1.983568536,-2.6805822951,-0.2425405481
	Au,0,-0.9735491036,-0.6178821509,1.1959753678
	P,0,-2.1467916784,-1.075653648,-0.7292365152
	C,0,-1.1742831066,-1.8812282097,-2.0317096524
	0,0,0.0870974547,-0.2235920961,2.961609265
	C,0,-1.8521636166,3.869889012,-1.0820472416
	C,0,-2.8660469605,0.36679343,-1.5669984934
	C,0,-3.5596361709,-2.1837632301,-0.4745352525
	H,0,4.0105245434,-1.7546563548,1.7978144491
	H,0,3.7933361962,0.0184061121,1.7967052891
	H,0,2.4577745252,-1.036711098,2.3124009919
	H,0,-1.7907386601,-2.0104324962,-2.9289258244
	H,0,-0.3054206214,-1.2592564017,-2.2767257703
	H,0,-0.8297773991,-2.8626238964,-1.6930990704
	H,0,-2.7978957485,3.7510102445,-0.5414568667
	H,0,-1.5464581231,4.9138902352,-0.9347046703
	H,0,-1.9920747805,3.6813488274,-2.1478796432
	H,0,0.3138579006,2.6616923839,1.2844043185
	H,0,-1.010427253,3.879208328,1.4404693576
	H,0,1.7162704184,-2.8817011578,-1.2838899392
	H,0,2.7158101435,-3.4255347252,0.0899310841
	H,0,1.085034503,-2.7516936064,0.380486968
	H,0,3.9350384155,-1.1793000686,-2.1579804677
	H,0,4.7573200618,-0.1301693237,-0.9810187779
	H,0,4.8325618419,-1.9031743346,-0.7951356821
	H,0,-3.4184981743,0.9884026431,-0.8561933643
	H,0,-2.0743832831,0.9625906172,-2.0299300973
	H,0,-3.5500109714,0.0241907071,-2.3521216198
	H,0,-4.2754694949,-1.7255444451,0.2141937771
	H,0,-4.0579178127,-2.3822830698,-1.4305766038 H,0,-3.2184174296,-3.1293279452,-0.0430258684
	H,0,-3.2184174296,-3.1293279452,-0.0430238684 H,0,-0.5489064745,-0.2791807261,3.6829634416
	H,0,-1.3824827708,2.1504107667,1.3329570507
6	
C	TT_3.log

	Low frequencies22.3903 -13.5170 -0.0009 0.0008 0.0012 10.8798
	Low frequencies 29.4003 37.4171 47.3057
	Zero-point correction= 0.328356 (Hartree/Particle)
	Thermal correction to Energy= 0.354569
	Thermal correction to Enthalpy= 0.355514
	Thermal correction to Gibbs Free Energy= 0.270276
	Sum of electronic and zero-point Energies= -1462.099518
	Sum of electronic and thermal Energies= -1462.073305
	Sum of electronic and thermal Entrapies= -1462.072360
	Sum of electronic and thermal Free Energies= -1462.072500
	C,0,0.558539764,-0.3958065306,0.2137758746
	P,0,0.3011746882,-0.1594751959,1.9937864855
	Au,0,2.2650766946,0.0300918125,3.1607910881
	0,0,4.1473435715,0.1769809069,4.1700402407
	C,0,4.91859321,1.2170251061,3.9309726784
	C,0,4.4942354763,2.4298246831,3.4924448682
	C,0,-0.7556959546,1.3103962607,2.0901211527
	C,0,-0.7803931237,-1.5276573925,2.4869670553
	Au,0,4.2372316177,-0.5871988171,0.8478649169
	P,0,4.1998782509,-2.8419953522,1.222492562
	C,0,2.5878252322,-3.6243943235,0.9572449034
	0,0,4.2942057566,1.6047549608,0.6115891589
	C,0,6.37270826,0.9401609227,4.1590673353
	C,0,4.6115985075,-3.2405343761,2.9415793406
	C,0,5.3595280593,-3.8145497903,0.2285396717
	H,0,-0.4107934817,-0.4274668795,-0.2976044571
	H,0,1.1496715206,0.4327679456,-0.1887366991
	H,0,1.1490715206,0.4527079450,-0.1887506991 H,0,1.0932270699,-1.3319054366,0.0256327044
	H,0,1.8310896164,-3.1429904645,1.5854609509
	H,0,2.2892822776,-3.5366970944,-0.0911754084 H,0,2.6550090878,-4.6851035888,1.2248918151
	H,0,7.0016499731,1.8177651637,3.9864524286
	H,0,6.5378522972,0.5864707744,5.1838357708
	H,0,6.703406373,0.134047485,3.4902054387
	H,0,3.4287666072,2.6378440355,3.3840229895
	H,0,5.1917201993,3.2564656099,3.3845362401
	H,0,-1.0837868909,-1.4058841149,3.5306347082 H,0,-1.6737280496,-1.5382601592,1.8518423499
	H,0,-0.2551764936,-2.4819996056,2.3851902661
	H,0,-1.0320509762,1.5091541008,3.1292079432
	H,0,-0.2191266662,2.1792866046,1.6979536313
	H,0,-1.6645003306,1.1504274909,1.4985133699
	H,0,5.5955441534,-2.837882385,3.1990057746
	H,0,3.8657273284,-2.8080042973,3.6155357215
	H,0,4.6224762765,-4.32938055,3.0697071023
	H,0,6.3825085175,-3.4709915798,0.4054799111
	H,0,5.2802090555,-4.8728845966,0.5026274473
	H,0,5.2802090555,-4.8728845966,0.5026274473 H,0,5.1290608126,-3.6993966608,-0.8342703228
	H,0,5.1290608126,-3.6993966608,-0.8342703228 H,0,5.0764278967,1.8555756441,0.1030220214
D	H,0,4.4371077147,1.9389246656,1.5309969353 TT final.log
	່ ເມຼົາເກດເ.ເບຮ
	Low frequencies2.2232 0.0006 0.0011 0.0012 11.0027 22.8741
	Low frequencies 40.8566 42.6058 51.9501
	Low nequencies = +0.0000 +2.0000 51.0001
L	

	Zene point connection 0.220040 (Hortuge (Denticle)
	Zero-point correction= 0.328919 (Hartree/Particle)
	Thermal correction to Energy= 0.355312
	Thermal correction to Enthalpy= 0.356257
	Thermal correction to Gibbs Free Energy= 0.271753
	Sum of electronic and zero-point Energies= -1462.116318
	Sum of electronic and thermal Energies= -1462.089924
	Sum of electronic and thermal Enthalpies= -1462.088980
	Sum of electronic and thermal Free Energies= -1462.173484
	C,0,-0.1922438165,-0.1317238251,-0.052234546
	P,0,-0.1179677238,-0.0861441105,1.756858617
	C,0,1.6540920363,-0.0427097101,2.1345863116
	Au,0,-1.2629364241,1.6699879843,2.6798377146
	Au,0,0.4993353732,2.7420527725,5.1831253632
	P,0,1.4827557148,0.9243087428,6.3055686158
	C,0,0.7191672748,-0.6857565505,5.9474286572
	C,0,-0.6835023878,-1.7202070335,2.2928572548
	0,0,-2.4076740605,3.2796309826,3.625674045
	C,0,-1.7687894701,4.138944015,4.3101066099
	C,0,-2.5496530282,4.8710929245,5.3500399763
	C,0,-0.3885041388,4.4257247163,4.1325915973
	C,0,1.4236599121,1.0424666559,8.1160798639
	C,0,3.2421057431,0.6599730582,5.9435843407
	H,0,0.4036510039,-0.9721570571,-0.4263884161
	H,0,-1.2281213565,-0.2504301942,-0.3817222214
	H,0,0.2031176916,0.8014770834,-0.464405286
	H,0,1.9092315536,0.1660628377,8.5607315478
	H,0,1.9409771304,1.9466054952,8.449702569
	H,0,0.3853654191,1.0890212924,8.4573096288
	H,0,-1.9033112956,5.3417198944,6.0948752354
	H,0,-3.1295072352,5.6625192596,4.8580640907
	H,0,-3.2628829853,4.204333862,5.8430250008
	H,0,-0.0284223215,4.2766282337,3.1101172348
	H,0,-0.0423421134,5.3519583167,4.5935943723
	H,0,1.811133065,-0.0455660785,3.216830125
	H,0,2.1491342211,-0.9161711024,1.6947375827
	H,0,2.0979190243,0.8681181833,1.7220152601
	H,0,-0.6507245305,-1.7943114604,3.3838115925
	H,0,-1.7138983607,-1.8804574737,1.9628629571
	H,0,-0.0408673481,-2.4937978544,1.857086526
	H,0,3.3847765298,0.5007865991,4.8703511346
	H,0,3.8215948482,1.5374813028,6.2450797091
	H,0,3.6095241196,-0.2171164218,6.48913658
	H,0,0.8874616921,-0.9530247111,4.8996541742
	H,0,1.1647908351,-1.4583674427,6.5850791363
	H,0,-0.3581099404,-0.6428443858,6.1321938233
	0,0,1.212707628,3.4065791347,0.9226589583
	H,0,0.3274992256,3.0185457362,0.9784639278
	H,0,1.614934847,3.2268166956,1.7815383761
TCP/C	
TS B/C	TS_5.log
	Low frequencies1502.2715 -18.7825 -16.0158 0.0002 0.0012 0.0012
	Low frequencies 18.6336 37.0910 42.6323
	Zero-point correction= 0.322769 (Hartree/Particle)
	Thermal correction to Energy= 0.348425
	Thermal correction to Enthalpy= 0.349370
	Thermal correction to Gibbs Free Energy= 0.265653

	Sum of electronic and zero-point Energies= -1462.094912
	Sum of electronic and thermal Energies= -1462.069255
	Sum of electronic and thermal Enthalpies= -1462.068311
	Sum of electronic and thermal Free Energies= -1462.15202
	C,0,-1.9048226329,-1.8385441777,-1.8429689227
	P,0,-2.711747848,-0.9665625348,-0.4738114398
	C,0,-3.3733055005,-2.2773367334,0.5871107788
	Au,0,-1.3015761172,0.5169903621,0.5543604393
	Au,0,1.3755476276,-0.0893901512,-0.87752605
	0,0,0.906518869,1.5259245775,-2.1981308991
	C,0,-4.1689186528,-0.1960043927,-1.2261637723
	0,0,0.095948968,1.9212277711,1.4670612252
	C,0,0.6209742963,2.843020705,0.7645797005
	C,0,1.9434500375,3.3404130627,1.2477653004
	C,0,0.0885728979,3.3145240414,-0.4502134272
	P,0,1.8565386176,-1.6744545538,0.7082123916
	C,0,3.1308424199,-2.8941794524,0.293831473
	C,0,0.4343516998,-2.6635986641,1.2448618936
	C,0,2.4464514678,-0.8971489339,2.2385329981
	H,0,-2.6207117516,-2.5176727242,-2.3204433054
	H,0,-1.5431664299,-1.1179130571,-2.5827815703
	H,0,-1.0539213416,-2.4172207537,-1.4709971104
	H,0,-0.356198366,-1.9957052101,1.6065057772
	H,0,0.0473089775,-3.2590872344,0.4129603541
	H,0,0.7413516912,-3.3362723452,2.0544468858
	H,0,1.8426779591,3.7321294832,2.2661042517
	H,0,2.6424643016,2.4957201651,1.3024816326
	H,0,2.3661064266,4.1167806373,0.6065012544
	H,0,-0.9822084909,3.140032857,-0.5912549481
	H,0,0.4439377128,4.2882602338,-0.7883532135
	H,0,-3.9563522322,-1.8394454925,1.4020281875
	H,0,-4.0190732708,-2.9368064083,-0.004191797
	H,0,-2.555917288,-2.8651270535,1.0154698597
	H,0,-4.7707731498,0.2990658676,-0.4591078455
	H,0,-3.854301648,0.5514389485,-1.9601852425
	H,0,-4.7764117966,-0.959062957,-1.7261555523
	H,0,3.3651465398,-0.3354106174,2.0465233062
	H,0,1.6854882329,-0.2100971327,2.6223299077
	H,0,2.647423184,-1.6662862765,2.9937466531
	H,0,4.0715607036,-2.3881903911,0.0593021294
	H,0,3.2842760181,-3.5672635551,1.1450381078
	H,0,2.8200775336,-3.4780792025,-0.5770305608
	H,0,1.7232491483,1.8148062139,-2.6233881699
TCO/D	H,0,0.5854401862,2.4358570792,-1.360723681
TS C/D	C
	p 1 pc2 c 2 cp3 1 cpc3
	c $2 \text{ cp}3 \text{ i cpc}3$ c $2 \text{ cp}4 \text{ 3 cpc}4 \text{ 1 dih}4 \text{ 0}$
	au 2 aup5 3 aupc5 4 dih5 0
	o 5 oau6 2 oaup6 3 dih6 0
	c 6 co7 5 coau7 2 dih7 0
	c 7 cc8 6 cco8 5 dih8 0
	au 5 auau9 2 auaup9 1 dih9 0
	p 9 paulo 5 pauaulo 2 dihlo 0 c 10 cp11 9 cpaul1 5 dihl1 0
	o 9 oau12 5 oauau12 2 dih12 0
	c 7 cc13 6 cco13 5 dih13 0

c 10 cp14 9 cpau14 5 dih14 0 c 10 cp14 2 kpq15 5 dih15 0 h 1 hc17 2 hcp16 4 dih16 0 h 1 hc17 2 hcp17 4 dih17 0 h 1 hc17 2 hcp17 4 dih17 0 h 1 hc17 2 hcp17 9 dih19 0 h 15 hc19 10 hcp19 9 dih19 0 h 15 hc20 10 hcp20 9 dih20 0 h 13 hc22 7 hc22 6 dih22 0 h 13 hc23 7 hc23 6 dih22 0 h 13 hc23 7 hcc23 6 dih25 0 h 8 hc26 7 hcc25 6 dih25 0 h 4 hc27 2 hcp27 1 dih27 0 h 4 hc28 2 hcp28 1 dih28 0 h 4 hc27 2 hcp29 1 dih28 0 h 4 hc28 2 hcp28 1 dih28 0 h 4 hc28 2 hcp28 1 dih28 0 h 3 hc31 2 hcp23 1 dih31 0 h 3 hc32 2 hcp28 1 dih34 0 h 11 hc33 10 hcp33 9 dih33 0 h 11 hc33 10 hcp35 9 dih34 0 h 11 hc36 10 hcp35 9 dih34 0 h 11 hc36 10 hcp35 9 dih34 0 h 11 hc38 10 hcp35 9 dih34 0 h 11 hc38 10 hcp35 9 dih37 0 h 14 hc28 1 hcp38 9 dih38 0 h 14 hc28 1 hcp38 9 dih38 0 h 11 hc38 10 hcp38 9 dih38 0 h 14 hc39 10 hcp38 9 dih38 0 h 14 hc38 10 hcp38 9 dih38 0 h 15 hcm38 0 h 16 hcm38 0 dih38 0 h 17 hcm38 0 dih38 0 h 18 hcm38 0 h 18 hcm38 0 h 18 hcm38 0 h 19 hcm39 0 dih38 0 h 19 hcm30 0 h 19 hcm30 0 h 10 hcm30 0 dih38 0 h 10 hcm30 0 h 10 hcm30 0 dih38 0 h 10 hcm30 0 h 1
h1hc162hcp164dih160h1hc172hcp174dih170h1hc182hcp184dih180h15hc1910hcp199dih120h15hc2010hcp209dih200h13hc227hcc236dih220h13hc237hcc236dih240h13hc247hcc256dih260h13hc247hcc256dih260h13hc247hcc271dih280h8hc267hcc266dih260h4hc272hcp281dih280h4hc282hcp381dih290h4hc282hcp381dih310h4hc282hcp339dih330h11hc3410hcp339dih330h11hc3610hcp369dih360h14hc3610hcp369dih370h14hc3810hcp389dih380h12hc399hca349dih380h1
h1hc172hcp174dih170h1hc182hcp134dih180h15hc120hcp199dih190h15hc2110hcp219dih210h13hc227hc226dih220h13hc227hc226dih220h13hc237hc226dih240h13hc247hc236dih240h8hc257hc2256dih250h8hc267hc2646dih240h4hc272hcp271dih270h4hc272hcp271dih280h4hc282hcp301dih300h4hc282hcp321dih300h3hc312hcp311dih310h11hc3310hcp359dih350h11hc3410hcp359dih360h12hc939hc9349dih360h12hc939hc9349dih360h12hc939hc9349dih360h12 <t< th=""></t<>
h1hc182hcp184dih180h15hc1910hcp199dih1200h15hc2010hcp209dih210h15hc2210hcp219dih210h13hc227hcc236dih220h13hc247hcc236dih240h13hc247hcc256dih250h13hc247hcc256dih260h8hc267hcc266dih260h4hc272hcp281dih280h4hc282hcp281dih290h4hc282hcp311dih310h4hc282hcp321dih310h3hc302hcp321dih310h11hc3310hcp339dih340h11hc3410hcp349dih340h14hc3810hcp339dih350h14hc3810hcp349dih350h14hc3810hcp389dih380h14hc3810hcp389dih380h
h 15 hc19 10 hcp19 9 dih19 0 h 15 hc20 10 hcp20 9 dih21 0 h 15 hc21 10 hcp20 9 dih21 0 h 13 hc22 7 hcc23 6 dih23 0 h 13 hc23 7 hcc24 6 dih24 0 h 13 hc24 7 hcc24 6 dih25 0 h 8 hc26 7 hcc24 6 dih26 0 h 4 hc27 2 hcp27 1 dih27 0 h 4 hc27 2 hcp23 1 dih29 0 h 4 hc27 2 hcp31 1 dih30 0 h hc33 lc2 hcp31 1 dih30 0 h hc33 lc2 hcp32 9 dih34 0 h hc34 10
h 15 hc20 10 hcp21 9 dih20 0 h 15 hc21 10 hcp21 9 dih21 0 h 13 hc22 7 hcp21 9 dih21 0 h 13 hc23 7 hcp24 6 dih22 0 h 13 hc24 7 hcp25 6 dih24 0 h 4 hc25 7 hcp25 6 dih26 0 h 4 hc27 7 hcp28 1 dih26 0 h 4 hc27 2 hcp29 1 dih26 0 h 4 hc28 2 hcp29 1 dih30 0 h 3 hc31 10 hcp33 9 dih34 0 h 11 hc33 10 hcp34 9 dih34 0 h 11 hc33 10 hcp35 9 dih34 0 h
h 15 hc20 10 hcp21 9 dih20 0 h 15 hc21 10 hcp21 9 dih21 0 h 13 hc22 7 hcp21 9 dih21 0 h 13 hc23 7 hcp24 6 dih22 0 h 13 hc24 7 hcp25 6 dih24 0 h 4 hc25 7 hcp25 6 dih26 0 h 4 hc27 7 hcp28 1 dih26 0 h 4 hc27 2 hcp29 1 dih26 0 h 4 hc28 2 hcp29 1 dih30 0 h 3 hc31 10 hcp33 9 dih34 0 h 11 hc33 10 hcp34 9 dih34 0 h 11 hc33 10 hcp35 9 dih34 0 h
h15hc2110hc229dih210h13hc227hc226dih220h13hc237hc226dih240h13hc247hcc246dih240h8hc257hcc256dih240h8hc267hcc266dih260h4hc272hcp281dih270h4hc282hcp281dih270h4hc282hcp281dih280h4hc282hcp281dih300h3hc312hcp311dih310h1hc3310hcp349dih340h11hc3310hcp349dih340h11hc3810hcp349dih360h14hc3810hcp349dih360h14hc3810hcp349dih360h14hc3810hcp349dih360h14hc3810hcp349dih360h14hc3810hcp349dih360h14hc3810hcp349dih360h
h13h<22
h13h<23
h13hc247hcc256dih240h8hc257hcc256dih250h8hc267hcc266dih260h4hc272hcp271dih270h4hc272hcp271dih280h4hc272hcp271dih290h4hc292hcp301dih290h3hc302hcp311dih300h3hc312hcp311dih310h11hc3310hcp349dih340h11hc3310hcp349dih350h11hc3310hcp359dih350h11hc3810hcp359dih350h12hc9399hc93195dih350h12hc9399hc93195dih350h12hc9399hc93195dih350h12hc9399hc93195dih350h12hc9399hc93195dih350h12hc9399hc93195dih350h12hc9399hc93195dih450 <td< th=""></td<>
h8h<25
h8hc267hc266dih260h4hc272hcp271dih270h4hc282hcp281dih280h4hc292hcp291dih290h3hc302hcp311dih310h3hc312hcp311dih310h3hc312hcp321dih330h11hc3310hcp339dih340h11hc3310hcp359dih350h11hc3710hcp359dih370h14hc3810hcp389dih380h14hc3810hcp389dih380h12hc909hoau<95dih400h12hc909hoau<95dih400Variables:yyhoau<95dih400Variables:yyyyyyycp31.81282yyyyyycp41.81356yyyyyycp41.81356yyyyyydih4-109.173yyyyyy
h4hc272hcp271dih270h4hc282hcp281dih280h4hc292hcp291dih290h3hc312hcp301dih300h3hc312hcp311dih310h3hc322hcp339dih330h11hc3310hcp339dih320h11hc3410hcp349dih350h11hc3510hcp359dih350h14hc3610hcp379dih350h14hc3810hcp379dih350h14hc3810hcp389dih350h14hc3810hcp389dih350h14hc3810hcp389dih350h14hc3810hcp389dih350h12hc909hc9199dih350h12hc939hc9389dih350h12hc939hc9389dih350h12hc939hc9389dih350h12hc949hc9485dih490h
h4hc282hc281dih280h4hc292hc291dih290h3hc312hcp301dih300h3hc312hcp311dih310h3hc322hcp321dih330h11hc3310hcp329dih30h11hc3310hcp339dih30h11hc3310hcp359dih30h11hc3310hcp359dih350h11hc3710hcp359dih350h14hc3810hcp359dih360h14hc3810hcp359dih360h14hc3810hcp359dih360h12hc939hcp350h0h12hc939hcp350h0h12hc939hcp350h0h12hc939hcp350h0h12hc939hcp350h0h12hc939hcp349dih360h12hc939hcp345dih360h12hc93<
h4hc292hcp291dih290h3hc302hcp301dih300h3hc312hcp311dih310h3hc322hcp321dih310h11hc3310hcp339dih330h11hc3310hcp339dih340h11hc3510hcp349dih340h11hc3510hcp359dih350h14hc3610hcp359dih360h14hc3610hcp379dih360h14hc3710hcp379dih360h12ho399hoau395dih360h12ho409hoau405dih400Variables:Variables:Variables:Variables:Variables:Variablescp31.812821.81282i.81285i.81285i.81285i.81285cp4104.358i.81285i.81285i.81285i.81285i.81285dih4-109.173i.81285i.81285i.81285i.81285dih4-109.173i.81285i.81285i.81285i.81285dih4-109.173i.81285i.81285i.81285i.81285dih4-109.173i.81285
h3hc302hc301dih300h3hc312hc311dih310h3hc322hc9321dih320h11hc3310hc9339dih320h11hc3310hc9339dih340h11hc3510hc9359dih350h11hc3610hc9359dih360h14hc3610hc9379dih370h14hc3710hc9379dih380h14hc3710hc9379dih380h14hc3810hc9389dih380h14hc3810hc9389dih380h14hc3810hc9389dih380h12hc399hcau395dih390h12hc399hcau395dih400Variables:variables:variables:variables:variables:variables:pc41.81356variables:variables:variables:variables:variables:dih4-109.173aup52.2946variables:variables:variables:
h3hc312hcp311dih310h3hc222hcp321dih320h11hc3310hcp339dih330h11hc3410hcp349dih340h11hc3510hcp359dih350h11hc3610hcp369dih360h14hc3710hcp379dih370h14hc3810hcp389dih380h14hc3810hcp389dih390h12ho409hoau405dih400Variables: </th
h3 $hc32$ 2 $hcp33$ 1 $dih32$ 0h11 $hc33$ 10 $hcp33$ 9 $dih33$ 0h11 $hc34$ 10 $hcp34$ 9 $dih34$ 0h11 $hc35$ 10 $hcp35$ 9 $dih35$ 0h14 $hc36$ 10 $hcp36$ 9 $dih36$ 0h14 $hc37$ 10 $hcp37$ 9 $dih37$ 0h14 $hc38$ 10 $hcp38$ 9 $dih38$ 0h12 $ho39$ 9 $hoau39$ 5 $dih40$ 0Variables: $pc2$ 1.81408 $cp3$ 1.81282 $cp3$ 1.81282 cpc3 104.069 $cp4$ 1.81356 $cp4$ 104.358 $dih4$ -109.173 $aup5$ 2.2946 2.2946 $adas$ $adas$ $adas$ $adas$
h11hc3310hcp339dih330h11hc3410hcp349dih340h11hc3510hcp359dih350h14hc3610hcp369dih360h14hc3710hcp379dih370h14hc3810hcp389dih380h12ho399hoau395dih390h12ho409hoau405dih400Variables:pc21.81408cp31.81282cp31.81282cp41.81356cp41.81356cpc4104.358dih4-109.173aup52.2946.
h11hc3410hcp349dih340h11hc3510hcp359dih350h14hc3610hcp369dih360h14hc3710hcp379dih370h12hc389hcau395dih380h12hc999hcau395dih390h12hc909hcau395dih400Variables:yyyyycp31.81282yyyyycp41.81356yyyyycp41.09.173yyyyyaup52.2946yyyyy
h 11 hc35 10 hcp35 9 dih35 0 h 14 hc36 10 hcp36 9 dih36 0 h 14 hc37 10 hcp37 9 dih37 0 h 14 hc37 10 hcp37 9 dih38 0 h 14 hc38 10 hcp38 9 dih39 0 h 12 ho39 9 hoau39 5 dih39 0 h 12 ho40 9 hoau40 5 dih40 0 Variables: variables: variables: variables: variables: variables: variables: pc2 1.81408 variables: variables: variables: variables: variables: cpc3 104.069 variables: variables: variables: variables: variables: dih4 -109.173 aup5 2.2946 variables: variables: variables:
h14hc3610hcp369dih360h14hc3710hcp379dih370h14hc3810hcp389dih380h12ho399hoau395dih400h12ho409hoau405dih400Variables:pc21.81408sssspc21.81408sssssscp31.81282sssssscp41.81356sssssscpc41.09.173ssssssaup52.2946ssssss
h14hc3610hcp369dih360h14hc3710hcp379dih370h14hc3810hcp389dih380h12ho399hoau395dih400h12ho409hoau405dih400Variables:pc21.81408sssspc21.81408sssssscp31.81282sssssscp41.81356sssssscpc41.09.173ssssssaup52.2946ssssss
h14hc3710hcp379dih370h14hc3810hcp389dih380h12ho399hoau395dih400h12ho409hoau405dih400Variables:pc21.81408cp31.81282555cpc3104.0695555cpc41.813565555cpc41.09.1735555aup52.29465555
h 12 ho39 9 hoau39 5 dih49 0 h 12 ho40 9 hoau40 5 dih40 0 Variables: pc2 1.81408 5 dih40 0 cp3 1.81282 5 dih40 0 cpc3 104.069 5 5 5 5 cpc4 1.81356 5 5 5 5 5 cpc4 1.04.358 5 5 5 5 5 5 dih4 -109.173 5 2.2946 5 5 5 5 5
h 12 ho39 9 hoau39 5 dih49 0 h 12 ho40 9 hoau40 5 dih40 0 Variables: pc2 1.81408 5 dih40 0 cp3 1.81282 5 dih40 0 cpc3 104.069 5 5 5 5 cpc4 1.81356 5 5 5 5 5 cpc4 1.04.358 5 5 5 5 5 5 dih4 -109.173 5 2.2946 5 5 5 5 5
h 12 ho40 9 hoau40 5 dih40 0 Variables: pc2 1.81408 1.81282 1.81282 cp3 1.81282 104.069 1.81356 1.81356 cpc4 1.81356 1.41358 1.41358 dih4 -109.173 1.41358 1.41356 aup5 2.2946 1.41358 1.41358
Variables: pc2 1.81408 cp3 1.81282 cpc3 104.069 cp4 1.81356 cpc4 104.358 dih4 -109.173 aup5 2.2946
pc2 1.81408 cp3 1.81282 cpc3 104.069 cp4 1.81356 cpc4 104.358 dih4 -109.173 aup5 2.2946
cp3 1.81282 cpc3 104.069 cp4 1.81356 cpc4 104.358 dih4 -109.173 aup5 2.2946
cpc3 104.069 cp4 1.81356 cpc4 104.358 dih4 -109.173 aup5 2.2946
cp4 1.81356 cpc4 104.358 dih4 -109.173 aup5 2.2946
cpc4 104.358 dih4 -109.173 aup5 2.2946
dih4 -109.173 aup5 2.2946
aup5 2.2946
aupc5 115.288
dih5 -127.04
oau6 2.14934
oaup6 177.44
dih6 167.433
co7 1.3131
coau7 117.478
dih7 99.555
cc8 1.36469
cco8 125.026
dih8 23.221
auau9 3.13864
auaup9 99.345
dih9 -6.781
pau10 2.30615
pauau10 89.972
dih10 -90.115
cp11 1.8145
cpau11 112.333
dih11 -78.788
oau12 2.34156
oauau12 99.151
dih12 69.195

cc13	1.49741
cco13	114.119
dih13	-156.794
cp14	1.81371
cpau14	117.008
dih14	160.479
cp15	1.81541
cpau15	114.021
dih15	38.556
hc16	1.09627
hcp16	109.496
dih16	52.154
hc17	1.09413
hcp17	109.796
dih17	171.926
hc18	1.09469
hcp18	110.473
dih18	-68.115
hc19	1.0961
hcp19	109.339
dih19	-54.335
hc20	1.09415
hcp20	110.341
dih20	65.697
hc21	1.09658
hcp21	109.491
dih21	-174.266
hc22	1.09348
hcc22	112.342
dih22	176.519
hc23	1.09716
hcc23	109.868
dih23	-62.815
hc24	1.09666
hcc24	110.653
dih24	54.676
hc25	1.09036
hcc25	119.856
dih25	11.071
hc26	1.08704
hcc26	120.416
dih26	175.752
hc27	1.09358
hcp27	110.161
dih27	-178.079
hc28	1.09626
hcp28	109.527
dih28	-58.051
hc29	1.09401
hcp29	110.216
dih29	61.987
hc30	1.09382
hcp30	110.097
dih30	173.132
hc31	1.09361
hcp31	110.134
dih31	-67.045
hc32	1.0962

hcp32	109.539
dih32	53.173
hc33	1.09391
hcp33	110.111
dih33	-59.999
hc34	1.09484
hcp34	109.712
dih34	59.792
hc35	1.09628
hcp35	109.746
dih35	179.742
hc36	1.09364
hcp36	110.155
dih36	58.276
hc37	1.0966
hcp37	109.732
dih37	178.51
hc38	1.09383
hcp38	109.87
dih38	-61.348
ho39	0.96537
hoau39	108.913
dih39	-140.998
ho40	0.96601
hoau40	108.405
dih40	103.768
	dih32 hc33 hcp33 dih33 hc34 hcp34 dih34 hc35 hcp35 dih35 hc36 hcp36 dih36 hc37 hcp37 dih37 hc937 dih37 hc938 dih38 hcp38 dih38 hc39 hoau39 dih39 ho40 hoau40

Table S2. Geometries and energetics for the calculated structures used for comparison of theoretical IR spectra with the helium tagging IRPD spectra. The structures were optimized at the B3LYP-D3/6-311+G*(SDD:Au) level of theory.

1a	Ac_vicAu2_a.log
	Low frequencies10.2622 -5.7938 -0.0016 -0.0015 -0.0010 4.6865 Low frequencies 17.5840 21.0821 24.7129
	Zero-point correction=0.305835 (Hartree/Particle)Thermal correction to Energy=0.330142Thermal correction to Enthalpy=0.331086Thermal correction to Gibbs Free Energy=0.246576Sum of electronic and zero-point Energies=-1386.139746Sum of electronic and thermal Energies=-1386.115440Sum of electronic and thermal Enthalpies=-1386.114495Sum of electronic and thermal Free Energies=-1386.199005
	C,0,-1.5794719191,-0.5911120762,-0.0575535581 O,0,-1.8761441338,-0.8476907576,1.1455715663 C,0,-0.3197996271,-0.0296457937,-0.4715909785 C,0,-2.6370048262,-0.9089194645,-1.0769973427 Au,0,1.0007442179,-1.730785051,-0.5176177114 H,0,2.554618238,-5.8206539961,-1.470541242 C,0,2.9652934085,-4.1842361272,1.0590367107 C,0,4.0702953402,-3.1781061529,-1.4240394504 C,0,1.8230459717,-5.0090016961,-1.4698884509 P,0,2.4813579896,-3.5438455922,-0.5902375004

	Au,0,-0.5294220071,-0.7799726894,2.7766284028
	P,0,0.8532091239,-0.7561073153,4.5863541822
	C,0,2.4570334318,-1.5761304528,4.2639513554
	C,0,1.2807804164,0.9316544896,5.1437620046
	C,0,0.168250492,-1.5929953116,6.0599750612
	H,0,3.881850471,-2.8696082454,-2.4534072422
	H,0,4.7172450164,-4.0585823349,-1.4282483225
	H,0,4.5807149644,-2.3610561408,-0.9118954665
	H,0,3.4528399696,-3.3942031886,1.6322380055
	H,0,2.0758474679,-4.5098529146,1.6008035242
	H,0,3.6516531483,-5.028603963,0.9610778708
	H,0,1.5843673824,-4.743196574,-2.500730562
	H,0,0.9079078172,-5.352283106,-0.985046097
	H,0,2.2896271827,-2.6242634775,4.0124908631
	H,0,3.1019253561,-1.5172816728,5.1436648867
	H,0,2.9520012179,-1.089968911,3.4220787352
	H,0,1.7699116945,1.4771419396,4.335635912
	H,0,0.3730698208,1.4693515353,5.4208458318
	H,0,1.9497948646,0.8899052771,6.006539065
	H,0,0.8815536066,-1.5513653703,6.8865303587
	H,0,-0.0531263176,-2.6354997632,5.8276871604
	H,0,-0.7589318006,-1.1046552218,6.3628964461
	H,0,-0.3323235763,0.4115058187,-1.4673708635
	H,0,-2.2071585652,-1.0984506753,-2.0609137775
	H,0,-3.2401922712,-1.7572258044,-0.7545285888
	H,0,-3.3001967841,-0.0411193989,-1.1634527353
	H,0,0.1155208153,0.6447951492,0.2682671823
1b	Ac_vicAu2_b.log
	Low frequencies0.9640 -0.0017 -0.0016 0.0010 3.0678 8.9078
	Low frequencies0.9640 -0.0017 -0.0016 0.0010 3.0678 8.9078 Low frequencies 13.9729 15.0821 22.7241
	Low frequencies0.9640 -0.0017 -0.0016 0.0010 3.0678 8.9078 Low frequencies 13.9729 15.0821 22.7241
	Low frequencies 13.9729 15.0821 22.7241
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle)
	Low frequencies13.972915.082122.7241Zero-point correction=0.306015 (Hartree/Particle)Thermal correction to Energy=0.330260
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065 Au,0,-2.2615103943,7.005626816,1.5966759311
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.11509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065 Au,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Energies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065 Au,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065 Au,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262 C,0,-0.6255825997,-1.4752868154,2.2130815815
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction= 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.599074648,5.1735489692,2.5763312065 Au,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262 C,0,-0.6255825997,-1.4752868154,2.2130815815 C,0,-1.4776223147,10.352852932,1.5771054494
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Energies= -1386.11509 Sum of electronic and thermal Free Energies= -1386.11509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.752752001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262 C,0,-0.6255825997,-1.4752868154,2.2130815815 C,0,-1.4776223147,10.352852932,1.5771054494 C,0,-0.8222951631,8.9328639856,-0.8728658387
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Enthalpies= -1386.111509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.7527522001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262 C,0,-0.6255825997,-1.4752868154,2.2130815815 C,0,-1.4776223147,10.352852932,1.5771054494 C,0,-0.8222951631,8.9328639856,-0.8728658387 H,0,2.2472133082,-0.6352817043,1.6587934454
	Low frequencies 13.9729 15.0821 22.7241 Zero-point correction = 0.306015 (Hartree/Particle) Thermal correction to Energy= 0.330260 Thermal correction to Enthalpy= 0.331204 Thermal correction to Gibbs Free Energy= 0.246159 Sum of electronic and zero-point Energies= -1386.136698 Sum of electronic and thermal Energies= -1386.112453 Sum of electronic and thermal Energies= -1386.11509 Sum of electronic and thermal Free Energies= -1386.11509 Sum of electronic and thermal Free Energies= -1386.196554 C,0,-0.1192432291,0.3072383951,-0.014223764 P,0,-0.0389572484,0.2132886889,1.8137193073 C,0,1.752752001,0.1783668031,2.1950348241 Au,0,-1.2217002529,1.8982795199,2.92807087 C,0,-2.3895195383,3.3468713905,4.0258918622 C,0,-1.9530105518,4.6075602529,3.5087045876 C,0,-0.7163436417,5.2708529039,4.0605429419 O,0,-2.2615103943,7.005626816,1.5966759311 P,0,-2.0342161673,8.9884595973,0.4949971214 C,0,-3.5907044653,9.5770392943,-0.2622213262 C,0,-0.6255825997,-1.4752868154,2.2130815815 C,0,-1.4776223147,10.352852932,1.5771054494 C,0,-0.8222951631,8.9328639856,-0.8728658387

	H,0,-1.6759782861,-1.578143605,1.9366926878
	H,0,-1.1581921388,0.2470654164,-0.3417175525
	H,0,0.2924696314,1.2586935516,-0.3540875378
	H,0,0.4466941762,-0.5098476662,-0.4681513088
	H,0,1.8984359051,0.0390544265,3.2672645736
	H,0,2.2112945028,1.1257656661,1.9077914232
	H,0,-2.1970120625,10.5029106934,2.3831773472
	H,0,-1.3839479566,11.2781515913,1.0038083838
	H,0,-0.511241815,10.1060844926,2.0187168719
	H,0,0.1596669818,8.6550084656,-0.4876391876
	H,0,-1.1280986774,8.1881459233,-1.6088178561
	H,0,-0.7535809709,9.9091642647,-1.3585153109
	H,0,-3.4259934791,10.5272161125,-0.7758798041
	H,0,-4.349548955,9.713291595,0.5093840761
	H,0,-3.9569062338,8.8406910887,-0.9787601358
	H,0,-2.1127011027,3.1697771863,5.0651325482
	H,0,-0.2034871973,4.653581213,4.7967069713
	H,0,-0.0260564731,5.5062457242,3.2460469563
	H,0,-1.0043867409,6.2177466468,4.5278940835 H,0,-3.4339761575,3.1248052248,3.8121444088
1c	Ac_gemAu2.log
	Low frequencies5.1170 -0.0016 -0.0013 -0.0006 5.2292 10.4035
	Low frequencies 13.1970 15.8705 23.6205
	Zara point correction _ 0.206322 (Hartroo/Darticla)
	Zero-point correction= 0.306233 (Hartree/Particle)
	Thermal correction to Energy= 0.330885
	Thermal correction to Enthalpy= 0.331829
	Thermal correction to Gibbs Free Energy= 0.245657
	Sum of electronic and zero-point Energies= -1386.121260
	Sum of electronic and thermal Energies= -1386.096609
	Sum of electronic and thermal Energies=-1386.096609Sum of electronic and thermal Enthalpies=-1386.095665
	Sum of electronic and thermal Energies= -1386.096609
	Sum of electronic and thermal Energies=-1386.096609Sum of electronic and thermal Enthalpies=-1386.095665Sum of electronic and thermal Free Energies=-1386.181836
	Sum of electronic and thermal Energies=-1386.096609Sum of electronic and thermal Enthalpies=-1386.095665Sum of electronic and thermal Free Energies=-1386.181836Au,0,1.5495822403,0.2351027817,-0.1662549717
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 -1386.18132428
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.2058784305,-3.2030167728,0.9152171423
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.2058784305,-3.2030167728,0.9152171423 H,0,-2.7784122188,-2.2186115604,2.2697801636
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.2058784305,-3.2030167728,0.9152171423 H,0,-2.7784122188,-2.2186115604,2.2697801636 H,0,-3.9239948373,-3.2417417934,1.3744725767
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.2058784305,-3.2030167728,0.9152171423 H,0,-2.7784122188,-2.2186115604,2.2697801636 H,0,-3.9239948373,-3.2417417934,1.3744725767 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.1729234513,0.4020028055,0.1333860662
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.2058784305,-3.2030167728,0.9152171423 H,0,-2.7784122188,-2.2186115604,2.2697801636 H,0,-3.9239948373,-3.2417417934,1.3744725767 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.1729234513,0.4020028055,0.1333860662 H,0,-4.6434263477,0.0355472911,1.7800993387
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4121884578,-1.2486249025,-2.1366223152 H,0,-4.2168384578,-3.2030167728,0.9152171423 H,0,-2.058784305,-3.2030167728,0.9152171423 H,0,-2.058784305,-3.2030167728,0.9152171423 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.1729234513,0.4020028055,0.1333860662 H,0,-4.6434263477,0.0355472911,1.7800993387 H,0,2.5155275066,-3.1952937735,-0.98437675
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4184962071,-2.5889889419,-1.0712032615 C,0,4.9917351301,-0.3932781743,-0.0201095959 H,0,-4.2168384578,-1.2486249025,-2.1366223152 H,0,-4.7666487355,-2.6725169241,-1.2244430751 H,0,-3.1030165493,-2.5912727754,-1.8487916404 H,0,-2.058784305,-3.2030167728,0.9152171423 H,0,-2.7784122188,-2.2186115604,2.2697801636 H,0,-3.9239948373,-3.2417417934,1.3744725767 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.1729234513,0.4020028055,0.1333860662 H,0,-4.6434263477,0.0355472911,1.7800993387 H,0,2.5155275066,-3.1952937735,-0.98437675 H,0,4.2921348725,-3.2207205341,-0.8935904158
	Sum of electronic and thermal Energies= -1386.096609 Sum of electronic and thermal Enthalpies= -1386.095665 Sum of electronic and thermal Free Energies= -1386.181836 Au,0,1.5495822403,0.2351027817,-0.1662549717 Au,0,-1.550287542,0.2357305319,-0.1641332428 C,0,-0.0003448306,1.6763161247,-0.5597055669 P,0,3.3612342591,-1.2120002825,0.1350886282 P,0,-3.3602582135,-1.2131913806,0.1361530328 C,0,-3.0406313589,-2.6047949484,1.2837817577 C,0,-4.8593902463,-0.3999299634,0.8033583871 C,0,-3.9185264258,-2.0108219036,-1.4151573898 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4107271822,-2.0290856543,1.7738784502 C,0,3.4121884578,-1.2486249025,-2.1366223152 H,0,-4.2168384578,-3.2030167728,0.9152171423 H,0,-2.058784305,-3.2030167728,0.9152171423 H,0,-2.058784305,-3.2030167728,0.9152171423 H,0,-5.6750878755,-1.1195387641,0.9056373711 H,0,-5.1729234513,0.4020028055,0.1333860662 H,0,-4.6434263477,0.0355472911,1.7800993387 H,0,2.5155275066,-3.1952937735,-0.98437675

	1105070202000000000000000000000000000000
	H,0,5.0788748938,0.4002932158,0.7229738827
	H,0,5.8004744434,-1.1123754058,0.128189808
	H,0,4.2795339455,-2.6870961246,1.849734003
	H,0,2.5037514923,-2.6170772183,1.9229960299
	H,0,3.4656698835,-1.2763975276,2.5615362859
	H,0,-0.0010305697,1.9501007485,-1.6143888413
	C,0,0.0007447207,2.7811556231,0.2715195658
	0,0,0.0017820521,2.7016715008,1.6068780499
	C,0,0.0010339382,4.205053583,-0.1773937113
	H,0,0.0002217497,4.2886656605,-1.2619260346
	H,0,-0.875828017,4.7181727582,0.2278165232
	H,0,0.8790659585,4.7173226503,0.2266315285
	H,0,0.0010274457,1.7722802564,1.8852761026
1d	Ac_OdiAu_a.log
	Low frequencies9.2500 -5.9645 -2.1026 -0.0013 -0.0012 -0.0010
	Low frequencies 10.7836 13.0896 16.2743
	Zero-point correction= 0.305449 (Hartree/Particle)
	Thermal correction to Energy= 0.329954
	1,
	Thermal correction to Gibbs Free Energy= 0.244410
	Sum of electronic and zero-point Energies= -1386.120601
	Sum of electronic and thermal Energies= -1386.096096
	Sum of electronic and thermal Enthalpies= -1386.095152
	Sum of electronic and thermal Free Energies= -1386.181640
	C,0,4.3085071212,-1.5275576504,-1.6332980999
	P,0,3.7583125378,-0.9998026826,0.0288729649
	Au,0,1.8081095784,0.1691370764,0.0101048291
	0,0,-0.0078125942,1.2573442811,0.0431939023
	Au,0,-1.806681622,0.1462274424,-0.0008134095
	P,0,-3.7269252487,-1.07475587,-0.0419572014
	C,0,-3.6162162459,-2.5947527013,-1.0525624025
	C,0,5.1537256874,-0.0402280062,0.7167899526
	C,0,3.6900598961,-2.5336684548,1.0223190062
	C,0,-0.0010218044,2.6412344476,-0.0752385503
	C,0,-0.9965232576,3.3238863343,0.8143565213
	C,0,0.8404504271,3.2685732212,-0.8971295922
	C,0,-4.2708293254,-1.6336784716,1.6120521027
	C,0,-5.1437002294,-0.1439325077,-0.7255035996
	H,0,3.4446058017,-2.2923208999,2.0571591931
	H,0,4.6531697061,-3.0484736137,0.9935297634
	H,0,2.9173711502,-3.1952591764,0.6289576505
	H,0,3.5565138124,-2.1766988786,-2.0841355043
	H,0,4.438765784,-0.6547317778,-2.2746253225
	H,0,5.2553316582,-2.0685968936,-1.5675939432
	H,0,6.0702630006,-0.6344952567,0.69438535
	H,0,4.9355953081,0.2453379619,1.7465429392
	H,0,5.3015068604,0.8682937453,0.1316208037
	H,0,-3.5022999514,-2.2636540783,2.0620993264
	H,0,-5.201020076,-2.201403142,1.5359632953
	H,0,-4.4301853727,-0.7700763216,2.259003642
	H,0,-5.3236102144,0.7477854983,-0.1236329908
	H,0,-4.9245978924,0.1678621051,-1.7475326434
	H,0,-6.0426131229,-0.7649008942,-0.7232405077
	H,0,-4.5681153953,-3.1308139762,-1.0351010212
	H,0,-2.8327574755,-3.2449830892,-0.6613191967
	11,0,-2.03273747030,-3.24443030032,-0.2013131307

	H,0,-3.3697320229,-2.3372975401,-2.0833810301	
	H,0,-3.369/320229,-2.33/29/5401,-2.0833810301 H,0,-2.0215652877,3.0496362584,0.5382434344	
	H,0,-0.8480209287,3.0217089014,1.8550624246	
	H,0,-0.9101689454,4.408341516,0.7475518188	
	H,0,1.5242025867,2.7224407492,-1.5375530897	
	H,0,0.8605497943,4.3489378816,-0.9490811471	
1e	Ac_gemAu2_c.log	
	Low frequencies5.9025 -3.6603 0.0004 0.0006 0.0009 3.2859	
	Low frequencies 10.3657 11.9710 23.8170	
	Zero-point correction = 0.306190 (Hartree/Particle) Thermal correction to Energy = 0.330737	
	Thermal correction to Energy=0.330737Thermal correction to Enthalpy=0.331681	
	Thermal correction to Gibbs Free Energy= 0.245642	
	Sum of electronic and zero-point Energies= -1386.117888	
	Sum of electronic and thermal Energies= -1386.093341	
	Sum of electronic and thermal Enthalpies= -1386.092397	
	Sum of electronic and thermal Free Energies= -1386.178436	
	C,0,-0.0021905943,-0.0190758362,-0.0088906727	
	Au,0,-0.0032176982,-0.0392459188,2.1297094137	
	Au,0,2.1358339743,-0.0388096736,0.0271623882	
	P,0,4.5326788456,0.0943468583,-0.1759931016	
	P,0,-0.2534112153,0.0909074062,4.5224184178	
	C,0,-2.0368777014,0.016356819,5.097240208	
	C,0,0.5985709332,-1.2739261351,5.4865803353	
	C,0,0.4073264426,1.6755781354,5.2764493581 C,0,5.5004471814,-0.6611948019,1.2420744248	
	C,0,5.1751097259,1.8521542878,-0.2933804892	
	C,0,5.2186656613,-0.7503694955,-1.7031991731	
	C,0,-0.6147254374,-1.0988478766,-0.633839577	
	0,0,-1.5606260363,-0.809363438,-1.5959123949	
	C,0,-0.3670391799,-2.5693458876,-0.3839809915	
	H,0,4.7345492048,2.34597764,-1.1642866778	
	H,0,6.2661898467,1.8514799435,-0.3914721604	
	H,0,4.8921942676,2.4086897792,0.6047473724	
	H,0,5.2383451564,-0.1550711422,2.1757514018	
	H,0,5.2504741244,-1.7222422061,1.333520936	
	H,0,6.5765516709,-0.5577450472,1.0643652946	
	H,0,6.305772203,-0.6235444141,-1.7500962951	
	H,0,4.7650605177,-0.3138737474,-2.5976540473 H,0,4.9804362622,-1.817602123,-1.673608174	
	H,0,1.4799864827,1.7584398785,5.0789470204	
	H,0,0.2365781337,1.6801114364,6.3585855374	
	H,0,-0.0997376037,2.534398057,4.8273240703	
	H,0,-2.6002400857,0.8421094889,4.6532310271	
	H,0,-2.4875975782,-0.9273472141,4.7768296663	
	H,0,-2.0864002266,0.0893711913,6.1891757105	
	H,0,0.4282535148,-1.1412374864,6.560640256	
	H,0,1.6735538374,-1.2515608105,5.2854058511	
	H,0,0.202670765,-2.24536279,5.1763406696	
	H,0,-0.3722742215,0.9407770658,-0.3842267594	
	H,0,0.3920556351,-2.7090880071,0.3864875024	
	H,0,-1.2921488198,-3.0669580341,-0.0593368659	
	H,0,-0.0275991605,-3.065435336,-1.3045877227	
	H,0,-1.9706467965,-1.5969350725,-2.0141630359	
1f	Ac_gemAu2_b.log	

Low frequencies 2.6662 0.0003 0.0006 0.0015 4.9081 7,9801 Low frequencies 12,9601 15.2028 2.6.0234 Zero-point correction to Enthalpy			
Zero-point correction to Energy= 0.330513 (Hartree/Particle) Thermal correction to Cibbs Free Energy= 0.245542 Sum of electronic and thermal Energies= -1386.117512 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.07803 Sum of electronic and thermal Energies= -1386.07803 C,0,-2.9081488129,-2.5704552742,1.3676085344 P,0,-3.2646477932,-1.246263532,0.1521117921 C,0,-3.70312083,-2.13885114,-1.3607083546 P,0,-3.2646477932,-1.246263532,0.01521174,-10924262133 C,0,-0.000596151,1.7331006649,-0.024262133 C,0,-0.000591652,4.240747337,0.1358015528 Au,0,-1.50129851,0.012704,-102803830,004841153626 P,0,3.2676701442,-1.2457028430,0.1395279616 C,0,4.3025159519,-0.472083830,0048419866 C,0,3.2315505182,-2.0986027622,1.760487927 C,0,3.315505182,-2.0986027622,1.760487927 C,0.330371296,-5.39917297,-2.8211350515,-1.15208580258 H,0,-4.69713711,-1.424347121,-2.1262317584 H,0,-4.697913711,-1.424347112,-2.1262317584 H,0,-2.0497917716,-3.154629465,1.575802768 H,0,-2.049791716,-3.154629458,1.1329705082 H,0,-2.049791716,-3.154629458,1.1329707834 H,0,-2.049791716,-3.1546294685,1.757017843 <t< th=""><th></th><th>Low frequencies2.6862 0.0003 0.0006 0.0015 4.9081 7.9801</th></t<>		Low frequencies2.6862 0.0003 0.0006 0.0015 4.9081 7.9801	
Thermal correction to Energy= 0.330156 Thermal correction to Gibbs Free Energy= 0.245642 Sum of electronic and thermal Energies= -1386.117512 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.17783 C.0, -2.9081488129, -2.5704552742, 1.3676085348 P.0, -3.2646477952, -1.2462635352, 0.1521117921 C.0, -3.07331058661, 0.2428012039, -0.1799842873 C,0, -0.0005996131, 1.7331008669, -0.6042262133 C.0, -0.000511652, 4.2467473375, -0.1858015528 Au, 0.1, 5.05296611, 0.241864246, -0.1881153626 P.0, 3.2676701442, -1.24570282430, 1395279616 C,0, 4.9265159519, -0.472088430, 0.06481154666 C.0, -3.03038221, -0.46946535, 0.7448498157 C,0, 0.00051670952, 2.16946535, 0.7448498157 O,0,0,0.0051670952, -0.0496027622, 1.760487927 C,0, 3.330371296, -2.5991622174, -1.0224431221 C.0, -4.93038221, -0.4594535, 0.7448498157 O,0,0,0,0061670952, -0.01024431712, -1.2420317584 H,0, -4.959937271, -2.8211350515, -1.1520458333 H,0, -2.93089326, -2.122037584 H,0, -4.93038221, -0.42633759,0.05783346 H,0, -2.93089326, -2.12263759,00734 H,0, -2.65893894, -1.122655621, -1.351597133 H,0, -2.65893894, -1.122655621, -1.351597133 <		Low frequencies 12.9601 15.2028 26.0234	
Thermal correction to Energy= 0.330156 Thermal correction to Gibbs Free Energy= 0.245642 Sum of electronic and thermal Energies= -1386.117512 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.02803 Sum of electronic and thermal Energies= -1386.17783 C.0, -2.9081488129, -2.5704552742, 1.3676085348 P.0, -3.2646477952, -1.2462635352, 0.1521117921 C.0, -3.07331058661, 0.2428012039, -0.1799842873 C,0, -0.0005996131, 1.7331008669, -0.6042262133 C.0, -0.000511652, 4.2467473375, -0.1858015528 Au, 0.1, 5.05296611, 0.241864246, -0.1881153626 P.0, 3.2676701442, -1.24570282430, 1395279616 C,0, 4.9265159519, -0.472088430, 0.06481154666 C.0, -3.03038221, -0.46946535, 0.7448498157 C,0, 0.00051670952, 2.16946535, 0.7448498157 O,0,0,0.0051670952, -0.0496027622, 1.760487927 C,0, 3.330371296, -2.5991622174, -1.0224431221 C.0, -4.93038221, -0.4594535, 0.7448498157 O,0,0,0,0061670952, -0.01024431712, -1.2420317584 H,0, -4.959937271, -2.8211350515, -1.1520458333 H,0, -2.93089326, -2.122037584 H,0, -4.93038221, -0.42633759,0.05783346 H,0, -2.93089326, -2.12263759,00734 H,0, -2.65893894, -1.122655621, -1.351597133 H,0, -2.65893894, -1.122655621, -1.351597133 <		Zero-point correction= 0.305913 (Hartree/Particle)	
Za Thermal correction to Gibbs Free Energy = 0.245642 Sum of electronic and thermal Energies =1386.117512 Sum of electronic and thermal Energies =1386.091359 Sum of electronic and thermal Free Energies =1386.091359 Sum of electronic and thermal Free Energies =1386.091359 Sum of electronic and thermal Free Energies =1386.175712 C, 02.9081488129, -2.5704552742,1.3676085348 P, 03.2646477952, -1.2462633532,0.1521117921 C, 02.9081938,1.1.7331008649, 0.60422133 C, 0.0000591052,1.7331008649, 0.60422133 C, 0.0000591052,1.7331008649, 0.60422133 C, 0.0000591052,1.741864246, 0.1881153260 P, 0.3.2676701442, -1.24570282430,0.1395279616 C, 0.4.3030321,0.405946536,0.7644948187 O, 0.00061570985,2.6045494686,1.5796802768 H, 0.4.079137111,-1.4243471121,-1262317584 H, 0.4.097937171,-531586240,511,53207689 H, 0.2.404797171,6-31548624051,1.032976089 H, 0.2.040797171,6-31548624051,1.032976089 H, 0.2.040797171,6-31548624051,1.032976089 H, 0.2.040797171,6-31548624051,0.329760893 H, 0.2.65893385,-2.12623573,0.2143877,0.288608306 H, 0.2.6167938,0.0212157085,7.294337932 H, 0.3.0736431313,0.0075079952,0.9109705186 H, 0.3.0736433131		, , , , , , , , , , , , , , , , , , , ,	
Sum of electronic and zero-point Energies-		Thermal correction to Enthalpy= 0.331566	
Sum of electronic and thermal Entregies -1386.092803 Sum of electronic and thermal Enthalpies -1386.092803 C, 0.2.9081488129, 2.5704552742,1.3676085348 -1386.177783 C, 0.3.773310883, 2.13858514,1.3660933264 -1386.177783 A, 0.0, 1.501338961,0.2428012093,-0.1799842873 -0.00029180378,2.81385814,1.360933264 A, 0.0, 1.5013938961,0.2428012093,-0.1799842873 -0.0021980378,2.8130187047,0.2453701063 C, 0.0.00029180378,2.8103187047,0.2453701063 -0.000021980378,2.8103187047,0.2458701063 C, 0.0.00021980378,2.8103187047,0.24581153626 -0.0325296611.0.24288602762,1.760487927 C, 0.436515519,0.4722903839,0.0648149666 -0.20351551919,0.47229038393,0.0648149666 C, 0.43603821,0064594658,0.7648498187 -0.00,0.0061670985,2.604594686,1.5796802768 H, 0.4087913711,1.4234371121,-2.162317584 -1.0329762189 H, 0.4087913711,1.423437121,-2.162317584 -0.230838267,-2.70918283,-1.758065023 H, 0.240972716,5.1548629451,0.10329762089 +0.0,-2.6658938954,-2.12826562012, 3351597193 H, 0.2407971716,3.1548629451,0.10329762089 +0.0,-5.5921035173,1.1224175624,0.891708734 H, 0.25921035173,1.212417563,2.094837393 +0.0,-5.5921035173,1.122417562,2.0945553346,-1.657203406 H, 0.55921035173,1.2124175654,0.8981211518 +0.0,5076531346,-1.65727477		Thermal correction to Gibbs Free Energy= 0.245642	
Sum of electronic and thermal Free Energies -1386.091859 Sum of electronic and thermal Free Energies -1386.177783 C0, 2. 9081488129, 2. 5704552742, 1.3676085348 0.386.177783 P,0, 3.2646477952, 1.2452633352, 0.1521117921 C,0,37733210883, 2.138858114, -1.3640933264 Au,0,1.501355861, 0.2426012033, 0.1799842873 C,0,-00059151, 1.7331008649, 0.6042262133 C,0,-0000511652, 4.2467473375, 0.188015528 Au,0,1.5025296611, 0.241846246, 0.1881153626 P,0,3.267501442, -1.2457028243, 0.1395279616 C,0,4265159519, 0.4729083839, 0.0648149666 C,0,4265159519, 0.4729083839, 0.0648149666 C,0,32315505182, 2.0986027622, 1.760487927 C,0,3.2315505182, 2.0986027622, 1.760487927 C,0,339037129, 5.2991622174, 1.0928431221 C,0,400579937271, -2.8211305015, -1520458333 H,0,4067193711, -1.424347121, -2.1262317584 H,0,4005793711, -1.424347121, -2.1262317584 H,0,2409797171, 5.3148629451, 1022762089 H,0,2,4047931, -1.24245521, 2.3351597193 H,0,24047933, -3.233089971, 1.4823667224 H,0,-4.66739352, -2.124255621, 2.3351597193 H,0,2.4147319675, -3.1270578, -0.9483170834 H,0,-5.921038173, -1.212475624, 0.891708734 H,0,2.4147319675, -3.167050124, -1.0610224542 H,0,-4.6173196328, 0.0012157085, 1.5821213138 H,0,3.0075079952, 0.9109705186 H,0,5.0736413131		Sum of electronic and zero-point Energies= -1386.117512	
Sum of electronic and thermal Free Energies= -1386.177783 C, 0, 2.908.1488.129, 2.5704552742, 1.3676085348 P,0.3.2646477552, 1.2462635352, 0.1521117921 C, 0, 3.7733210883, 1.3640933264 Au,0,-1.5019358961, 0.2428012093, 0.179842873 C, 0, 0.0005996151, 1.7331008649, 0.6042262133 C,0,0.00021980378, 2.8103187047, 0.2453701663 C, 0, 0.000511652, 2.4267473375, 0.1858015528 Au,0,1.502296611, 0.241846246, 0.1881153626 P,0,3.2676701442, -1.2457028243, 0.1395279616 C,0.4.9265159519, 0.4729083830, 0.648149666 C, 0, 3.2315505182, -2.0980627622, 1.760487927 C,0,3.3310371296, -2.5991622714, 1.0928431221 C, 0, -4.00438321, 0.46594655, 0.5764498187 O,0.0061670985, 2.6045944686, 1.5796802768 H, 0, -4.09791711, -4.243471121, -2.1263317584 H,0, -4.09791711, -4.243471121, -2.1263317584 H, 0, -4.09791717, -2.8211350515, 1.1520458333 H,0, -4.09797171, -2.8211350515, 1.1520458333 H,0, -4.09797171, -2.8211350515, 1.1322762089 H,0, -4.667949383, -3.233098971, 1.4823667224 H,0, -4.667949382, 0.021157083, 1.0327762089 H,0, -4.667949733, -1.2124175624, 0.891708734 H,0, -5.921035173, -1.21241756124, 0.891708734 H,0, -5.921035173, -1.21241756124, 0.891708734 H,0, -5.921035173, -1.21241756124, 0.891708734 H,0, -3.413172225, 0.2916283793, 0.0055783326 H,0, -5.921035173, -1.2124755128, -1.2083			
C0.2.9081488129.2.5704552742,1.367085348 P.0.3.2646477952,1.246263352,0.1521117921 C,0.3.773210883,2.13885114,1.3640933264 Au,0.1.5019358961,0.2428012093,0.1799842873 C,0.0000511652,4.2467473375,0.1358015528 Au,0.1.502596611,0.241846246,0.1881153626 P,0.3.2676701442,1.2457028243,0.1395279616 C,0.4.9265159519,0.472908389,0.0648149666 C,0.3.2315505182,-2.0986027622,1.760487927 C,0.3.330371295,-5991622174,10928431221 C,0.4.8043083221,0.46594668,1.5796802768 H,0.40879137111,1.4234371121,-21262317584 H,0.2.093939267-2.70918258,-1.7580650523 H,0.2.093939267,-2.70918258,-1.7580650523 H,0.2.093939277,-2.8211350515,-1.1520458333 H,0.2.6558938954,-2.1282656201,2.3351597193 H,0.2.6558938954,-2.1282656201,2.3351597193 H,0.2.6558938954,-2.1282656201,2.3351597193 H,0.2.657938951,-1.2124175624,0.891708734 H,0.4617196328,0.0212157085,1.7228317447 H,0.2.46739344793,-3.230989971,1.48236724 H,0.4617196328,0.0212157085,1.7228317447 H,0.2.00579383316 H,0.46167196328,0.0212157085,1.7228317447 H,0.2.00570842,0.007507952,0.9109705186 H,0.5.0094303288,0.3014288787,0.8288608306 H,0.5.007443181088			
P.0.3.2646477952.1.2462635352.0.1521117921 C,0.3.7733210883, 2.13885114, 1.3640933264 Au,0.1.5019358961,0.2428012093, 0.1799842873 C,0.00005996151,1.7331008649,0.6042262133 C,0.0000511652,4.2467473375,0.1858015528 Au0,1.50125296611,0.2418464246,0.1881153626 P,0.3.2676701442,1.2457022430,0.1395279616 C,0.4,9265159519,0.4729083839,0.0648149666 C,0.3.339037126,0.25991622174,1.0928431221 C,0.4.804303221,0.465946536,0.7648498187 O,0.000161670852,6.00454946656,1.5796802768 H,0.4.0879137111,-14243471121,2.1262317584 H,0.2.930839267,2.70918258,1.7580650523 H,0.2.0497971716,-3.1548629451,1.0329762089 H,0.2.6458938954,-2.1282656021,2.3351597193 H,0.3.7693447933,-3.2330989971,14823667224 H,0.3.7693447933,-3.2330989971,1482366724 H,0.4.813947765,-3.26202400,2.839176374 H,0.4.813947765,-3.26202400,2.83917834 H,0.4.813947765,-3.26202400,0.88954393 H,0.4.813947765,-3.26202400,0.88954393 H,0.4.813947765,-3.26202400,0.2889739382 H,0.4.8148100711,-1.2190896147,0.22640573 H,0.4.814810071,-1.2190896147,0.22640573 H,0.4.08311870688,2.7780700893,1.859831467 H,0.2.3055585224,-2.6672006455,1.881211318		Sum of electronic and thermal Free Energies= -1386.177783	
24 C,0.3.7733210883.2.138858114,1.3640933264 Au,0.1.5019358961,0.2428012093,0.1799842873 C,0.0000591651,1.7331008649.0.604256133 C,0.0.000591651,1.7331008649.0.604256133 C,0.0.000511652,2.446747375,7.0.1850115528 Au,0.1.5025296611,0.2418464245,0.1881153626 P,0.3.267701442,-1.2457028243,0.1395279616 C,0.4.0000511652,0.42694293,0.0648149666 C,0.3.2315505182,-2.0986027622,1.760487927 C,0.3.2315505182,-2.0986027622,1.760487927 C,0.3.3390371296,-2.5991622174,-1.0928431221 C,0.4.0437932171,0.465946536,0.766489486 F,796802768 H,0.4.087913711,1.4243471121,-2.1262317584 H,0.4.087913711,-1.4243471121,-2.1262317584 H,0.2.4087913711,-1.4243471121,-2.1262317584 H,0.2.909393267,-2.70918258,-1.7500650523 H,0.2.2097971716,-3.154629451,10.0329762089 H,0.2.6658938954,-2.1282656201,2.3351597193 H,0.2.6658938954,-2.1282656201,2.3351597193 H,0.2.46167196328,0.0212157085,1.7228317447 H,0.2.44613172250,0.2916283759,0.0557839316 H,0.418033287,0.51282,1.758060573 H,0.4.1835347765,-3.26022406,0.889543993 H,0.5.0736431313,0.007507932,0.9109705186 H,0.5.0736431313,0.007507932,0.9109705186 H,0.5.0736431313,0.007507932,0.9109705186 H,0.5.004310288,0.3014288787,0.828800306 H,0.2.3055585224,2.6672000455,1.35821211318 H,0.0.8282116497,4.7647			
Au, 0, -1.5019358961, 0.2428012093, 0.1799842873 C, 0, 00002996151, 1.7331008649, 0.064262133 C, 0, 000021980378, 28.103187047, 0.2453701063 C, 0, 0000211652, 4.2467473375, 0.1858015528 Au, 0, 1.502259611, 0.241864246, 0.1881158263 P, 0, 3.2676701442, -1.2457028243, 0.1395279616 C, 0, 4.9265159519, 0.4729083839, 0.0648149666 C, 0, 3.3390371296, -2.5991622174, -1.0928431221 C, 0, -4.8043083221, 0.046594656, 0.7648498187 O, 0, 0.0061670985, 2.6045494666, 1.5796802766 H, 0, -4.0879137111, -1.4243471121, -2.1262317584 H, 0, -4.039932277, 1.28211350515, -1.1520468333 H, 0, -2.9308398267, -2.70918258, 1.7580650523 H, 0, -2.0499797176, -3.1136429451, 1.0329762089 H, 0, -5.1413172225, 0.2916283759, 0.0557839316 H, 0, -5.1413172225, 0.2916283759, 0.0557839316 H, 0, -5.1413172225, 0.2916283759, 0.0557839316 H, 0, -5.041393882, 0.3014288787, 0.258452 H, 0, 4.815347765, -3.262022406, 0.889543993 H, 0, -139447933, -1.2124175624, 0.891768 H, 0, -2.04979776, -3.2650202406, 0.889543993 H, 0, -2.0497977176, -3.12705758, -2.0948379382 H, 0, -2.0497973 H, 0, -2.049797 H, 0, -2.049797 H, 0, -2.049786, -1.36277777776, -2.55502			
C00.0005996151,1.73310086490.6042262133 C,00.0005996151,52,8.103187047,0.2453701063 C,00.000511652,4.2467473375,-0.1858015528 Au,0,1.5025296611,0.2418464246,-0.1881153626 P,0,3.2676701442,-1.2457028243,0.1395279616 C,0.4.295159,-0.4729083839,.0064149666 C,0.3.2315505182,-2.0986027622,1.760487927 C,0.3.39037126,-2.5991622174,-1.0928431221 C,0.4.8043083221,-0.465946536,0.7648498187 O,0.0061670985,2.604594686,1.5796802768 H,0,-4.087913711,-1.4243471121,-2.126217584 H,0,-4.087913711,-1.4243471121,-2.126217584 H,0,-2.0497971716,-3.1548629451,1.0327752089 H,0,-2.0497971716,-3.1548629451,1.0327762089 H,0,-2.0497971716,-3.154829451,10.327762089 H,0,-2.0497971765,-3.127605124,-1.061022542 H,0,-55912035173,-1.2124175624,0.891708734 H,0,-51921035173,-1.2124175624,0.891708734 H,0,-4147319675,-3.1776950124,-1.0610225452 H,0,41431038,-2.7780700833,1829317447 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0736431313,-0.007507952,-0.9109705186 H,0,5.0736431313,-0.007507952,-0.9109705186 H,0,0.00267741424,43437131304,-1.2649089732 H,0,-0.0026771424,43437131304,-1.2649089732 H,0,-0.0026771424,43473131304,-1.2649			
C,0.0.0021980378,2.8103187047,0.2453701063 C,0.0.0000511652,4.2467473375,-0.1858015528 Au,0.1.5025296611,0.241846246,0.1881153626 P,0.3.2676701442,-1.2457028243,0.1395279616 C,0.4.9265159519,-0.472908389,0.0648149666 C,0.3.2315505182,-2.098602762,1.760487927 C,0.3.309371296,-2.5991622174,-1.0928431221 C,0.4.8043083221,-0.465946536,0.7648498187 O,0.00016709285,26045494686,1.5796802768 H,0.4.4599337111,-1.4243471121,-2.1262317584 H,0,-2.990838267,-2.70918258,-1.7580650523 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-2.6658938954,-2.12826550124,-1.0610225452 H,0,-5.041372225,0.2916238759,0.0557893166 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1270250124,-1.0610225452 H,0,0.5073643131,-0.007507955,-0.9109705186 H,0,5.073643131,-0.007507955,-0.9109705186 H,0,5.073643131,-0.007507955,-0.9109705186 H,0,5.073643131,-0.007507955,-0.9109705186 H,0,5.073643131,-0.007507955,-0.9109705186 H,0,0.20757424,-2.6720046,-38954374 H,0,0.20757424,-2.6720046,51, 8581211318 H,0,0.20757424,-2.6720046,51, 8581211318 H,0,0.002788124,-2.0256533346,-1.652856254 <th></th> <th></th>			
C,0,-0.0000511652,4.2467473375,-0.1858015528 Au,0,1.5025296611,0.2418464246,-0.1881153626 P,0,3.2676701444,-1.245702243,0.1395279616 C,0,4.9265159519,-0.4729083839,0.0648149666 C,0,3.2315505182,-2.0986027622,1.760487927 C,0,3.3035505182,-2.0986027622,1.760487927 C,0,4.8043083221,-0.465946536,0.7648498187 O,0,0.0061670985,2.604594666,1.5796802768 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-2.0999372771,-2.8211350515,-1.1520458333 H,0,-2.0497971716,-3.1548629451,10.329762089 H,0,-2.0497971716,-3.1548629451,10.329762089 H,0,-2.0497971716,-3.1548629451,10.329762089 H,0,-2.049797175,-3.127695107814 H,0,-5.592103573,-1.21241756240,891708734 H,0,-5.592103573,-1.2241756240,891708734 H,0,-5.616196328,0.0212157085,1.7228317447 H,0,5.708467204005,-2.1812705788,-20948379382 H,0,5.0784813,0.007507958,-099487933 H,0,4.814318108 H,0,5.008403288,0.3014288787,0.8288608306 H,0,4.08148118088,-2.7780700585,1.8581211318 H,0,5.009430288,0.3014288787,0.8288608306 H,0,0.0036585224,2.6672006455,1.8581211318 H,0,0.0038321964937,1.4527822741,02085156448			
Au,0,1,5025296611,0.2418464246,-0.1881153626 P,0,3,2676701442,-1.2457028243,0.1395279616 C,0,4,92651591,0,4729083830,0.0648149666 C,0,3,2315505182,-2.0986027622,1.760487927 C,0,3,330371296,-2.5991622174,-1.0928431221 C,0,4,804308221,-0.465946536,0.7644948187 O,0,00061670985,2.6045494686,1.5796802768 H,0,-4,0879137111,-1.4243471121,-2.1262317584 H,0,-4,0879137717,-2.8211350515,-1.1520458333 H,0,-2.9308398267,-2.70918258,-1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.658939854,-2.1282656212,3331597193 H,0,-2.658939854,-2.1282656212,31597193 H,0,-3.599103173,-1.21241750458333 H,0,-2.661939854,-2.1282656214,2331597193 H,0,-4.5693172225,0.29106283759,0.0557839316 H,0,-5.41417225,0.29106283759,0.0557839316 H,0,-4.147319675,-3.17669124,-1.0610225452 H,0,4.1483547765,-3.26022406,-0.889543993 H,0,5.0094303288,0.301428870,0.8288608306 H,0,5.0094303288,0.301428870,0.8288608306 H,0,5.0094303288,0.301428870,0.22640573 H,0,4.0814181088,-1.3627777762,2560208452 H,0,0.00398215,2.0256533346,-1.16528562954 H,0,0.00398215,947,4.7647299432,0.2045556448 H,0,0.00382196497,4.7647299432,0.2045556448 </th <th></th> <th></th>			
P.0.3.2676701442,-1.2457028243,0.1395279616 C,0.4.9265159519,-0.4729083839,0.0648149666 C,0.3.231505182,-2.0986027622,1,760487927 C,0.3.3390371296,-2.5991622174,-1.0928431221 C,0.4.8043083221,-0.465946536,0.7648498187 O,0.0061670985,2.604549468,1.579602768 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-4.9999372771,-2.8211350515,-1.1520458333 H,0,-2.9308398567,-2.70918258,-1.7580650523 H,0,-2.94097971716,-3.1548629451,1.0329762089 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,0.50736431313,-0.0075079552,-0.9169705186 H,0,0.50736431313,-0.0075079552,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,0.2065771424,43437131304,-1.2694089732 H,0,0.0026771424,43437131304,-1.2694089732 H,0,0.0026771424,43437131304,-1.2694089732 H,0,0.003821197,3.438271			
C,0.4.9265159519,-0.4729083839,0.0648149666 C,0.3.2315505182,-2.0986027622,1,760487927 C,0.3.3300371266,-2.5991622174,-102924312211 C,0.4.8043083221,-0.465946536,0.7648498187 O,0.0.0061670985,2.6045494686,1.5796802768 H,0.4.989912771,-2.8211350515,-1.1520458333 H,0.2.9308398267,-2.20918258,1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.7693447933,-3.2330989971,1.4823667224 H,0,-5.413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.3176950124,-1.0610225452 H,0,4.183547765,-3.26202406,-0.889543993 H,0,5.073643131,0.007507952,-0.9109705186 H,0,5.0073643131,0.007507952,-0.9109705186 H,0,5.00746431313,0.007507952,-0.9109705186 H,0,5.003403288,0.301428878,0.828608306 H,0,5.00344845,-1.3627777776,2.5652083062 H,0,0.0039825,0.205533346,-1.528562954 H,0,0.0026771424,4.3437131304,-1.2694089732 H,0,0.882716026,4.762532241,0.2085193074 H,0,0.882716026,4.762532241,0.208595448 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0016 7.8828			
C,0,3,2315505182,-2.0986027622,1.760487927 C,0,3,390371296,-2.5991622174,-1.0928431221 C,0,-3,804308221,-0,465946536,0.7648498187 O,0,00061670985,2.6045494686,1.5796802768 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-2.9308398267,-2.70918258,1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.658938954,-2.1282655201,2.3351597193 H,0,-3.6693447933,-3.233098971,1.4823667224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-4.6167196328,0.0212157085,1.728317447 H,0,-5.073643131,0.0075079952,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,0.3065783947,0.8288608306 H,0,5.7081600711,-1.2190896147,0.26652083062 H,0,0.0026771424,4.343713104,-1.2694089732 H,0,0.0026771424,4.343713104,-1.2694089732 H,0,0.0026771424,4.343713120,-1.2694089732 H,0,0.0026771424,4.343713120,-1.2694089732 H,0,0.0026771424,4.343713130,-1.2694089732 H,0,0.0026771424,4.343713130,-1.2694089732 H,0,0.0026771424,4.343713130,-1.2694089732 H,0,0.0079881197,3.4382714794,2.0679640725 2a 2a 2a <			
2a C,0,3.3390371296,-2.5991622174,-1.0928431221 C,0,-4.8043083221,-0.465946536,0.7648498187 O,0.00061670985,2.6045494686,1.5796802768 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-4.6599337711,-2.8211350515,-1.1520458333 H,0,-2.9308398267,-2.70918258,-1.7580650523 H,0,-2.0658938954,-2.1282656201,2.3351597193 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.7693447933,-3.2330989971,1.4823667224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4167319675,-3.1776950124,-1.0610225452 H,0,4.813547765,-3.26202406,0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0094303288,0.3014288787,0.828608306 H,0,5.0094303288,0.301428787,0.828608306 H,0,5.009430328,0.2012157085,1.752852083062 H,0,0.205578224,2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,0.00349825,2.0256533346,-1.6528562954 H,0,0.00039881197,3.4382714794,2.0679640725 H,0.00019881197,3.4382714794,2.0679640725 Za AuAcetone.log Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
0,0,0.0061670985,2.6045494686,1.5796802768 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-2.3908398267,-2.70918258,1.7580650523 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.659347933,-2.330989971,14823657224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.616719628,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0736431313,-0.0075079952,0.9109705186 H,0,2.30558524,-2.6672006455,1.8581211318 H,0,2.30558524,-2.6672006455,1.8581211318 H,0,-3.06748436,1.302777776,2.5652083062 H,0,-0.00349825,2.025653346,-1.65287562954 H,0,-0.00349825,2.025653346,-1.6528756448 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828			
H,0,-4.0879137111,-1.4243471121,-2.1262317584 H,0,-4.5999372771,-2.8211350515,-1.1520458333 H,0,-2.9308398267,-2.70918258,-1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-3.7693447933,-3.2330989971,1.482367224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.51413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,0.32657885224,-2.6672006455,1.8581211318 H,0,3.365783436,-1.6527777776,2.5652083062 H,0,0.0026771424,4.3437131304,-1.2694089732 H,0,0.0079825,0.20565324,0.204555648 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.007981197,3.4382714794,2.0797640725 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.007981197,3.4382714794,2.0797640725 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.007981197,3.4382714794,2.0679640725 H,0,0.		C,0,-4.8043083221,-0.465946536,0.7648498187	
H,0,-4.5999372771,-2.8211350515,-1.1520458333 H,0,-2.9308398267,-2.70918258,-1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.1617196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.305585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,0.2056533346,-1.5628562954 H,0,0.0079881197,3.4382714794,2.0679640725 H,0,0.0079881197,3.4382714794,2.0679640725 H,0,0.0079881197,3.4382714794,2.0679640725 H,0,0.0079881197,3.4382714794,2.0679640725 H,0,0.0079881197,3.4382714794,2.0679640725 H,0,0.0079881197,3.4382714794,2.0679640725 Low frequencies 12.1723 -		O,0,0.0061670985,2.6045494686,1.5796802768	
H,0,-2.9308398267,-2.70918258,-1.7580650523 H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.7693447933,-3.233098971,1.4823667224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.722817447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.305585224,-2.6672006455,1.8581211318 H,0,0.3049825,20256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.08827116026,4.7625322241,0.2086193074 H,0,0.079881197,3.432714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478		H,0,-4.0879137111,-1.4243471121,-2.1262317584	
H,0,-2.0497971716,-3.1548629451,1.0329762089 H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.7693447933,-3.2330989971,1.4823667224 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.26022406,-0.89543993 H,0,5.0736431313,-0.007507955,-2.09109705186 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.305558524,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.362777776,2.5552083062 H,0,0.000349825,2.0256533346,-1.6528562954 H,0,0.0079881197,3.4382714794,2.0286193074 H,0,0.0079881197,3.4382714794,2.0286193074 H,0,0.0079881197,3.4382714794,2.024555648 H,0,0.0079881197,3.4382714794,2.024555648 H,0,0.0079881197,3.4382714794,2.0204555648 H,0,0.0079881197,3.4382714794,2.02015 2a AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0010 0.0016 7.8288 Low frequencies 12.1723 -0.200705 (Hartree/Particle) Thermal correction =		H,0,-4.5999372771,-2.8211350515,-1.1520458333	
H,0,-2.6658938954,-2.1282656201,2.3351597193 H,0,-3.7693447933,-3.2330989971,1.4823667224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.191035173,-1.2124175624,0.891708734 H,0,-6.1617196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-0.9108705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,0,5.0094303288,0.3014288787,0.8288608306 H,0,0,00349825,2.0256533346,-1.362777776,2.5652083062 H,0,0.00349825,2.0256533346,-1.6528562954 H,0,0.00349825,2.0256533346,-1.6528562954 H,0,0.00349825,2.0256533346,-1.6528562954 H,0,0.0034981197,3.4382714794,2.0694089732 H,0,0.0079881197,3.4382714794,2.0286193074 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (H			
H,0,-3.7693447933,-3.2330989971,1.4823667224 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.176950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.07364303288,0.3014288787,0.8288608306 H,0,5.07364303288,0.3014288787,0.8288608306 H,0,5.07364303288,0.3014288787,0.8288608306 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.0055585224,-2.6672006455,1.8581211318 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,0.30349825,2.0256533346,-1.6528562954 H,0,0.00349825,2.0256533346,-1.6528562954 H,0,0.08321196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842		H,0,-2.6658938954,-2.1282656201,2.3351597193	
H,0,-5.5921035173,-1.2124175624,0.891708734 H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.07084303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.362777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,0-0.00349825,2.0256533346,-1.6528562954 H,0,0.0026771424,4.3437131304,-1.2694089732 H,0,0.003981197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,-5.1413172225,0.2916283759,0.0557839316 H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,5.0736431313,-0.007507952,-2.0948379382 H,0,5.0736431313,-0.007507952,-0.9109705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.362777776,2.5652083062 H,0,0-0.00349825,2.025653346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.0827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,-4.6167196328,0.0212157085,1.7228317447 H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.07036431313,-0.0075079952,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,0.08827116026,4.7625322241,0.2086193074 H,0,0.0882196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,2.4147319675,-3.1776950124,-1.0610225452 H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,2.305558224,-2.6672006455,1.8581211318 H,0,2.305558224,-2.6672006455,1.8581211318 H,0,2.3055785224,-2.6672006455,1.8581211318 H,0,2.30557488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,0.8827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,4.1835347765,-3.262022406,-0.889543993 H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,0.08827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,3.4467204005,-2.1812705758,-2.0948379382 H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.362777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.0827116026,4.7625322241,0.2086193074 H,0,0.0832196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,5.0736431313,-0.0075079952,-0.9109705186 H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,5.0094303288,0.3014288787,0.8288608306 H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.08827116026,4.7625322241,0.2086193074 H,0,0.0879881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,5.7081600711,-1.2190896147,0.22640573 H,0,4.0814181088,-2.7780700893,1.8598314167 H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.362777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction = 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,2.3055585224,-2.6672006455,1.8581211318 H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842		H,0,5.7081600711,-1.2190896147,0.22640573	
H,0,3.2667488436,-1.3627777776,2.5652083062 H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,-0.8827116026,4.7625322241,0.2085556448 H,0,0.0079881197,3.4382714794,2.0679640725 Za AuAcetone.log\ Low frequencies 12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842		H,0,4.0814181088,-2.7780700893,1.8598314167	
H,0,-0.00349825,2.0256533346,-1.6528562954 H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.0832196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842		H,0,2.3055585224,-2.6672006455,1.8581211318	
H,0,-0.0026771424,4.3437131304,-1.2694089732 H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.8832196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,-0.8827116026,4.7625322241,0.2086193074 H,0,0.8832196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,0.8832196497,4.7647299432,0.2045556448 H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
H,0,0.0079881197,3.4382714794,2.0679640725 2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= Thermal correction to Energy= 0.215842			
2a AuAcetone.log\ Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy=			
Low frequencies12.1723 -4.3393 -0.0015 -0.0010 0.0016 7.8828 Low frequencies 18.4298 41.8366 42.4478 Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842	22		
Low frequencies18.429841.836642.4478Zero-point correction=0.200705 (Hartree/Particle)Thermal correction to Energy=0.215842			
Zero-point correction= 0.200705 (Hartree/Particle) Thermal correction to Energy= 0.215842			
Thermal correction to Energy= 0.215842			
		Zero-point correction= 0.200705 (Hartree/Particle)	
		Thermal correction to Enthalpy= 0.216786	
Thermal correction to Gibbs Free Energy= 0.155361		Thermal correction to Gibbs Free Energy= 0.155361	

	Sum of electronic and zero-point Energies=	-789.814526
	Sum of electronic and thermal Energies=	-789.799389
	Sum of electronic and thermal Enthalpies=	-789.798445
	Sum of electronic and thermal Free Energies=	-789.859870
	C,0,0.0421257506,0.0767488842,-0.0198878796	5
	P,0,0.0281537107,0.0437741085,1.8057971291	L
	C,0,1.7797740977,0.0144374327,2.3208595263	3
	C,0,-0.6257103758,1.6647513837,2.3341306695	
	Au,0,-1.1664275656,-1.7027842547,2.6641799967	
	0,0,-2.2438244359,-3.3232921229,3.6057766001	
	C,0,-3.0463183232,-4.170795803,3.1954723414	
	C,0,-3.4693343544,-4.2535370757,1.762634562	24
	C,0,-3.610411623,-5.1567056479,4.1670335259	9
	H,0,0.4811393947,-0.8439231799,-0.40616883	
	H,0,0.6287292162,0.9281519066,-0.37295444	
	H,0,-0.9764972334,0.163490999,-0.400080208	4
	H,0,-1.6572851493,1.7782548514,1.998707265	
	H,0,-0.6044919439,1.7379064318,3.422167331	
	H,0,-0.0200926798,2.4687632828,1.909294417	
	H,0,2.3077409949,0.8713179437,1.895651866	-
	H,0,2.2546022124,-0.9053043377,1.977064032	1
	H,0,1.8492603264,0.0551369324,3.4085485363	
	H,0,-3.2315480451,-3.3397882071,1.21774554	
	H,0,-2.9348879857,-5.0894276869,1.29524826	
	H,0,-4.5347241384,-4.4788644781,1.67776961	
	H,0,-3.0601571523,-5.1417186836,5.10575384	
	H,0,-4.6565370316,-4.8918832861,4.36280422	
	H,0,-3.6206137188,-6.1632714859,3.74072827	
	11.03.020013/1000.1032/14033.3./40/202/	67
2h		65
2b	Au_enol_1.log	
2b	Au_enol_1.log	
2b		-0.0002 0.0014 5.0207
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005	-0.0002 0.0014 5.0207
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401	-0.0002 0.0014 5.0207
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401	-0.0002 0.0014 5.0207 5 (Hartree/Particle)
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457
2b	Au_enol_1.logLow frequencies7.0519 -4.5348 -0.0005Low frequencies 15.3260 45.1480 55.401Zero-point correction=0.201888 (Thermal correction to Energy=0.2164Thermal correction to Energy=0.217	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401
2b	Au_enol_1.logLow frequencies7.0519-4.5348-0.0005Low frequencies15.326045.148055.401Zero-point correction=0.201888 (Thermal correction to Energy=0.216Thermal correction to Enthalpy=0.217Thermal correction to Gibbs Free Energy=0	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401).157455
2b	Au_enol_1.log Low frequencies7.0519 Low frequencies 15.3260 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= Sum of electronic and zero-point Energies=	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401).157455 -789.793703
2b	Au_enol_1.log Low frequencies7.0519 Low frequencies 15.3260 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies=	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135
2b	Au_enol_1.logLow frequencies7.0519Low frequencies15.326045.148055.401Zero-point correction=0.201888 (Thermal correction to Energy=0.216Thermal correction to Enthalpy=0.217Thermal correction to Gibbs Free Energy=Sum of electronic and zero-point Energies=Sum of electronic and thermal Free Energies=	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136
2b	Au_enol_1.logLow frequencies7.0519-4.5348-0.0005Low frequencies15.326045.148055.401Zero-point correction=0.201888 (Thermal correction to Energy=0.216Thermal correction to Enthalpy=0.217Thermal correction to Gibbs Free Energy=Sum of electronic and zero-point Energies=Sum of electronic and thermal Energies=Sum of electronic and thermal Energies=Sum of electronic and thermal Enthalpies=Sum of electronic and thermal Free Energies=Sum of electronic E	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136
2b	Au_enol_1.logLow frequencies7.0519 -4.5348 -0.0005Low frequencies 15.3260 45.1480 55.401Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216Thermal correction to Enthalpy= 0.217Thermal correction to Gibbs Free Energy= 0Sum of electronic and zero-point Energies=Sum of electronic and thermal Enthalpies=Sum of electronic and thermal Enthalpies=Sum of electronic and thermal Enthalpies=Sum of electronic and thermal Free Energies=C,0,0.0789471426,-0.0084880419,0.0088081999P,0,-0.0201710013,-0.0430863124,1.833891800	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401. Zero-point correction = 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081995 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401. Zero-point correction = 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081995 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401. Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216. Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0. Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.83389180 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.241926963	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.2419269633 O,0,4.2740585819,-2.2404705242,4.414731475	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401. Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.241926963: O,0,4.2740585819,-2.2404705242,4.414731475 H,0,-2.0208882454,-1.4213368862,1.73860484	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7 1 5 5 5 7 7
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401. Zero-point correction= 0.201888 (Thermal correction to Energy= 0.2166 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.2419269633 O,0,4.2740585819,-2.2404705242,4.414731475 H,0,-2.0208882454,-1.4213368862,1.738604844 H,0,-1.1845836509,1.428911291,3.3753519454	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7 1 5 1 5
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.241926963 O,0,4.2740585819,-2.2404705242,4.414731475 H,0,-2.0208882454,-1.4213368862,1.73860484 H,0,-1.1845836509,1.428911291,3.3753519454 H,0,-1.9890953109,1.3820648173,1.790397508	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7 1 5 65 6 66
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.2419269633 O,0,4.2740585819,-2.2404705242,4.414731475 H,0,-2.0208882454,-1.4213368862,1.73860484 H,0,-1.1845836509,1.428911291,3.3753519454 H,0,-1.9890953109,1.3820648173,1.790397508 H,0,-0.5012755262,2.330348076,2.0129179478	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7 1 5 6 5 6 6 6 6 6 6 6 6 6 6 6 6 6
2b	Au_enol_1.log Low frequencies7.0519 -4.5348 -0.0005 Low frequencies 15.3260 45.1480 55.401 Zero-point correction= 0.201888 (Thermal correction to Energy= 0.216 Thermal correction to Enthalpy= 0.217 Thermal correction to Enthalpy= 0.217 Thermal correction to Gibbs Free Energy= 0 Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Free Energies= Sum of electronic and thermal Free Energies= C,0,0.0789471426,-0.0084880419,0.0088081999 P,0,-0.0201710013,-0.0430863124,1.833891800 Au,0,2.079206396,-0.0768243479,2.855408247 C,0,4.1404974026,0.0287773985,3.6753045388 C,0,3.9744119559,-0.9709513236,4.632502986 C,0,3.4632663574,-0.7410682985,6.012521793 C,0,-1.0215463803,1.4145961962,2.296861047 C,0,-1.053882889,-1.4951925015,2.241926963 O,0,4.2740585819,-2.2404705242,4.414731475 H,0,-2.0208882454,-1.4213368862,1.73860484 H,0,-1.1845836509,1.428911291,3.3753519454 H,0,-1.9890953109,1.3820648173,1.790397508	-0.0002 0.0014 5.0207 5 (Hartree/Particle) 457 7401 0.157455 -789.793703 -789.779135 -789.778191 -789.838136 5 07 3 1 7 1 5 65 4 65 4 66 4 66

H,0,-0.9245220726,0.0104637964,-0.4228263848
H,0,-1.2166481749,-1.5461603724,3.3193082722
H,0,-0.5548853952,-2.4111039107,1.9227003936
H,0,4.1828606704,1.0495048805,4.0450830809
H,0,3.0864259925,0.2714448425,6.1405804302
H,0,2.6829851087,-1.4647809271,6.2558095625
H,0,4.2855665312,-0.9085276553,6.7156869457
H,0,4.791074929,-0.1756280317,2.8257381776
H,0,4.6673410287,-2.3884313625,3.5407893413