Supporting Information

π-Bonding of Group 11 Metals to a Tantalum Alkylidyne Alkyl Complex Promotes Unusual Tautomerism to Bis-Alkylidene and CO_2 to Ketenyl Transformation

Abdelhak Lachguar,[a] Iker Del Rosal,[b] Laurent Maron,[b] Erwann Jeanneau,[c] Laurent Veyre,[a] Chloé Thieuleux,[a] and Clément Camp*[a]

[a] Laboratory of Catalysis, Polymerization, Processes and Materials (CP2M UMR 5128), CNRS, Universite Claude Bernard Lyon 1, CPE-Lyon, Institut de Chimie de Lyon, 43 Bd du 11 Novembre 1918, F-69616 Villeurbanne, France.
[b] Université de Toulouse, CNRS, INSA, UPS, UMR 5215, LPCNO, 135 Avenue de Rangueil, F-31077 Toulouse, France.
[c] Université de Lyon, Centre de Diffractométrie Henri Longchambon, 5 Rue de la Doua, 69100 Villeurbanne, France.

*clement.camp@univ-lyon1.fr

Content

A. NMR and DRIFT spectroscopic data

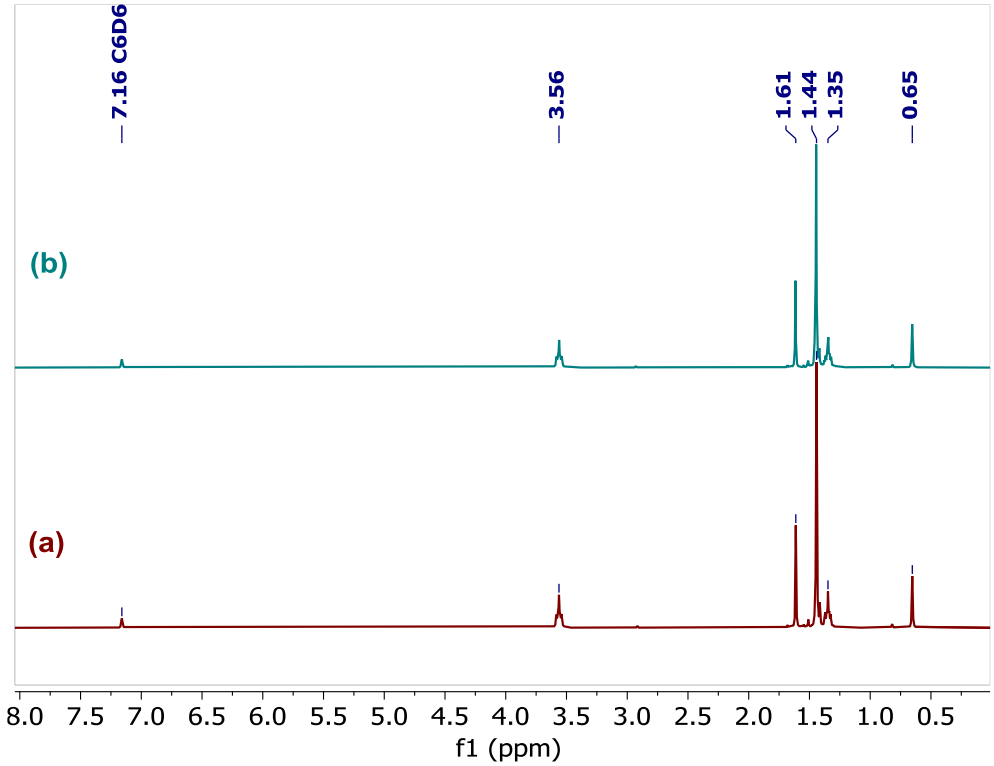


Figure S1. ^{1}H-NMR spectrum (300 MHz, C_6D_6, 298K) of compound **(1)**: **(a)** at t_0 **(b)** after 24h in C_6D_6.

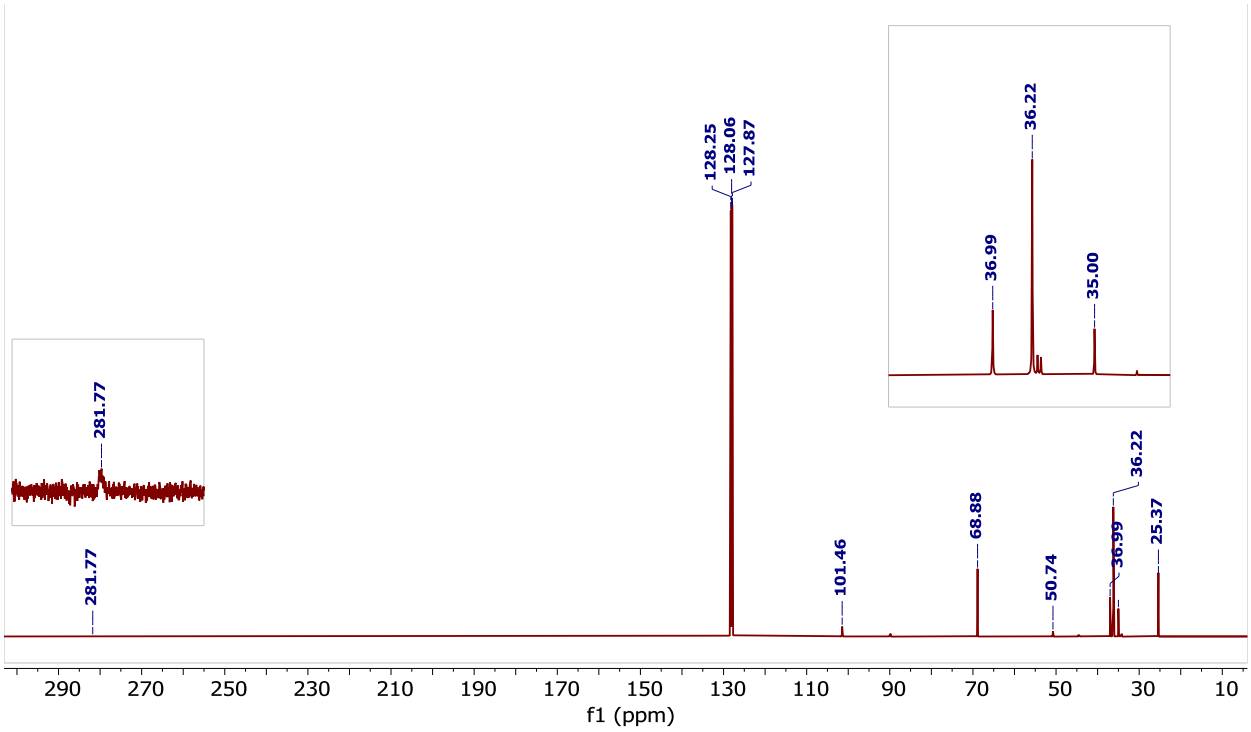


Figure S2. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(1)**.

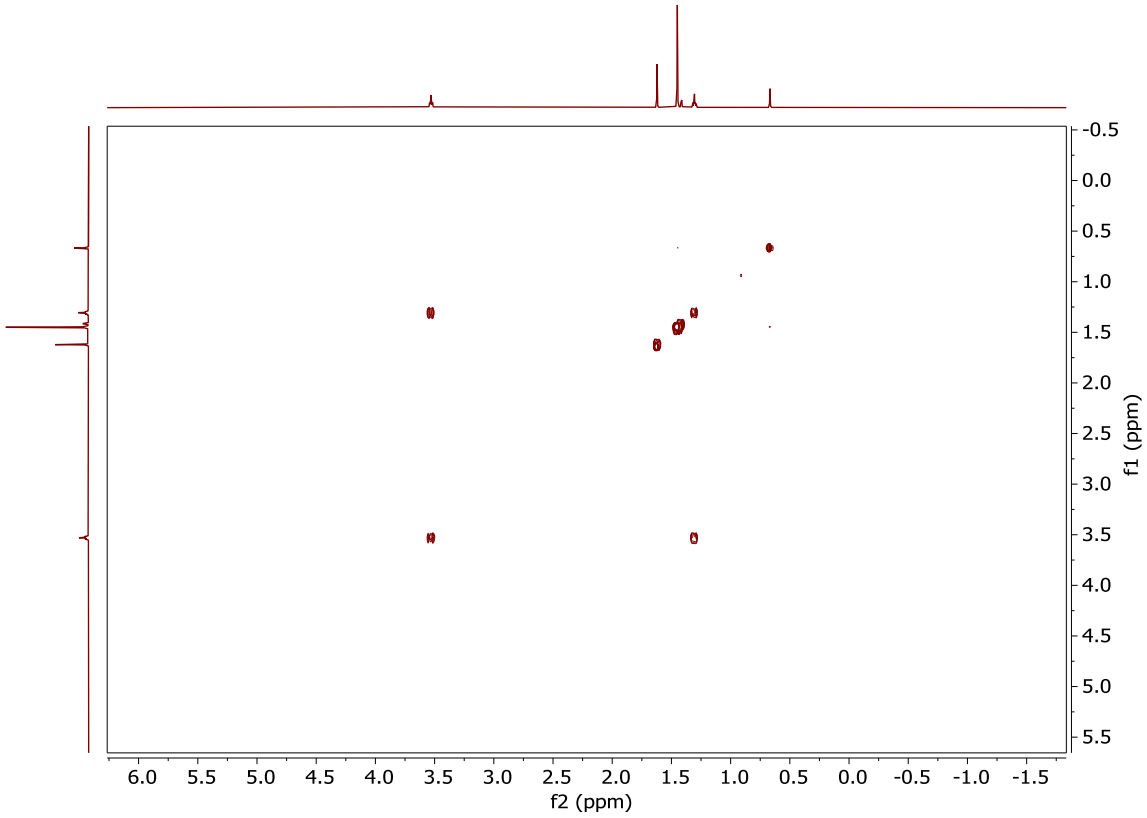


Figure S3. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(1)**.

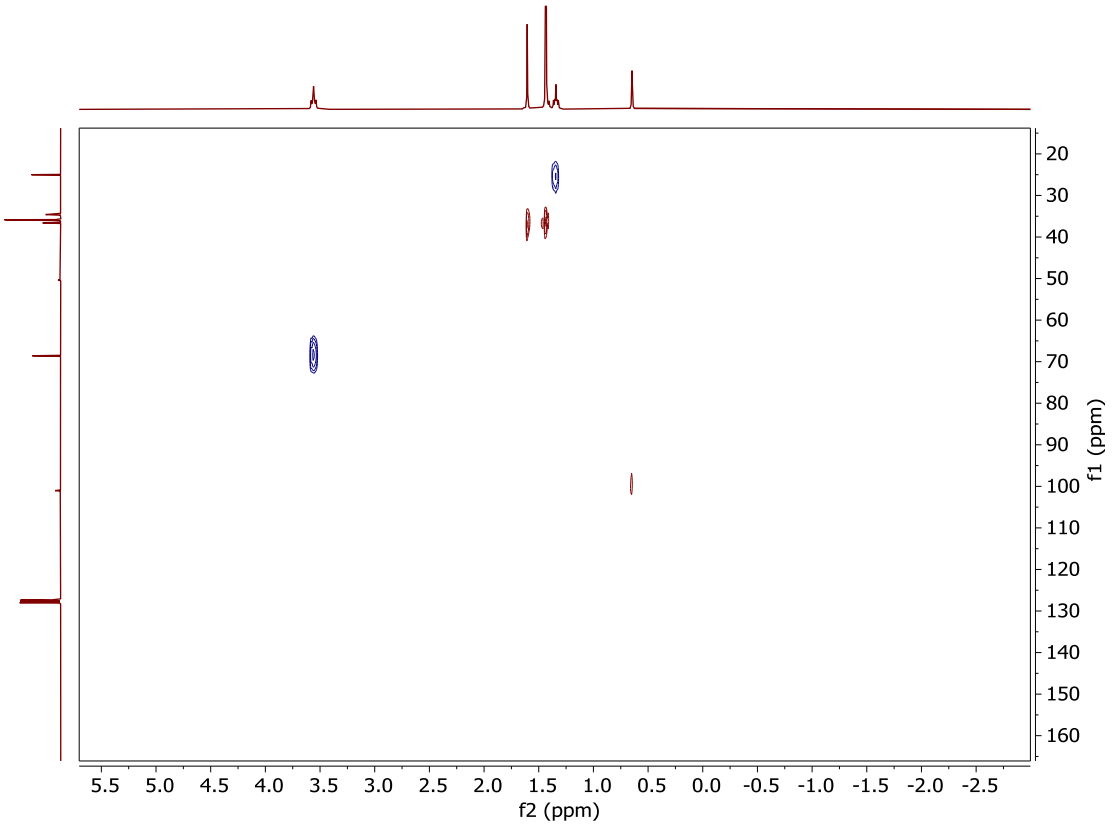


Figure S4. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(1)**.

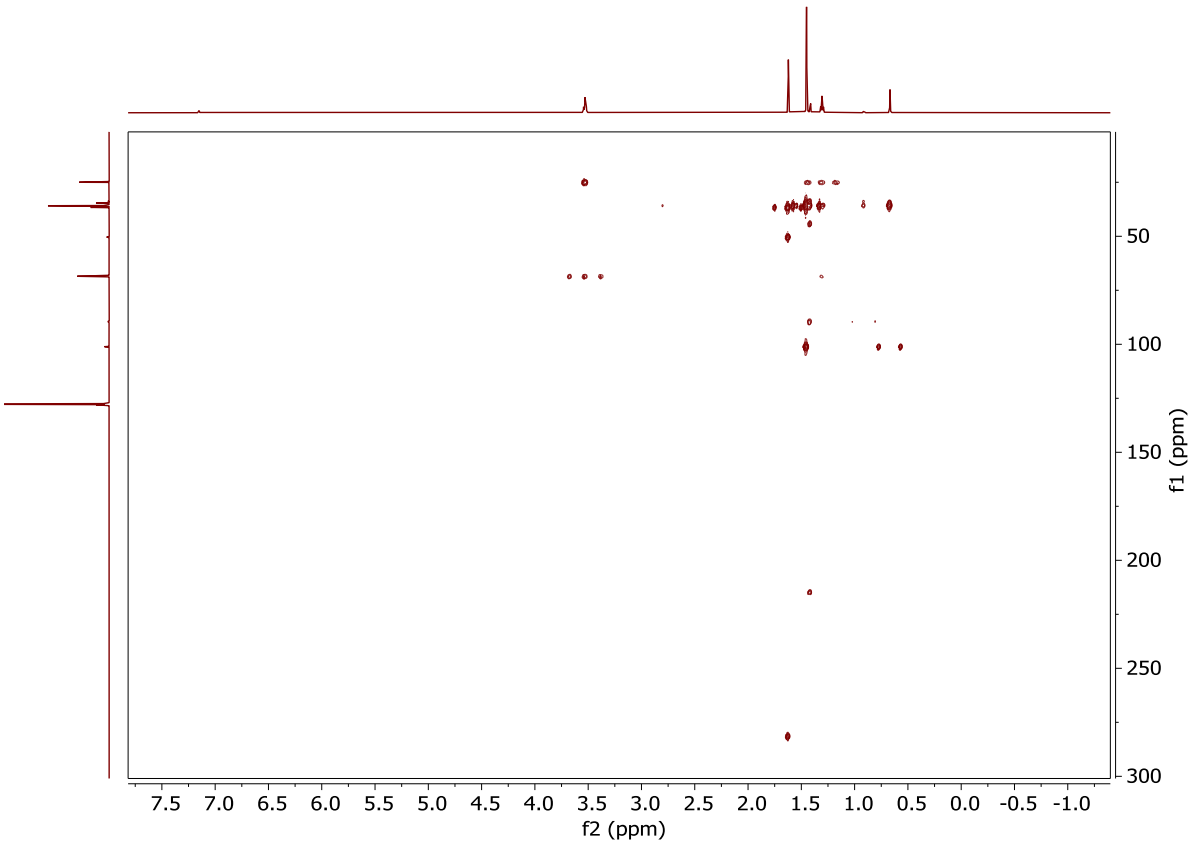


Figure S5. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(1)**.

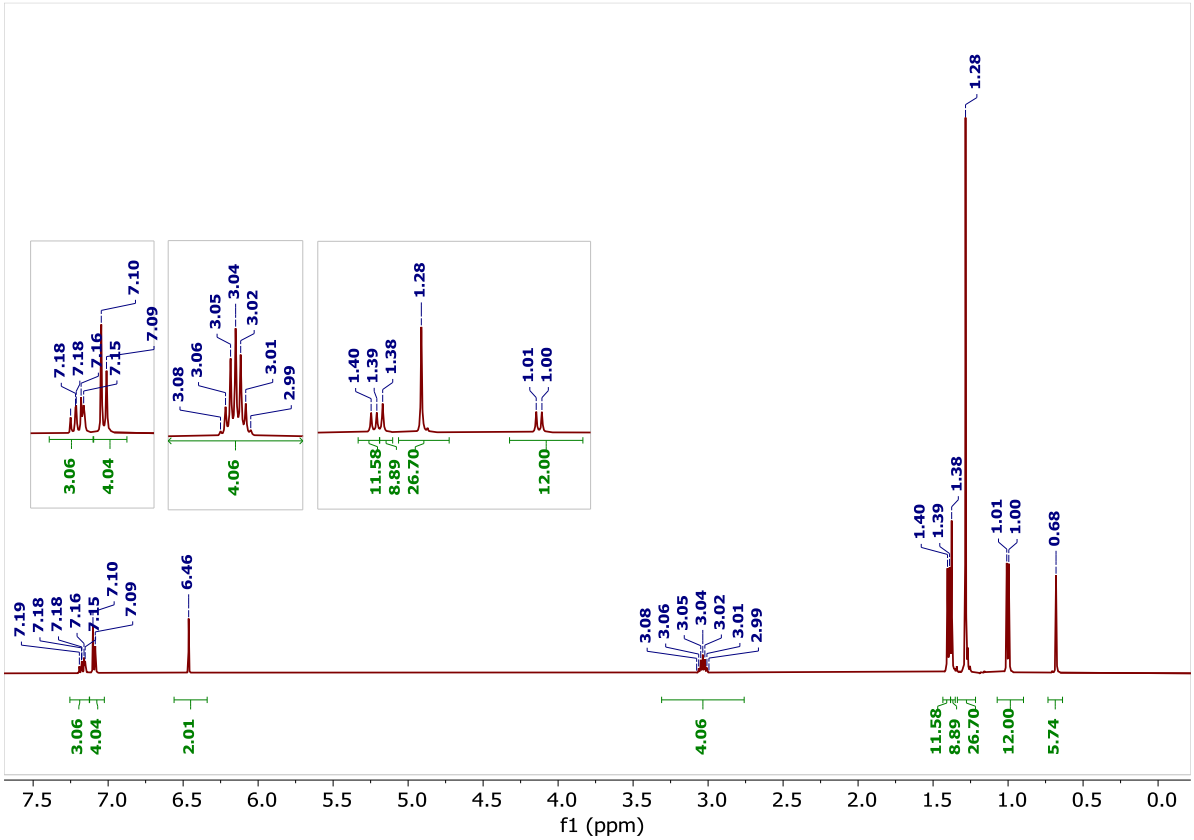


Figure S6. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)**.

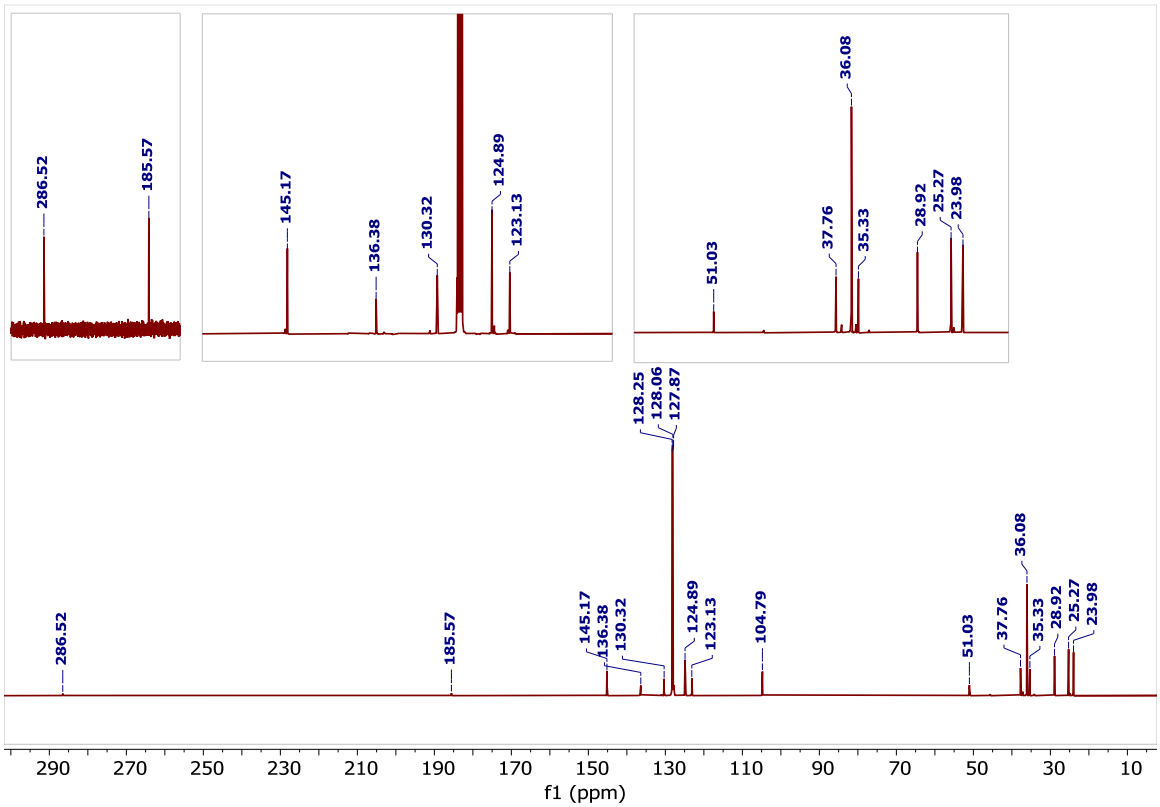


Figure S7. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(2-Cu)**.

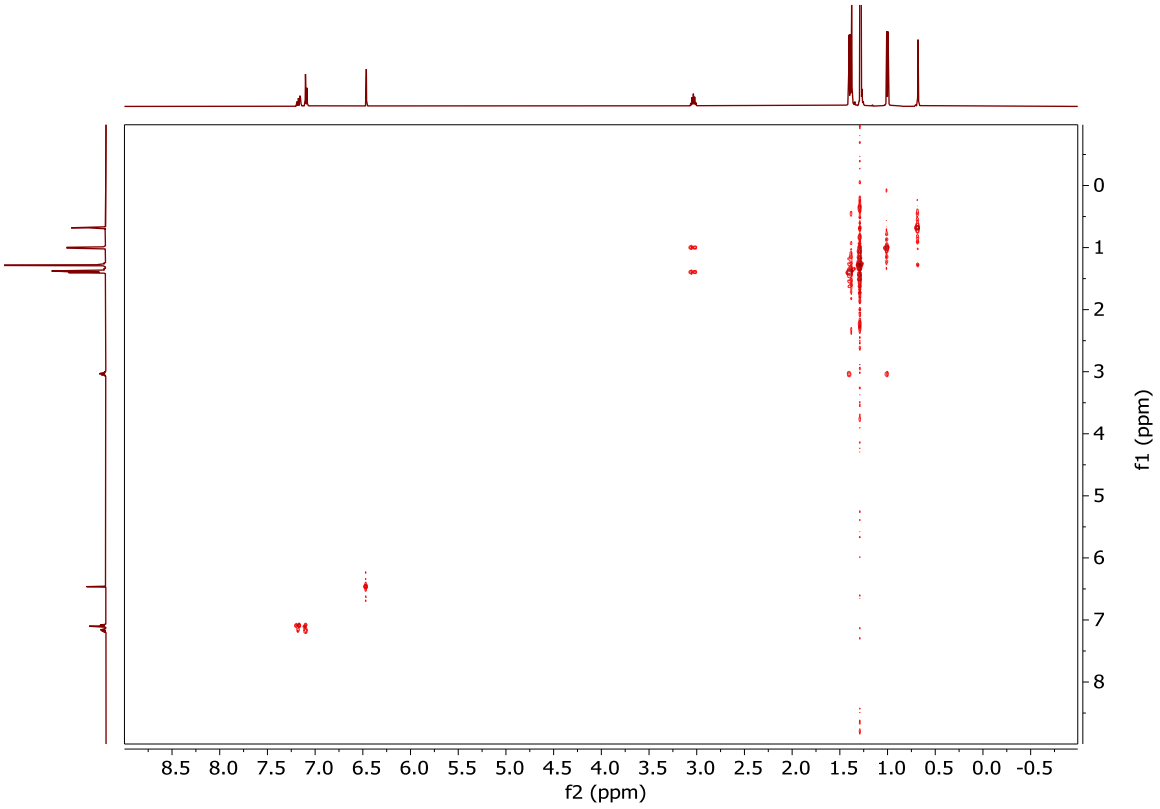


Figure S8. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)**.

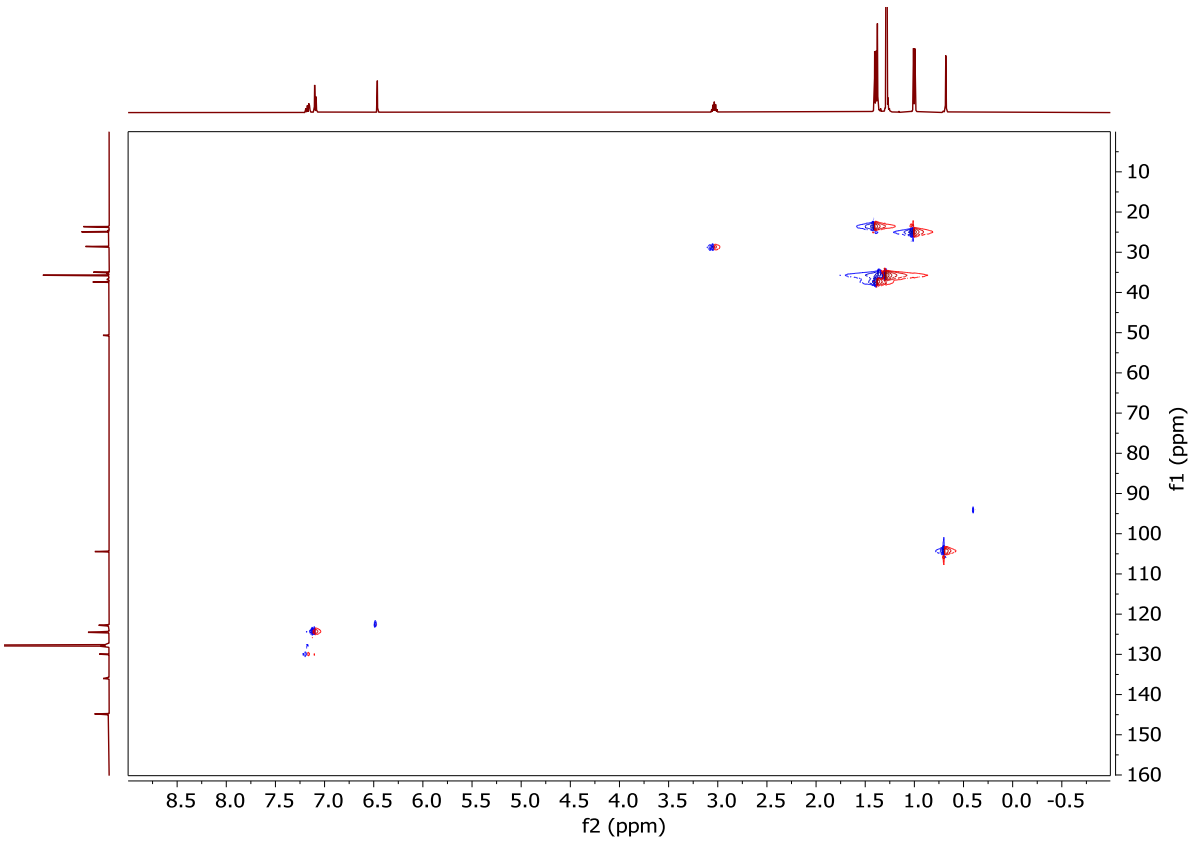


Figure S9. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)**. Part 1: from 0 ppm to 160 ppm in f1.

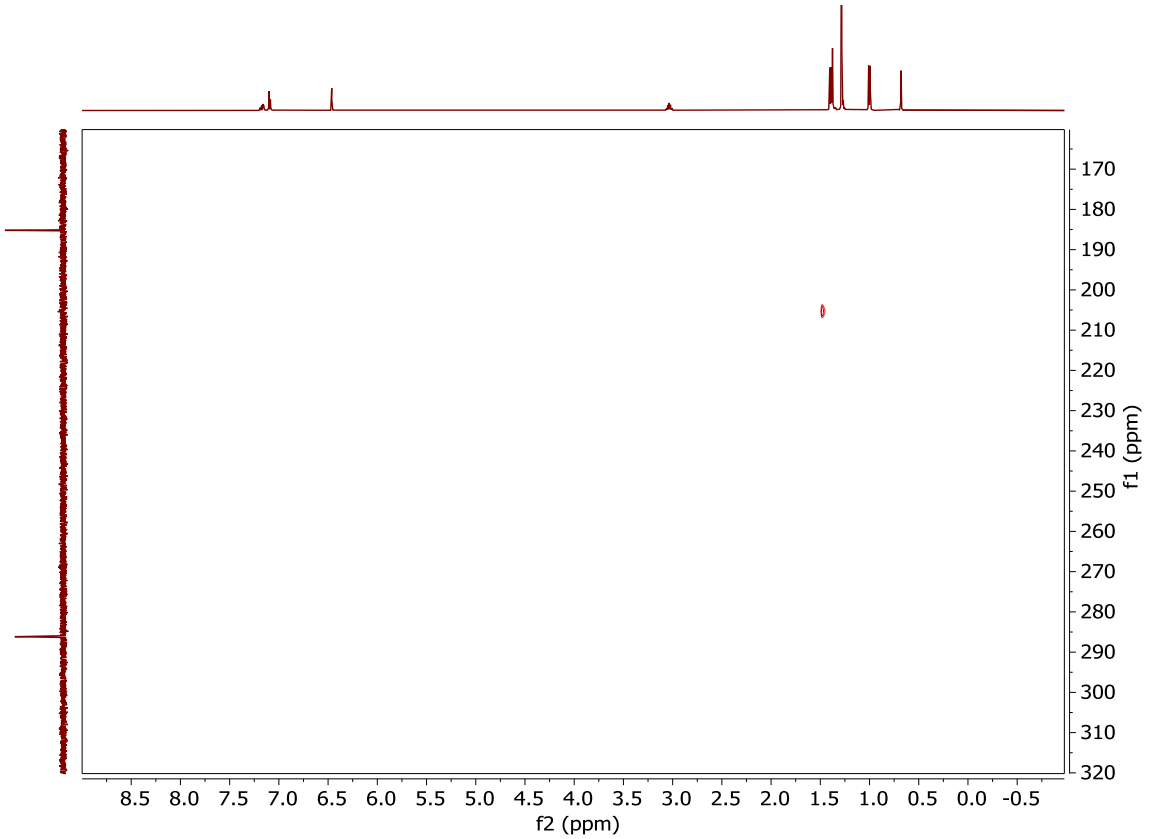


Figure S10. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)**. Part 2: from 160 ppm to 320 ppm in f1.

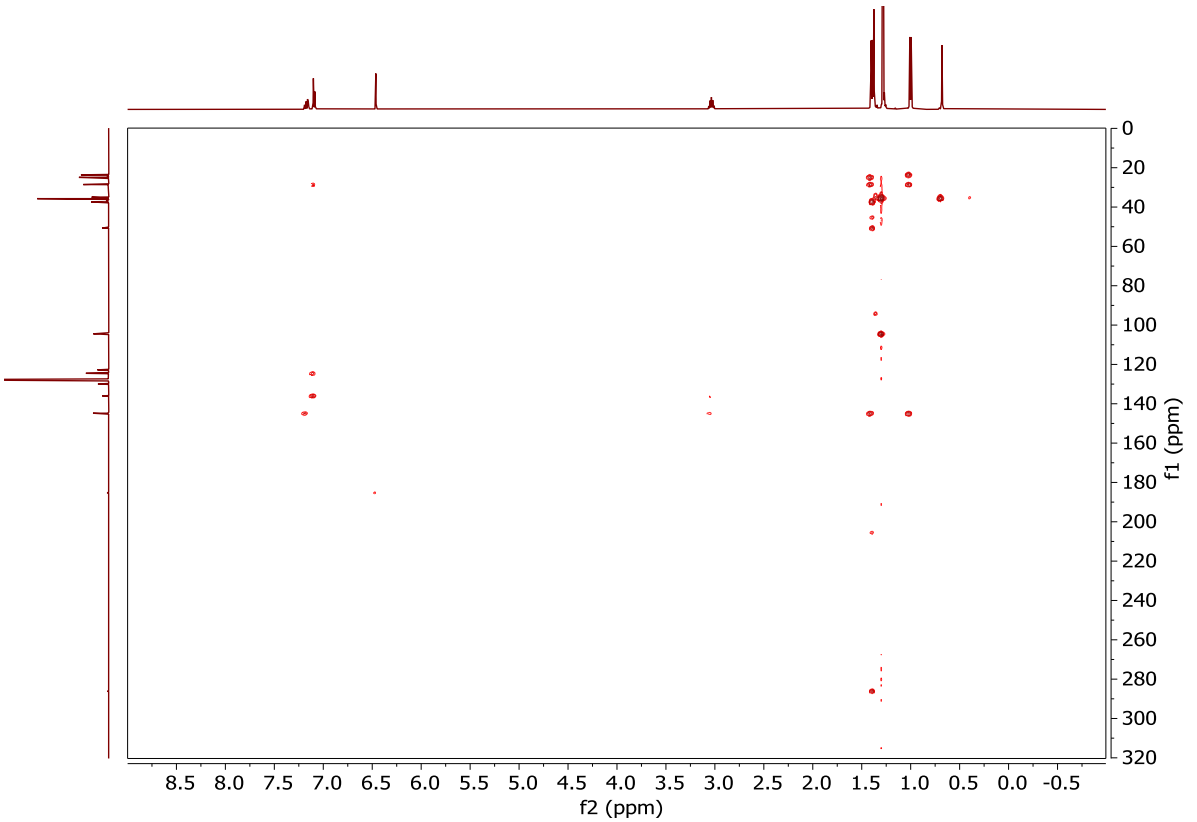


Figure S11. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)**.

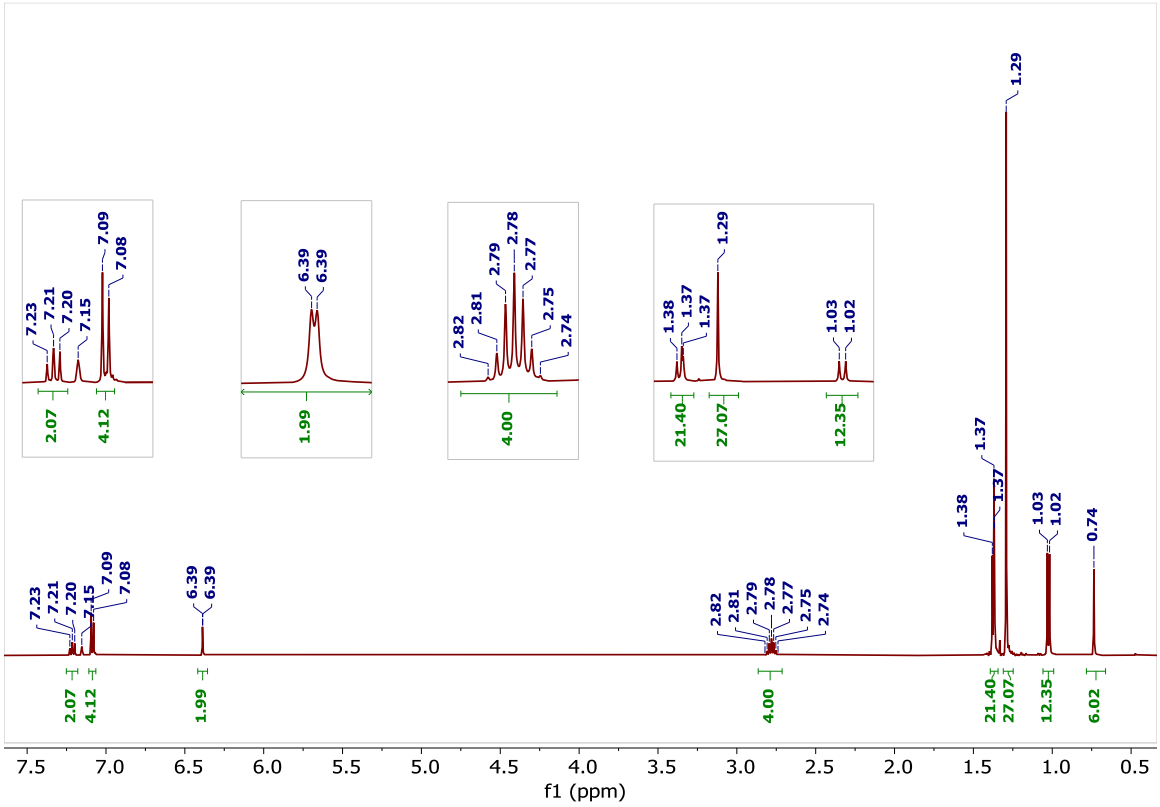


Figure S12. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)**.

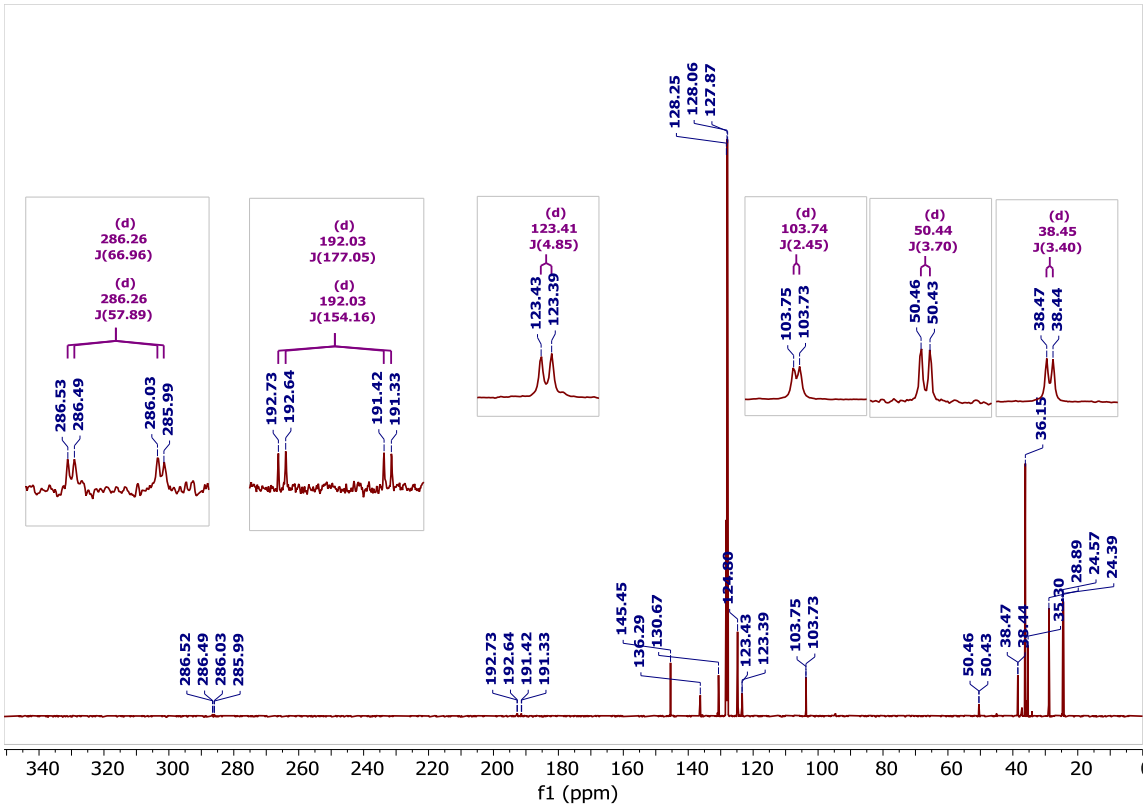


Figure S13. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(2-Ag)**. Naturally occurring silver (Ag) is composed of the two stable isotopes, both being NMR active: ^{107}Ag (51.8% abundance, S = 1/2) and ^{109}Ag (48.2% abundance, S = 1/2).

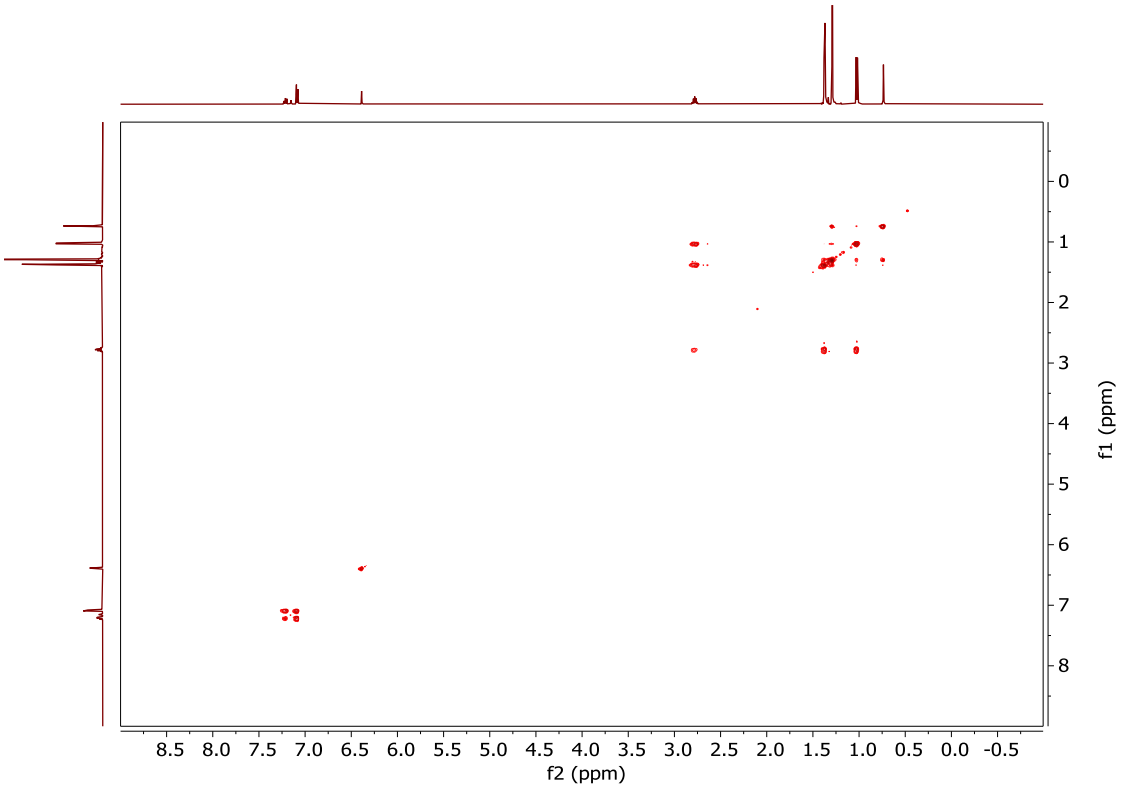


Figure S14. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)**.

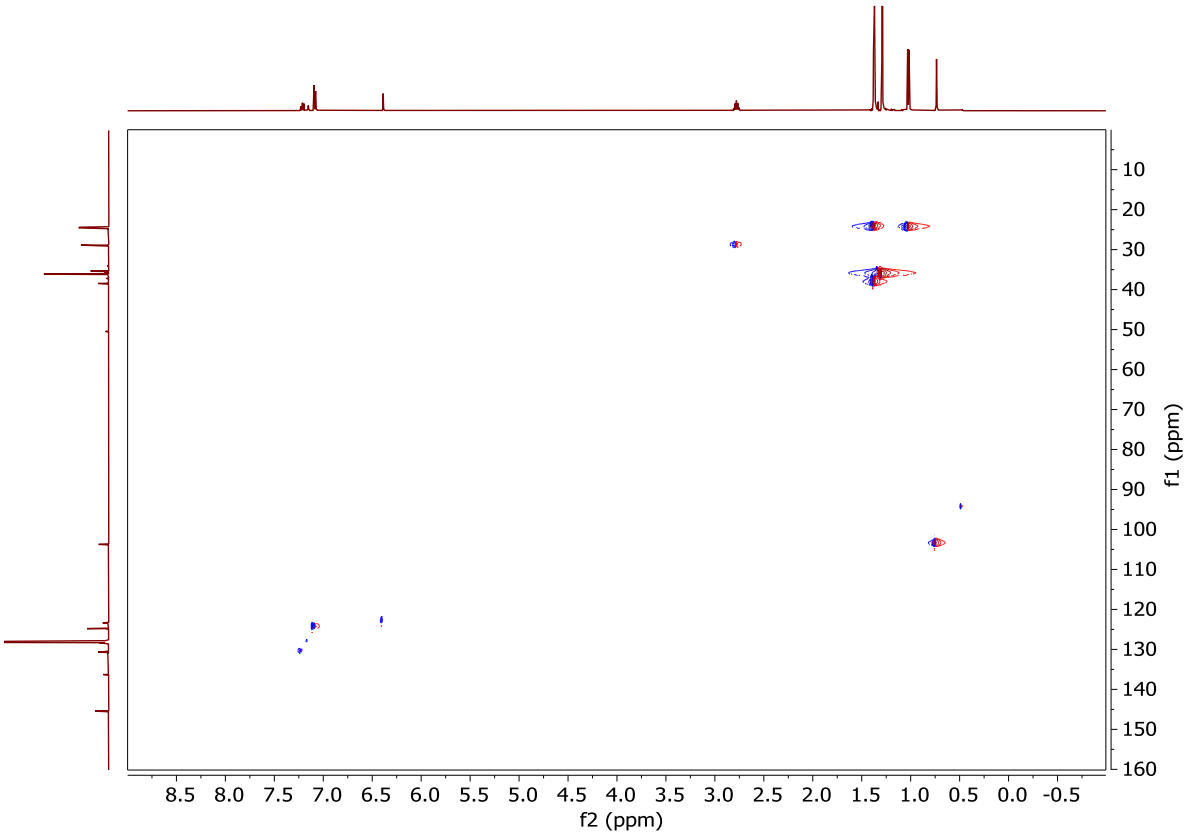


Figure S15. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)**. Part 1: from 0 ppm to 160 ppm in f1.

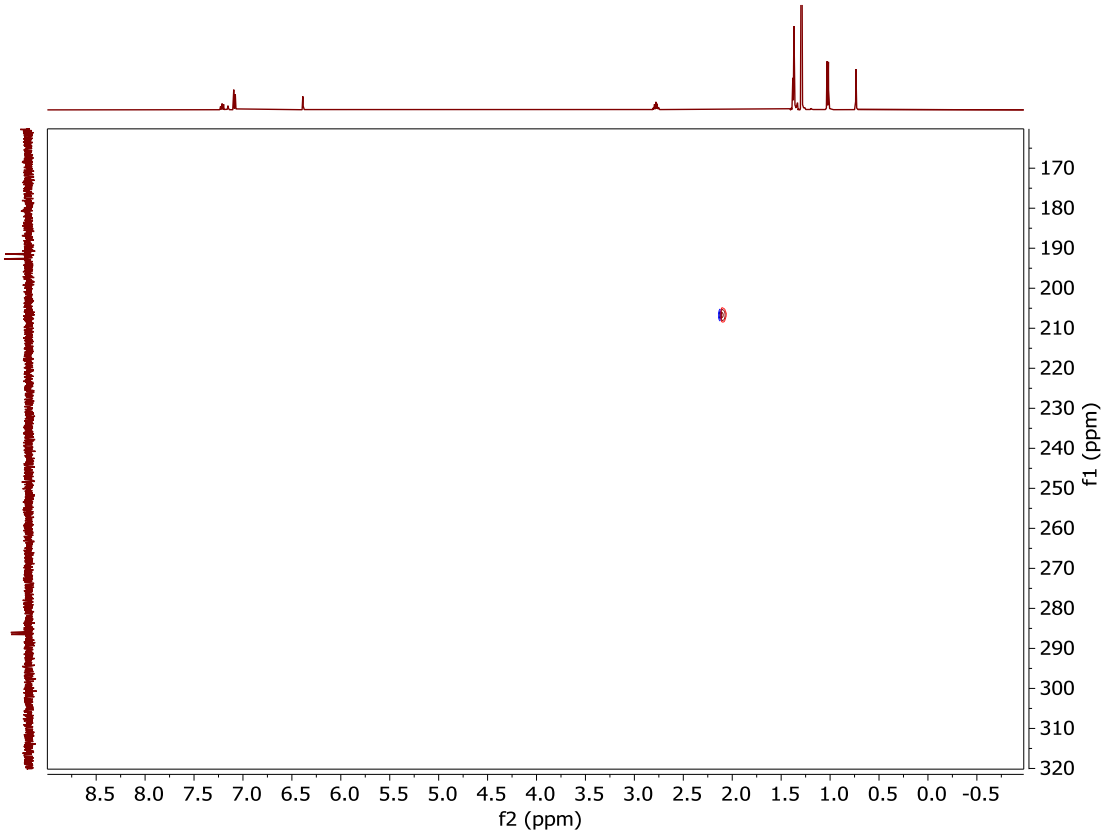


Figure S16. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)**. Part 2: from 160 ppm to 320 ppm in f1.

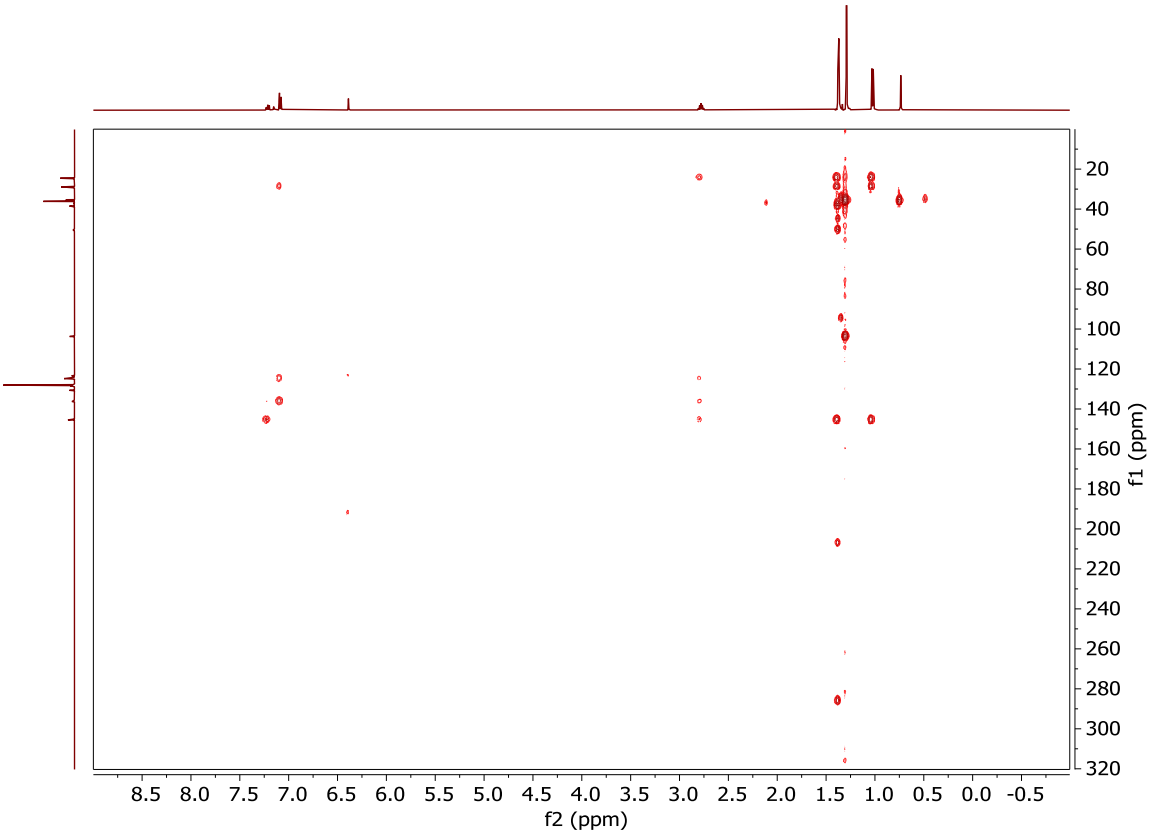


Figure S17. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)**.

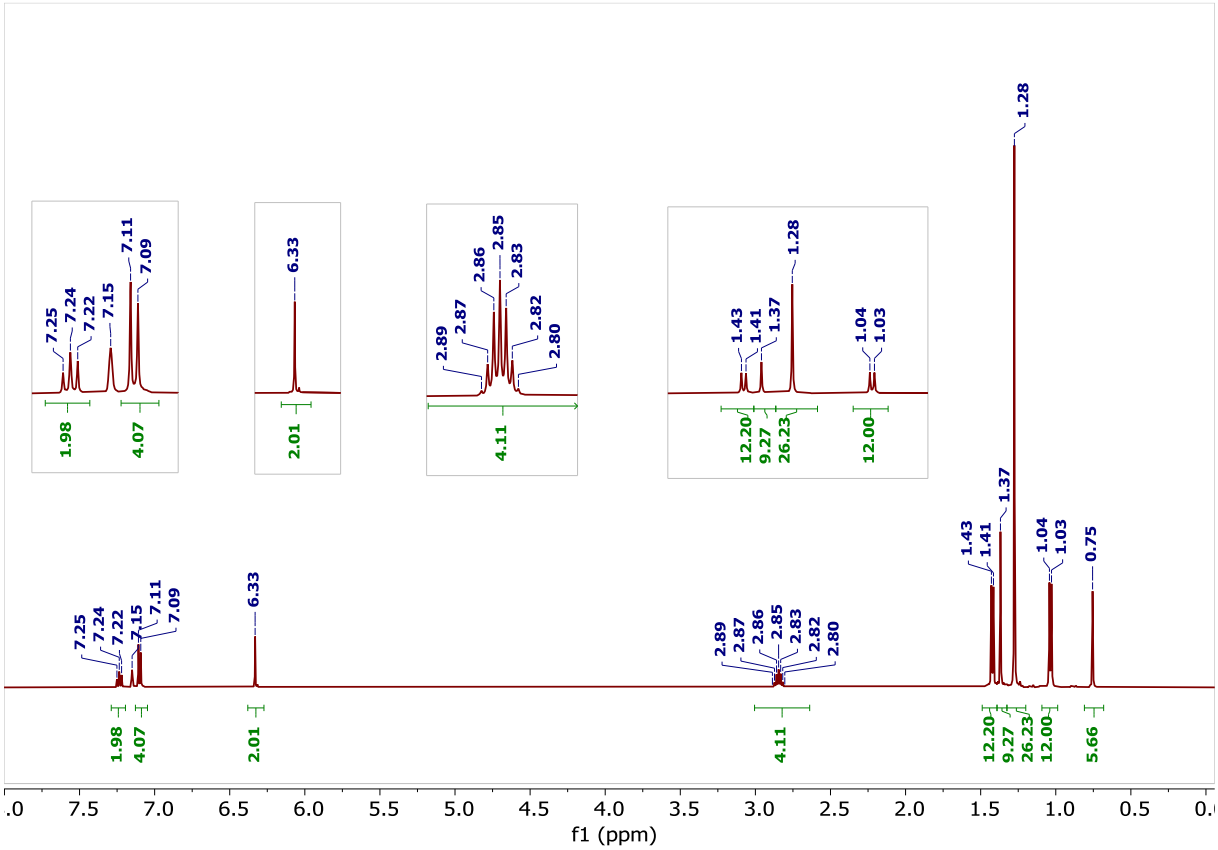


Figure S18. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Au)**.

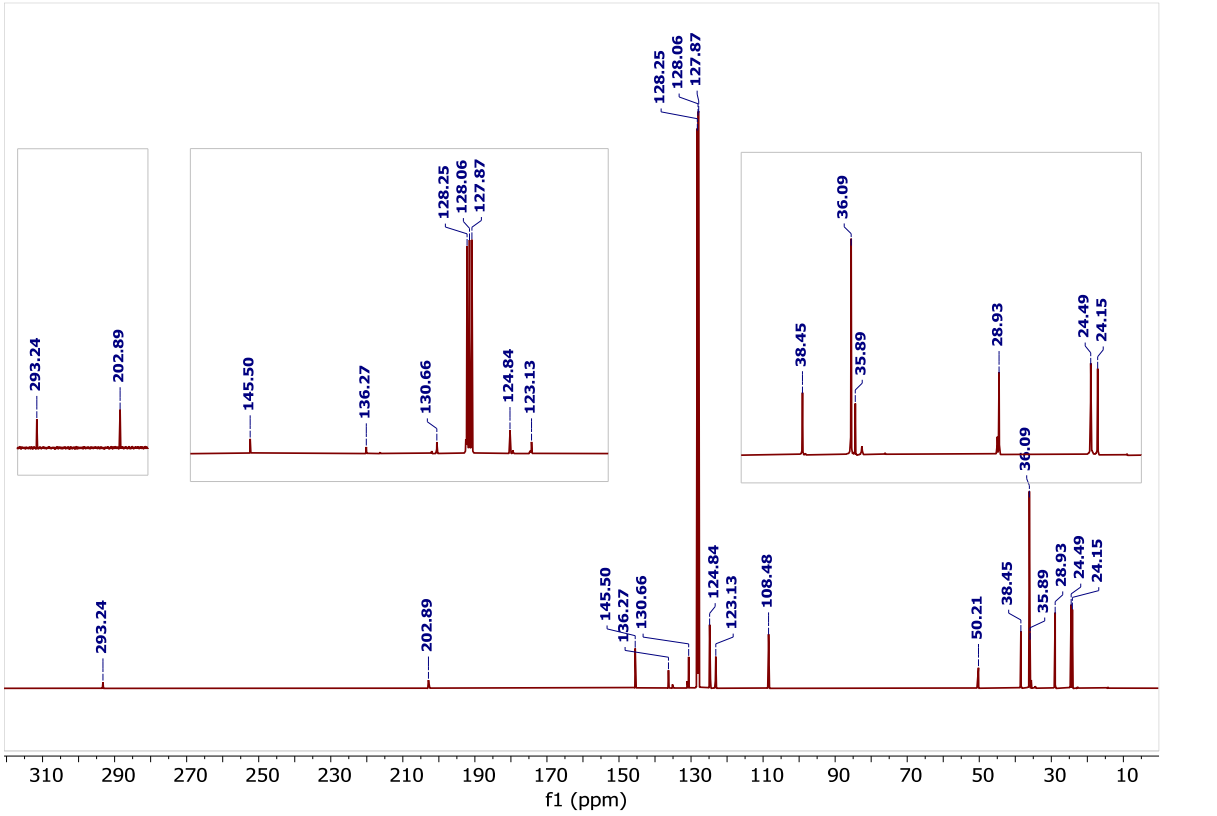


Figure S19. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(2-Au)**.

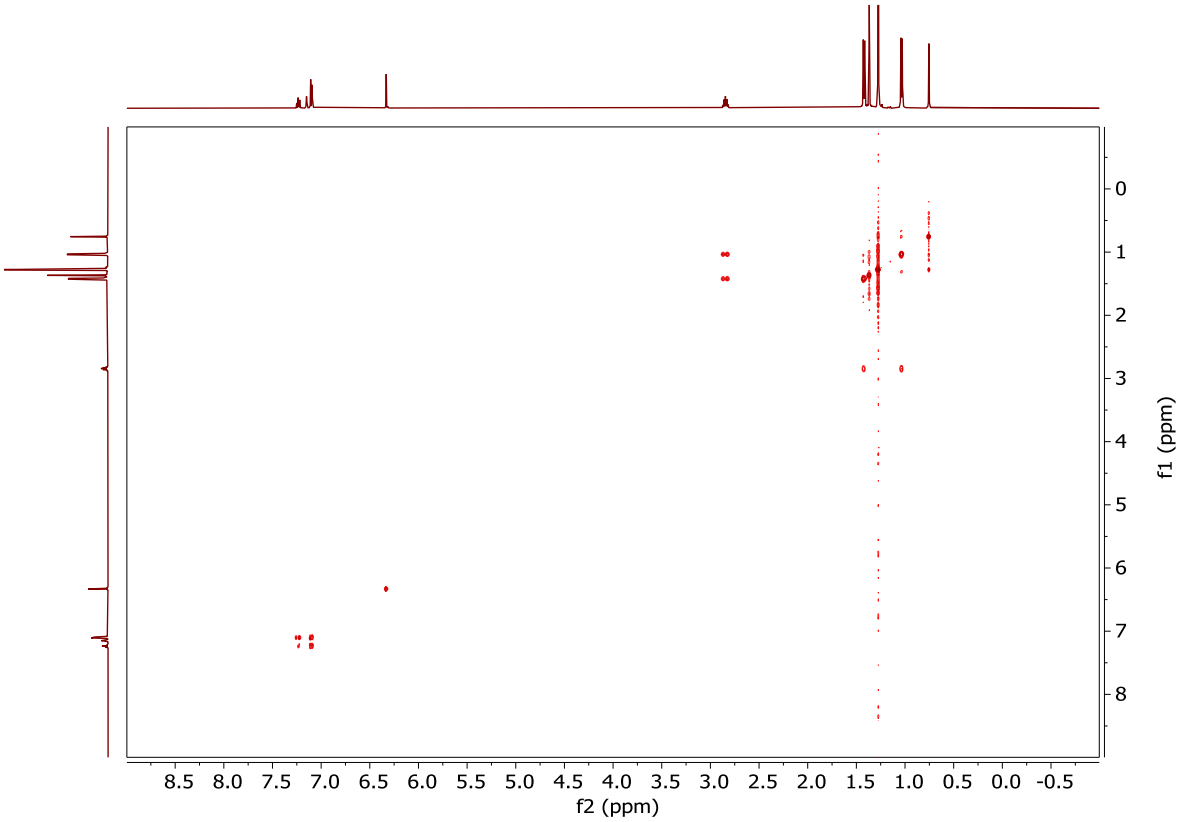


Figure S20. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Au)**.

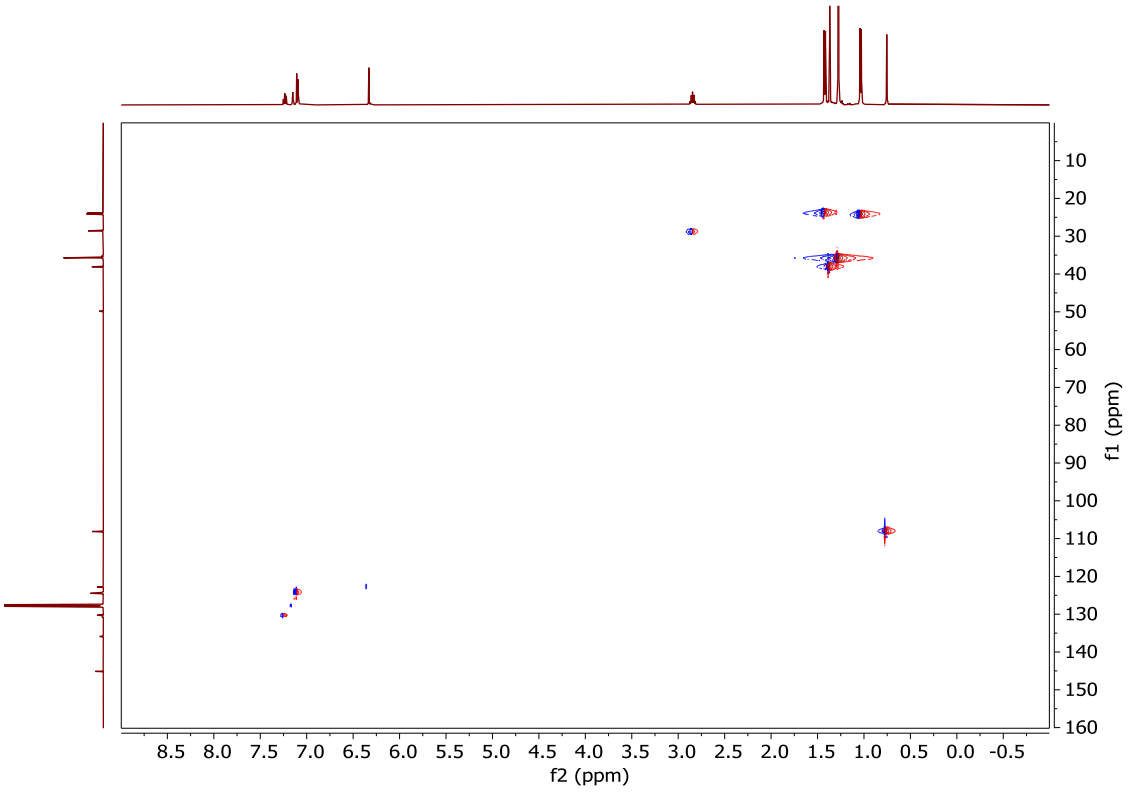


Figure S21. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Au)**. Part 1: from 0 ppm to 160 ppm in f1.

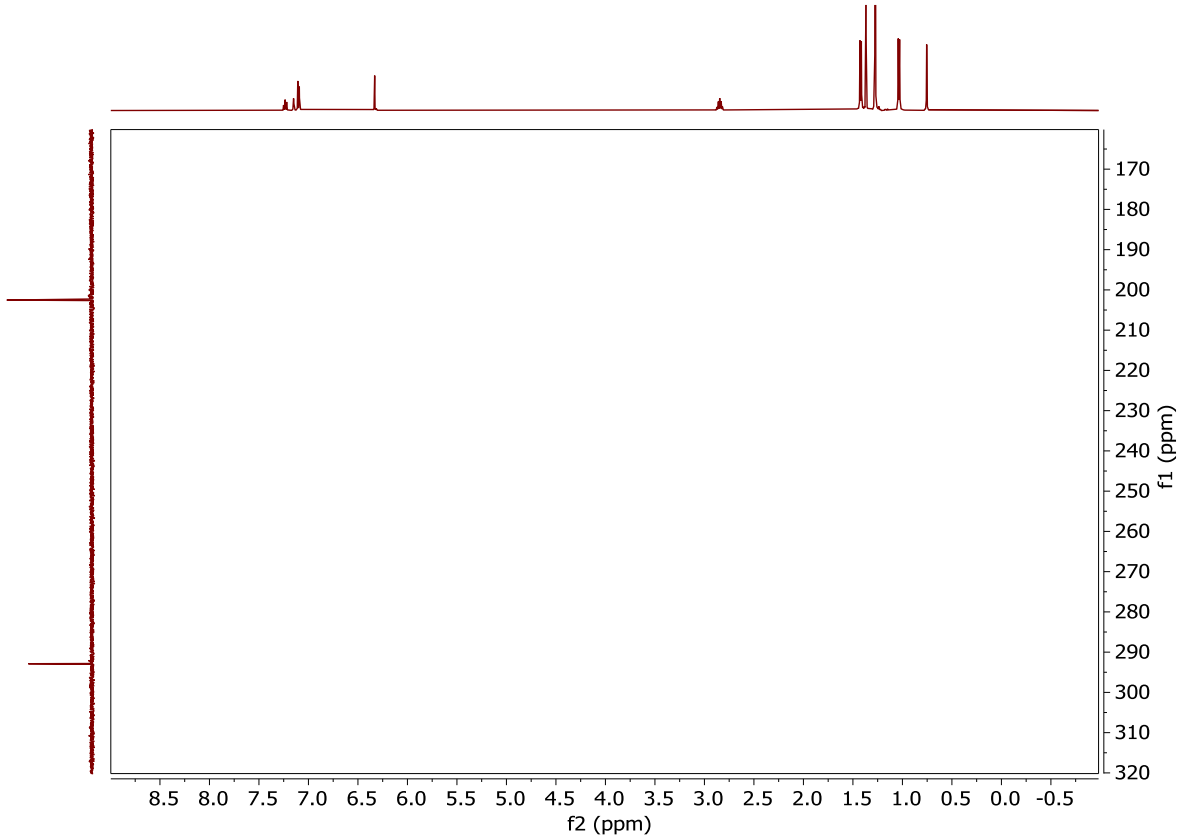


Figure S22. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Au)**. Part 2: from 160 ppm to 320 ppm in f1.

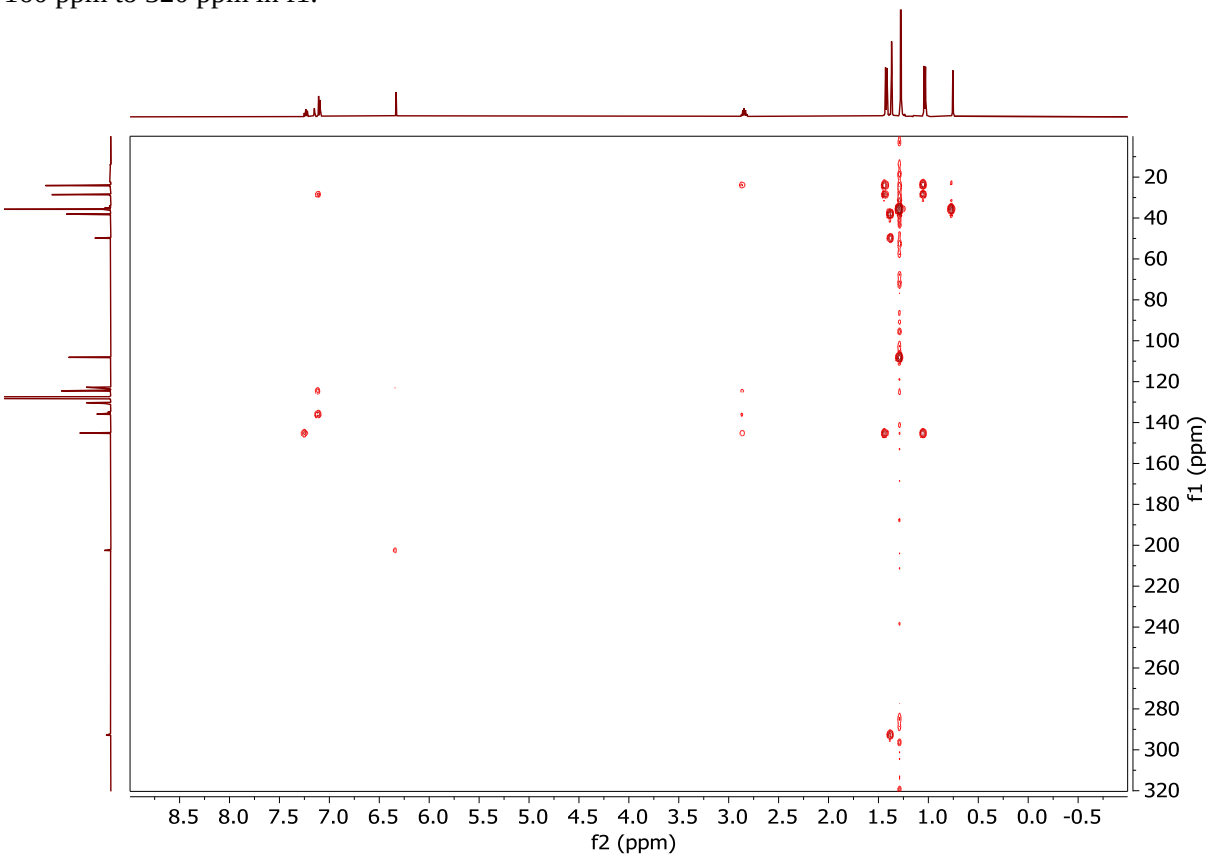


Figure S23. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Au)**.

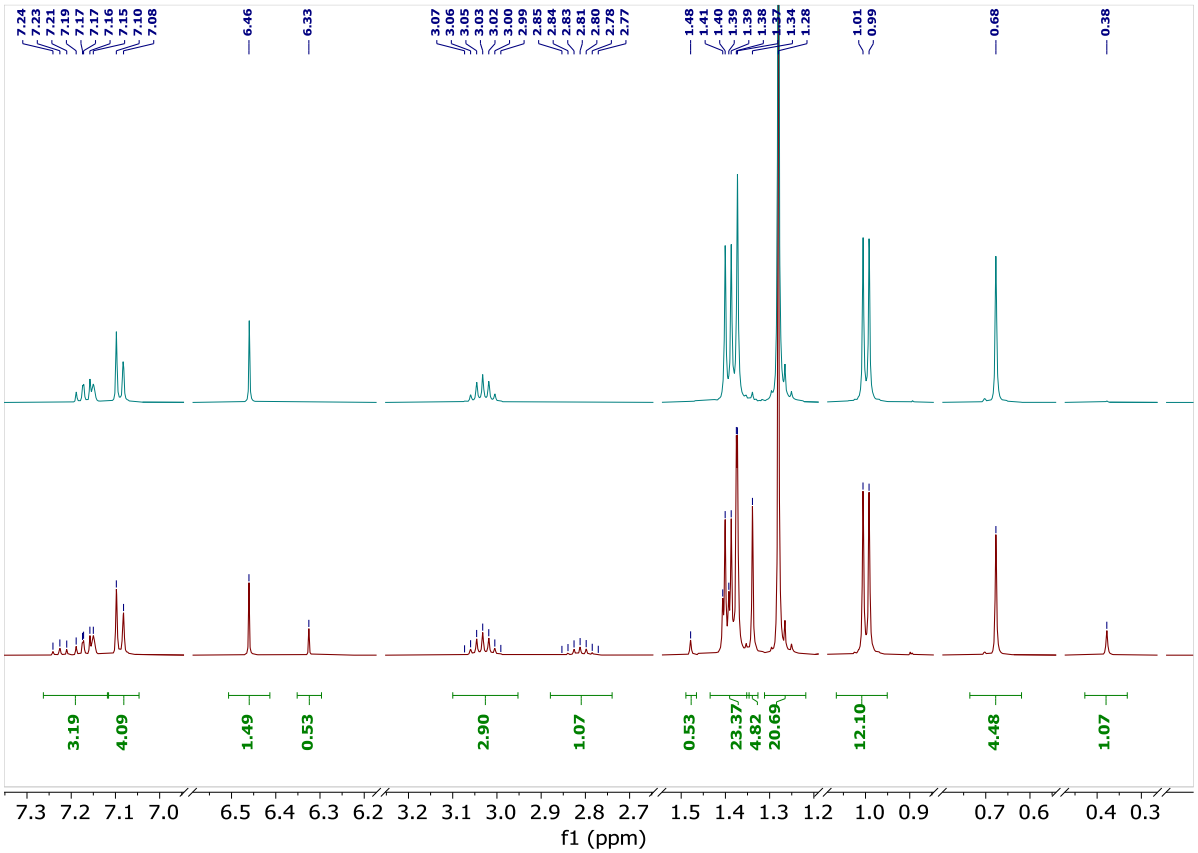


Figure S24. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Cu)** is shown at the top. The same sample was analysed after one day in C_6D_6 at room temperature (bottom).

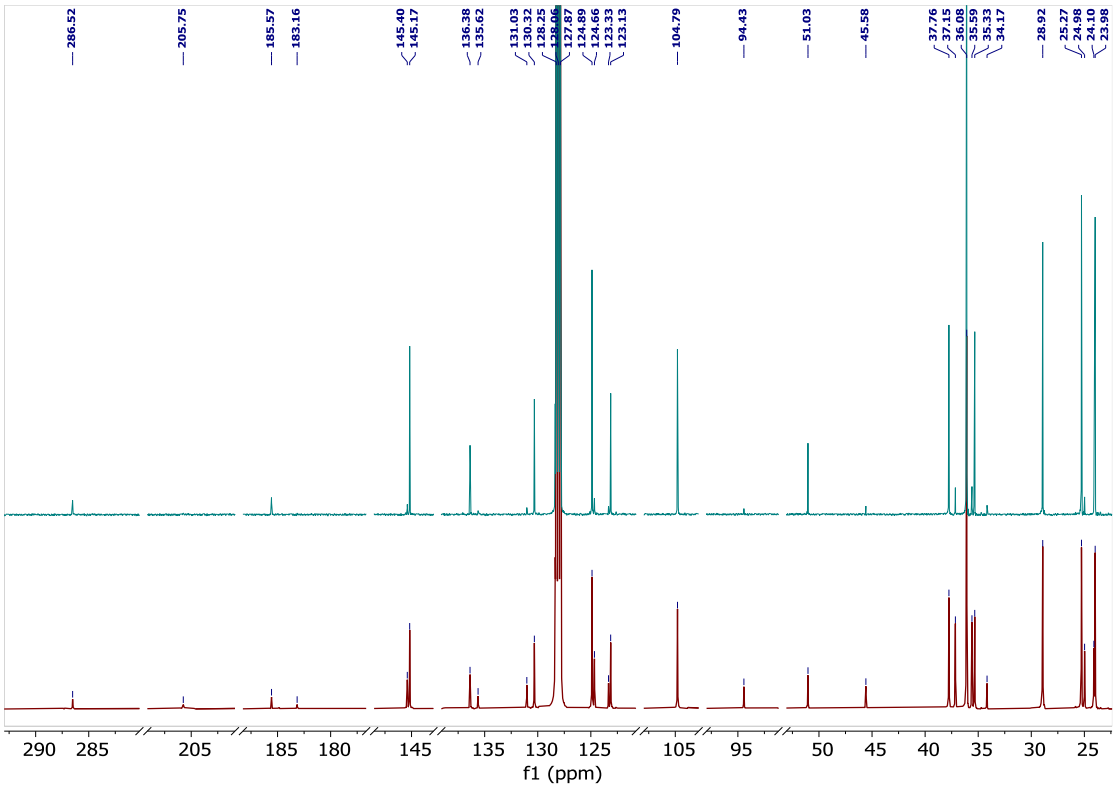


Figure S25. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(2-Cu)** is shown at the top. The same sample was analysed after one day in C_6D_6 at room temperature (bottom).

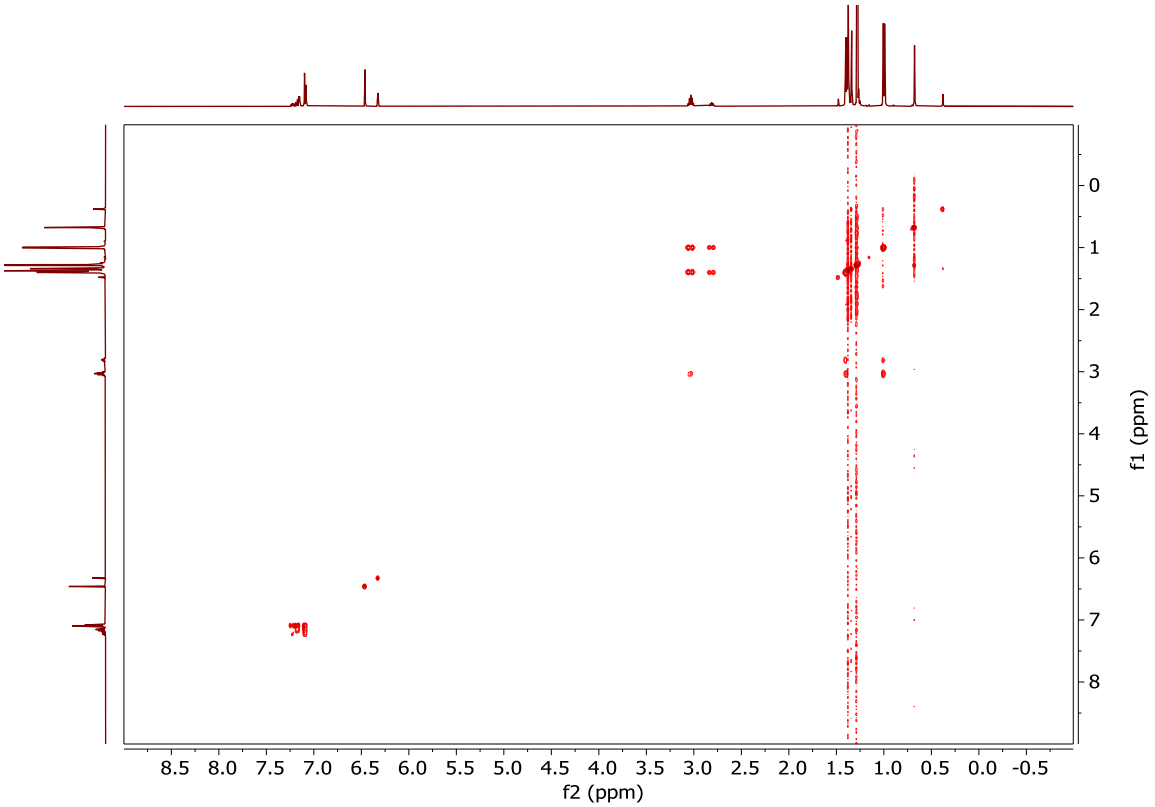


Figure S26. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2-Cu)** and **(3-Cu).**

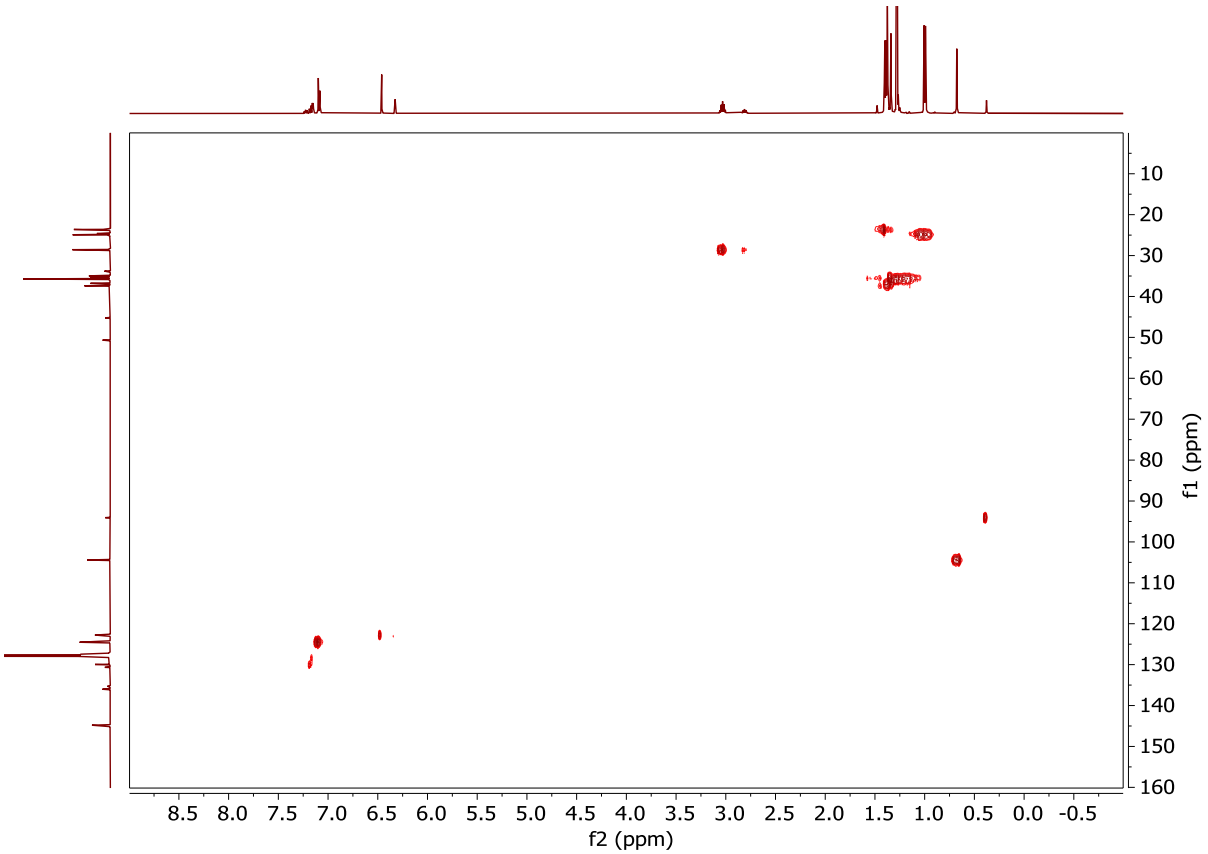


Figure S27. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2-Cu)** and **(3-Cu).** Part 1: from 0 ppm to 160 ppm in f1.

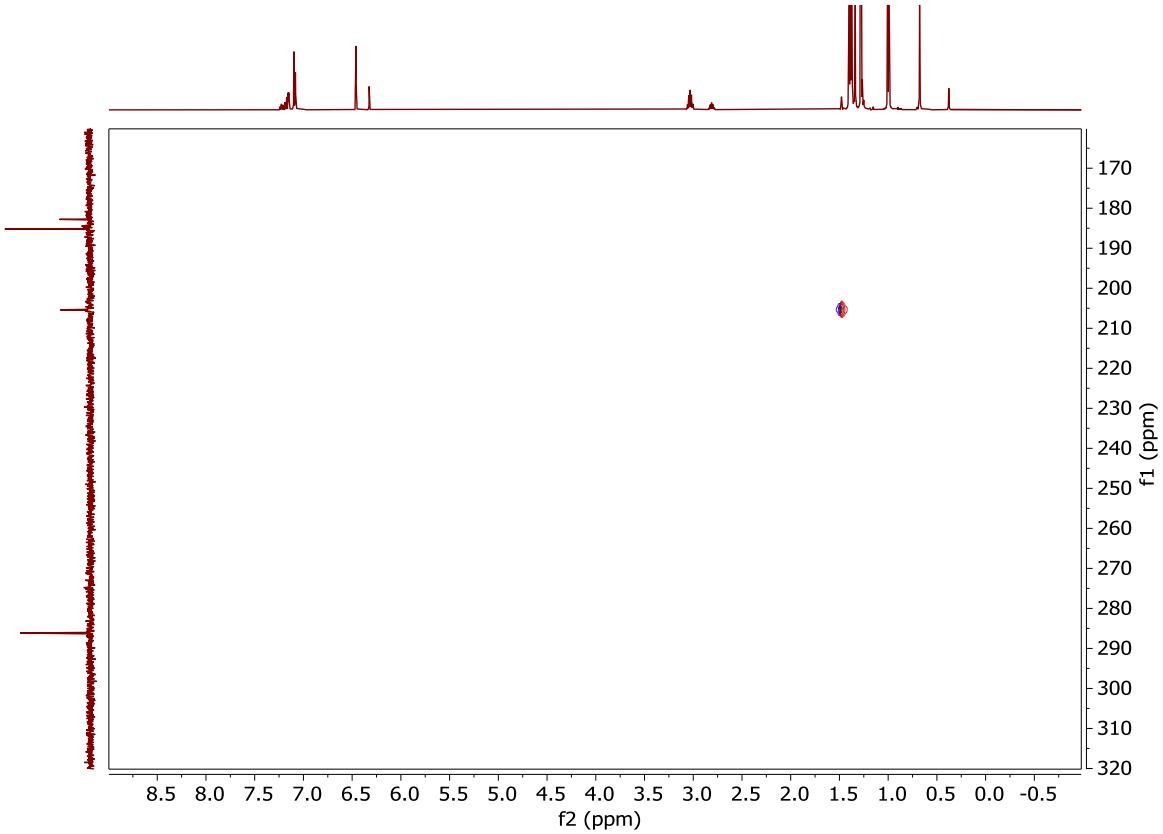


Figure S28. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2-Cu)** and **(3-Cu).** Part 2: from 160 ppm to 320 ppm in f1.

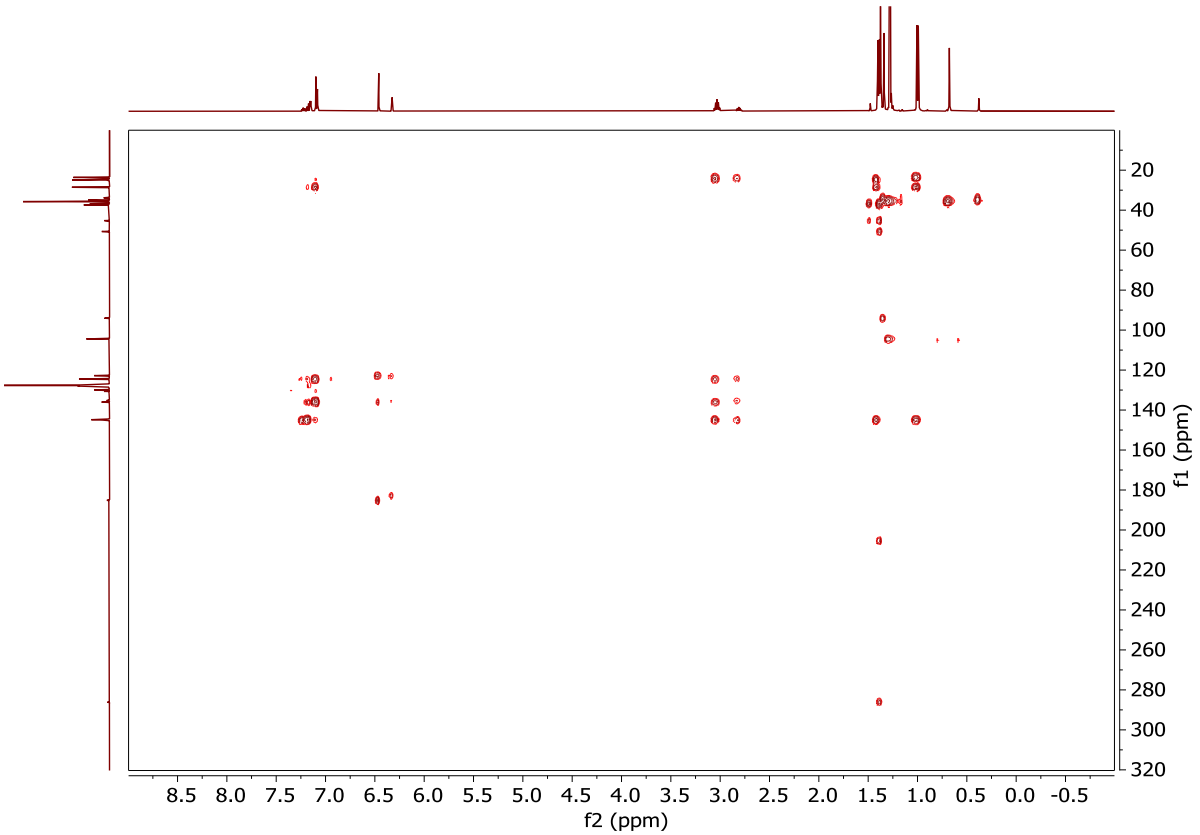


Figure S29. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2-Cu)** and **(3-Cu).**

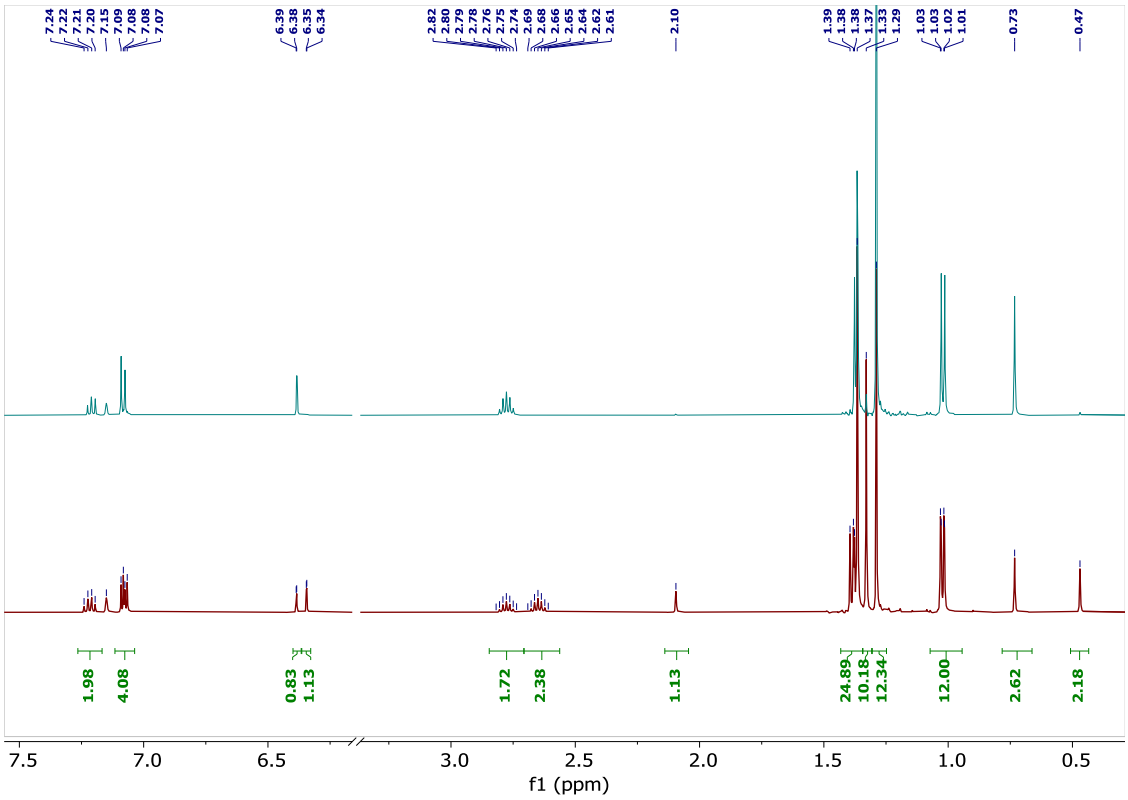


Figure S30. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(2-Ag)** is shown at the top. The same sample was analysed after one day in C_6D_6 at room temperature (bottom).

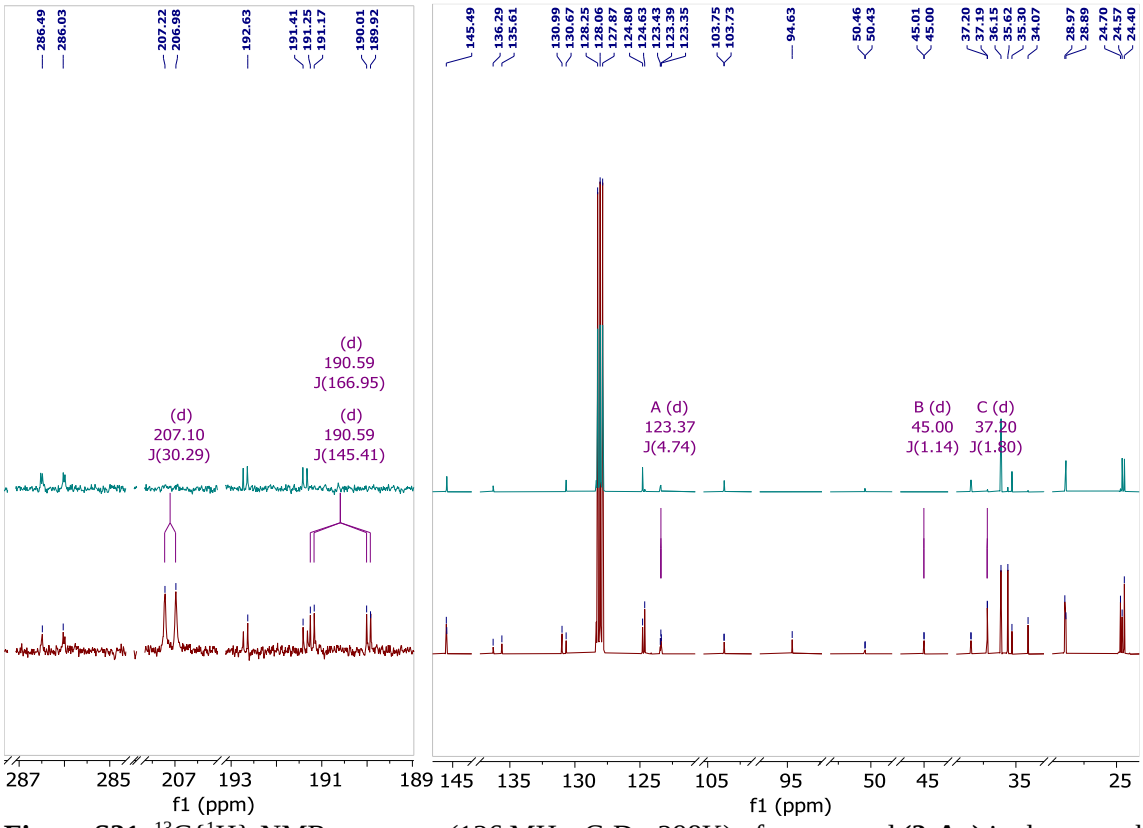


Figure S31. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(2-Ag)** is shown at the top. The same sample was analysed after one day in C_6D_6 at room temperature (bottom).

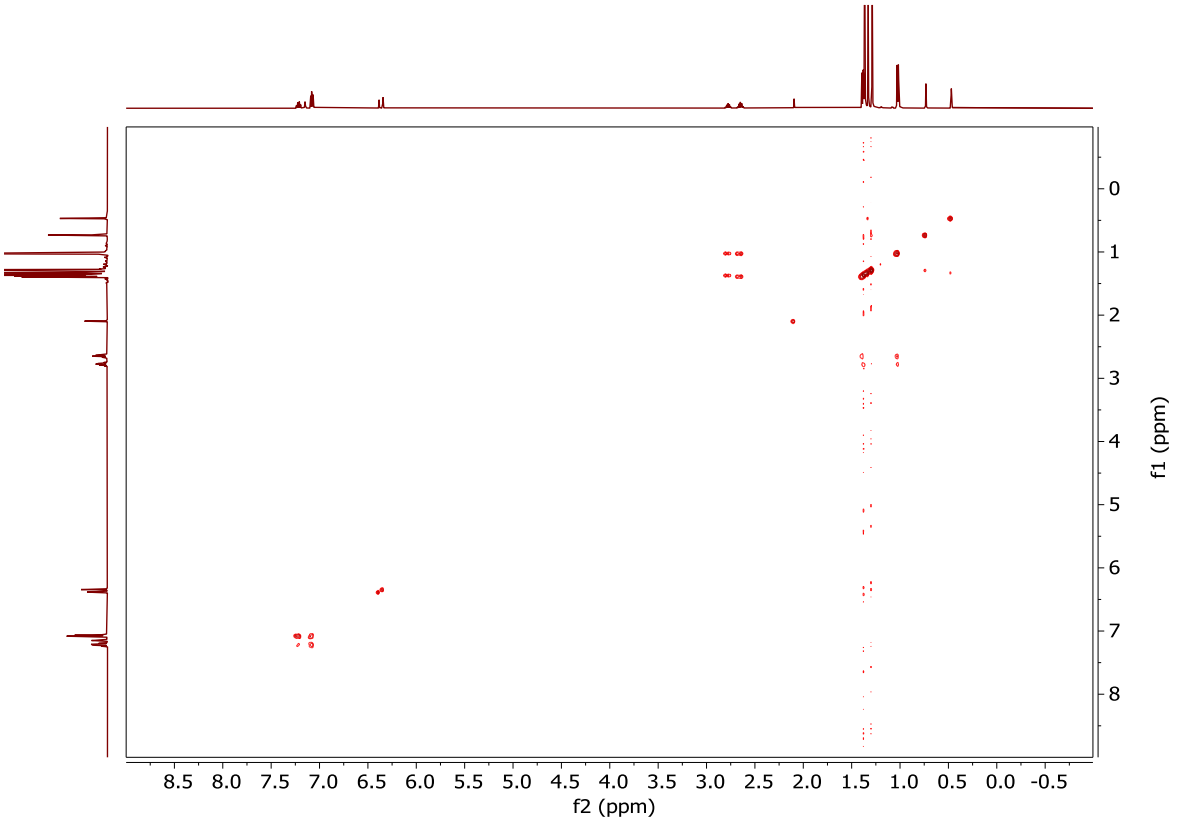


Figure S32. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2- Ag)** and **(3-Ag).**

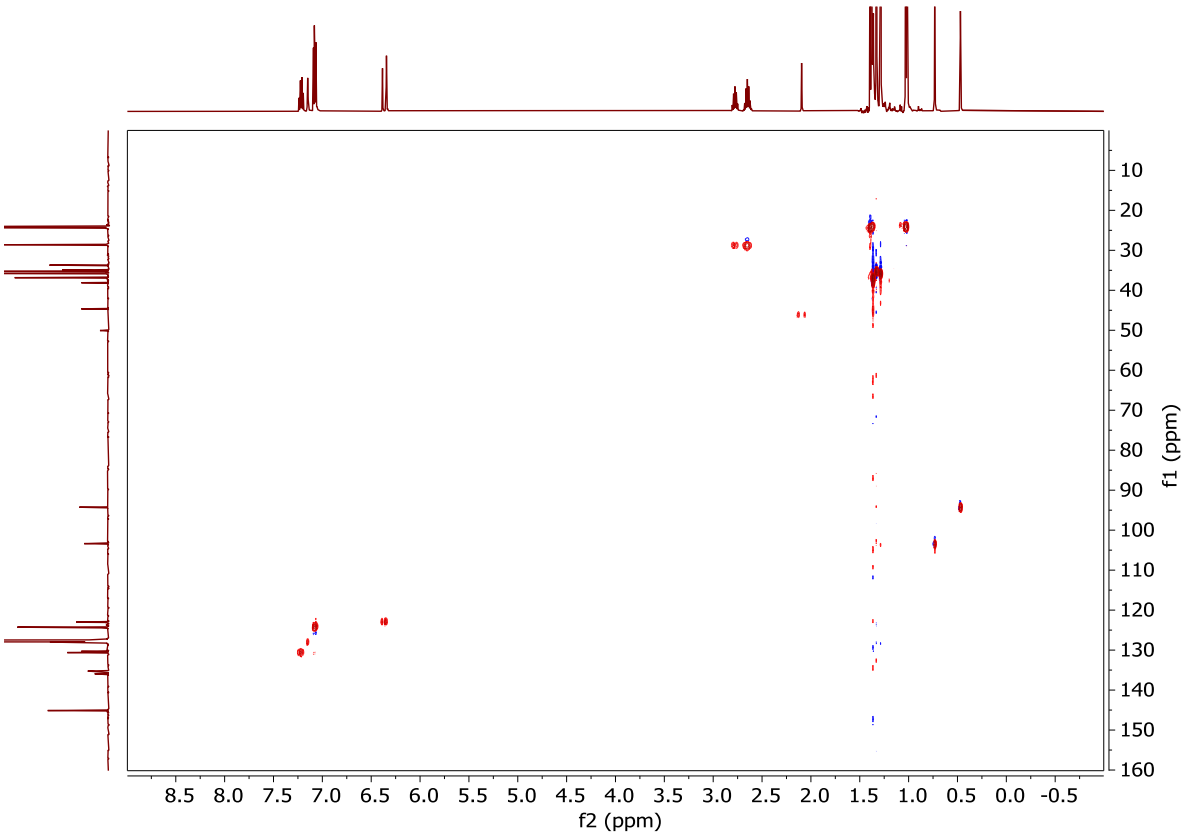


Figure S33. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2- Ag)** and **(3-Ag).** Part 1: from 0 ppm to 160 ppm in f1.

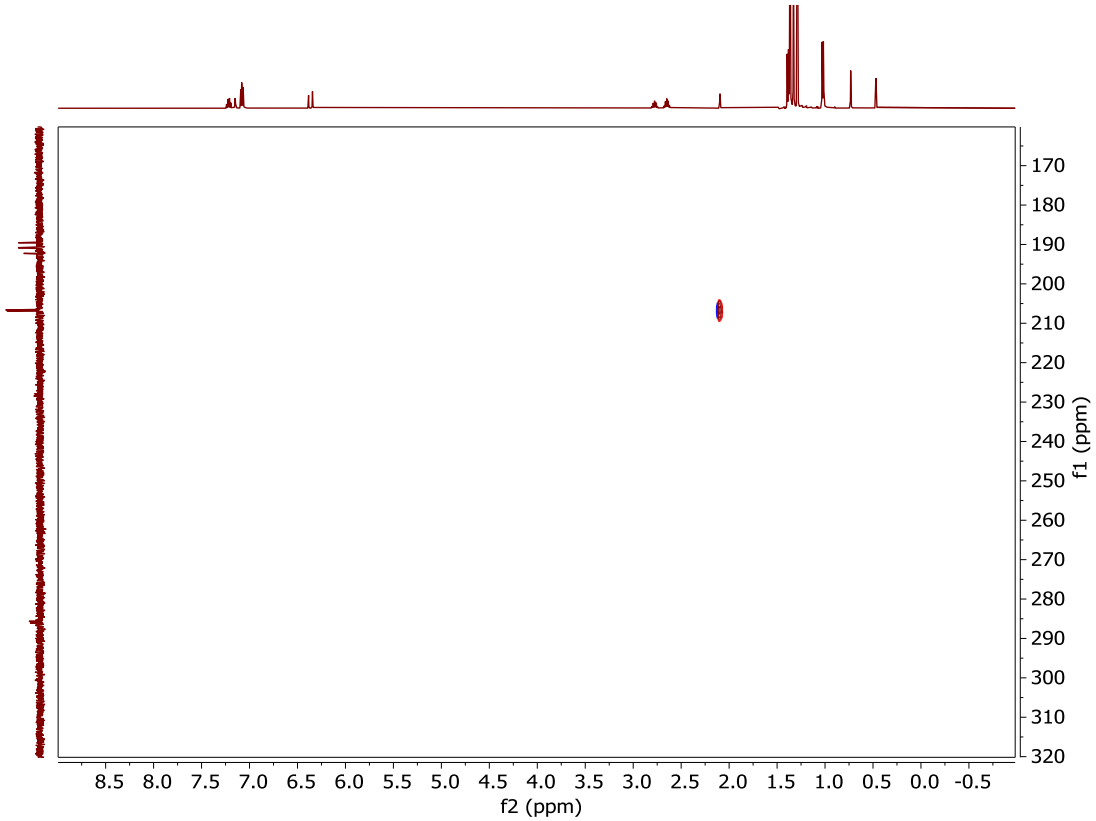


Figure S34. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2- Ag)** and **(3-Ag).** Part 2: from 160 ppm to 320 ppm in f1.

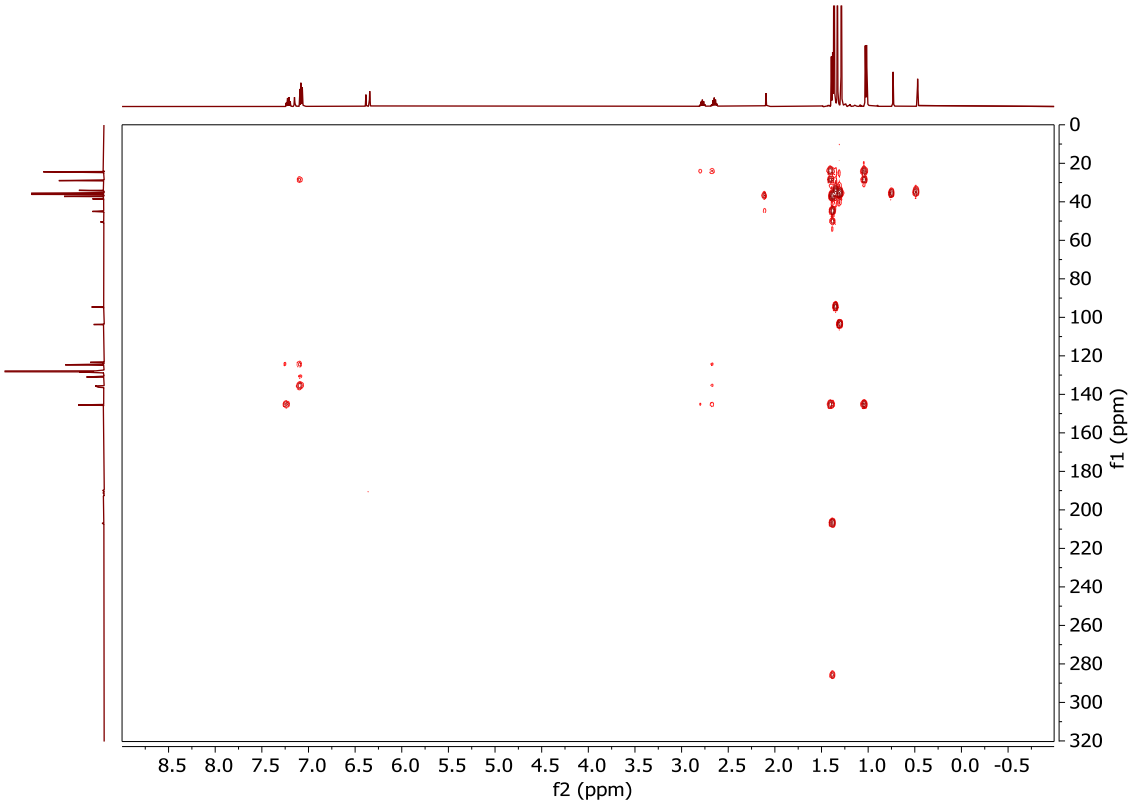


Figure S35. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2- Ag)** and **(3-Ag).**

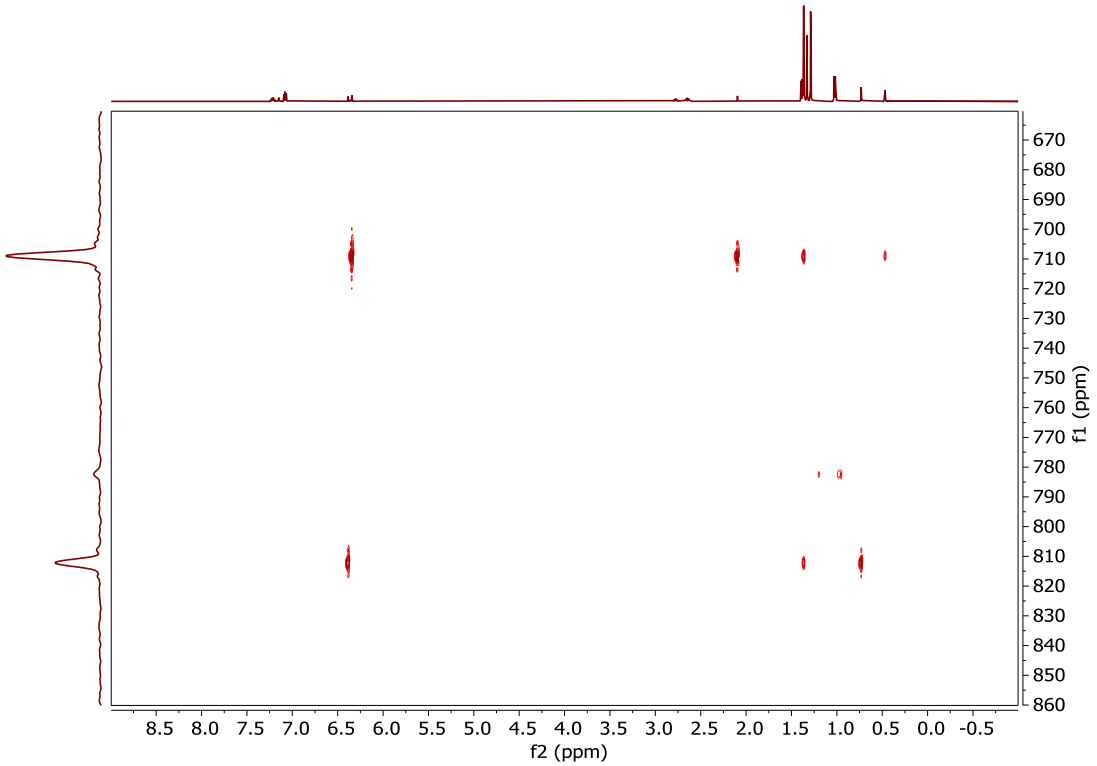


Figure S36. ^{1}H-^{109}Ag HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of the mixture of products **(2-Ag)** and **(3-Ag).**

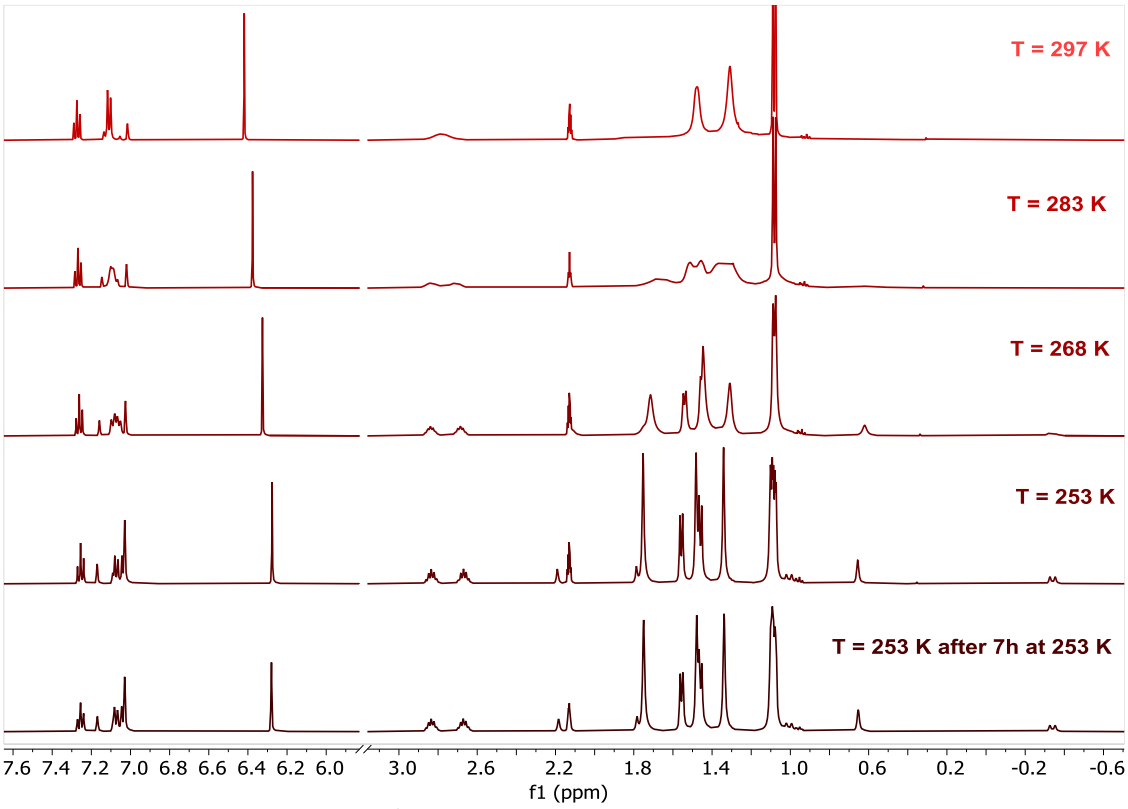


Figure S37. Variable temperature ^{1}H-NMR spectra (500 MHz, toluene-d_8) of compound **(3-Au)**, ranging from 253 K up to 297 K. The spectrum at the bottom was acquired after 7 hours at 253 K. The fluxionality is attributed to the rapid exchange between the two Ta=CH*t*Bu motifs on the NMR timescale at 297K.

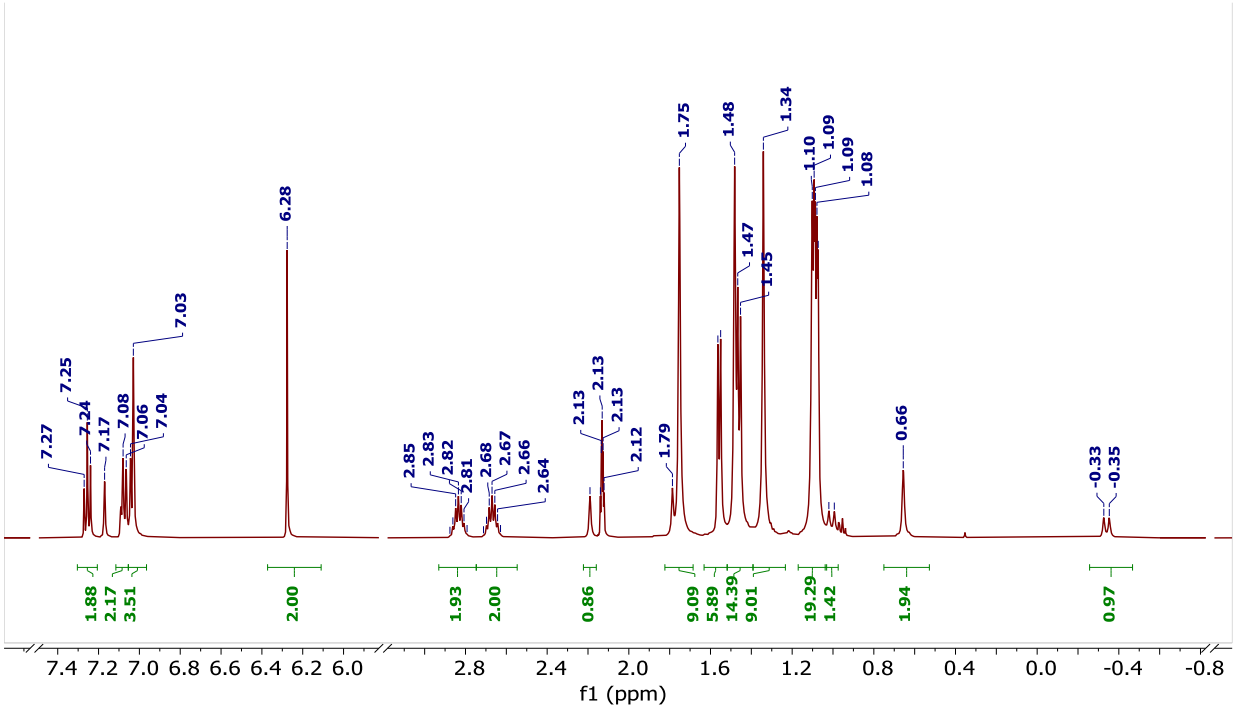


Figure S38. ^{1}H-NMR spectrum (500 MHz, toluene-d_8, 253K) of compound **(3-Au)**.

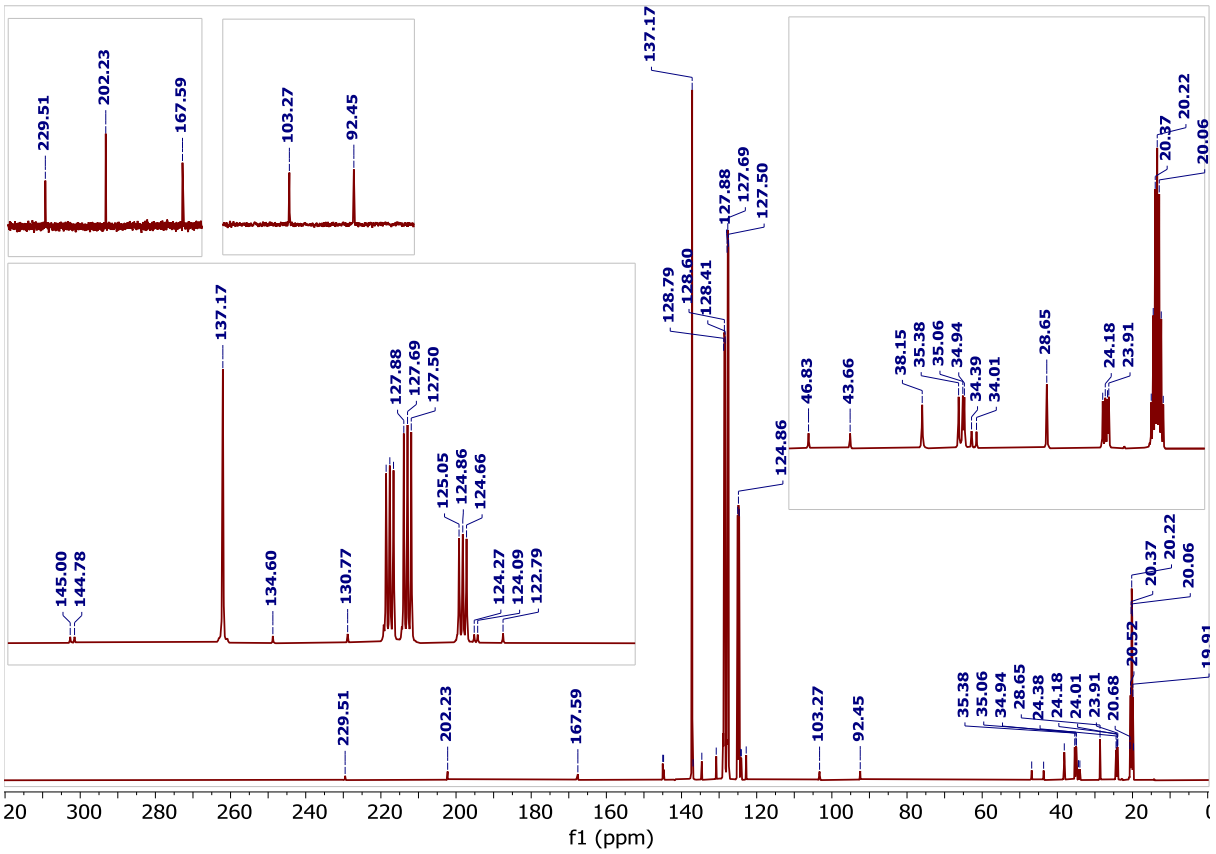


Figure S39. ^{13}C{^{1}H}-NMR (126 MHz, toluene-d_8, 253K) of compound **(3-Au)**.

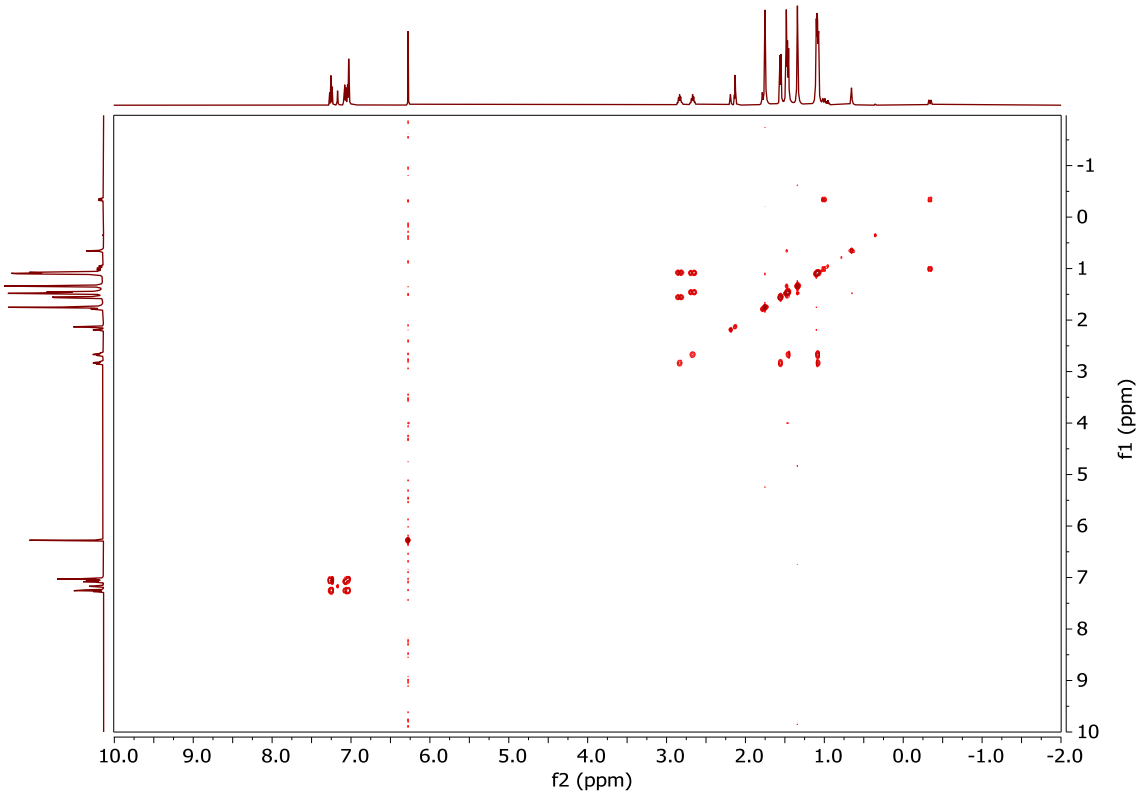


Figure S40. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, toluene-d_8, 253K) of compound **(3-Au)**.

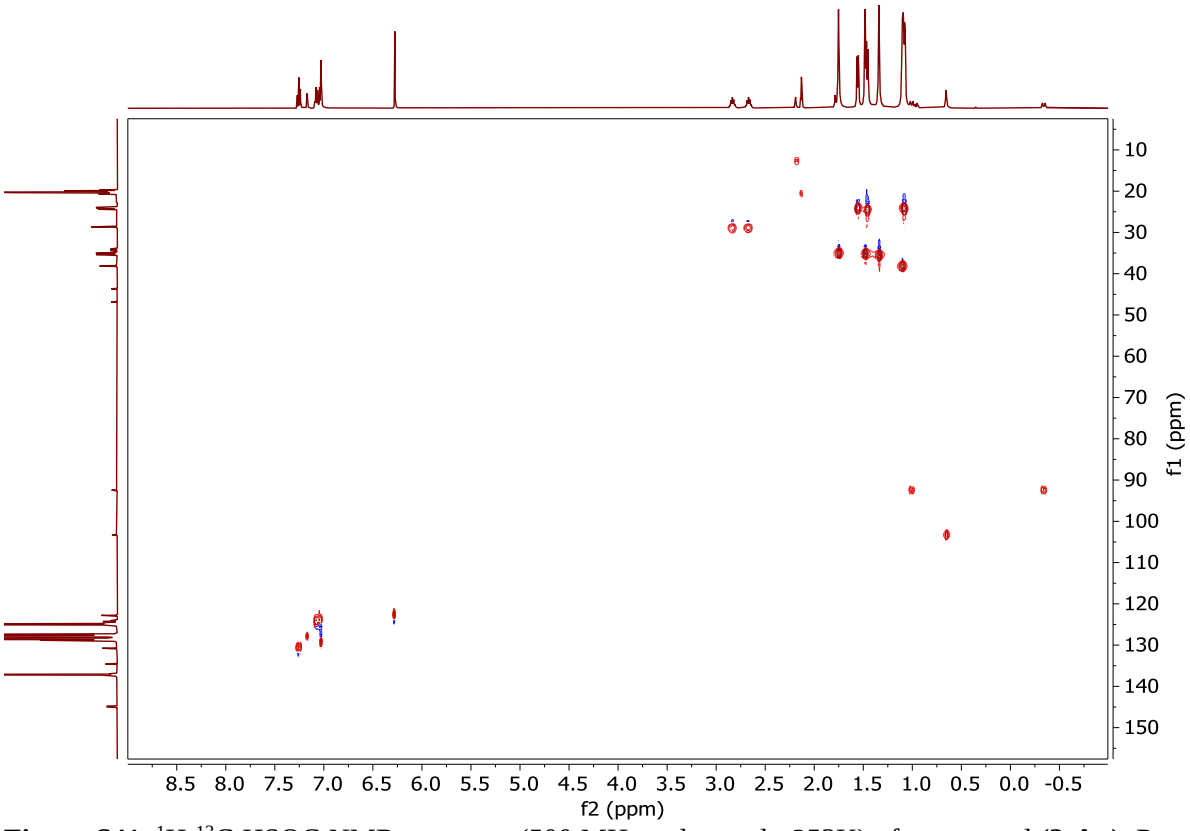


Figure S41. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, toluene-d_8, 253K) of compound **(3-Au)**. Part 1: from 0 ppm to 155 ppm in f1.

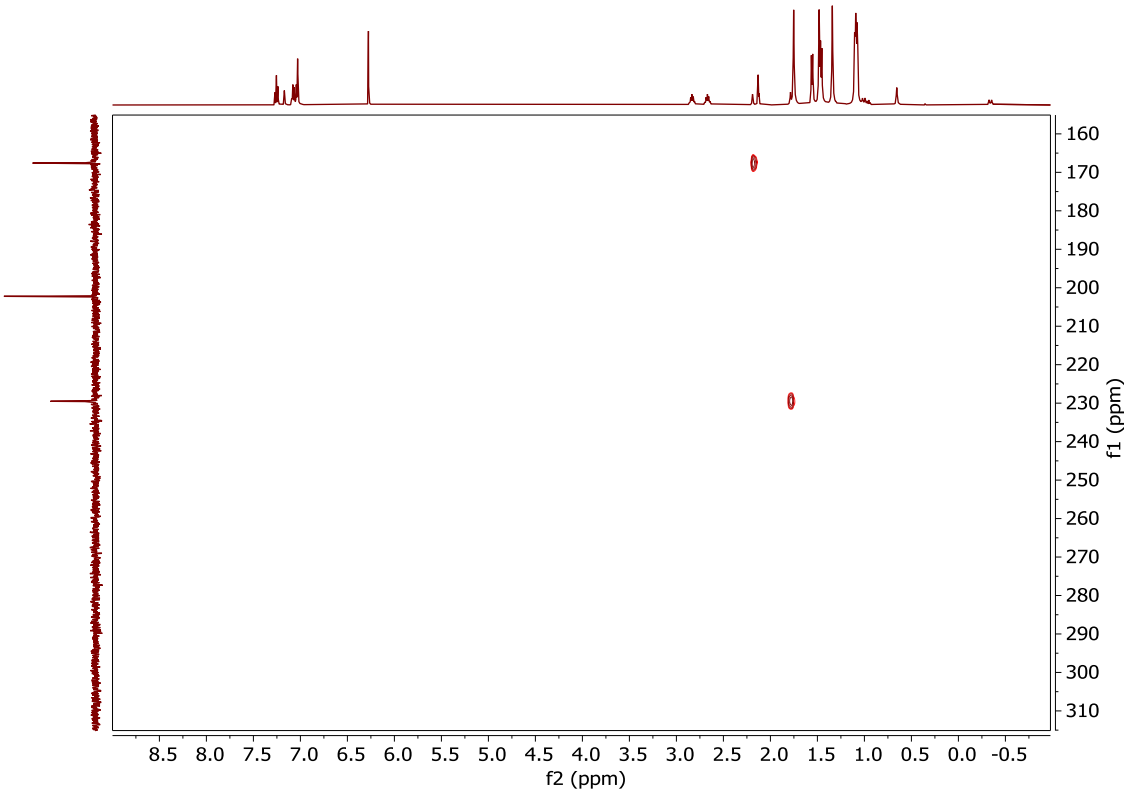


Figure S42. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, toluene-d_8, 253K) of compound **(3-Au)**. Part 2: from 155 ppm to 315 ppm in f1. Part 1: from 0 ppm to 155 ppm in f1.

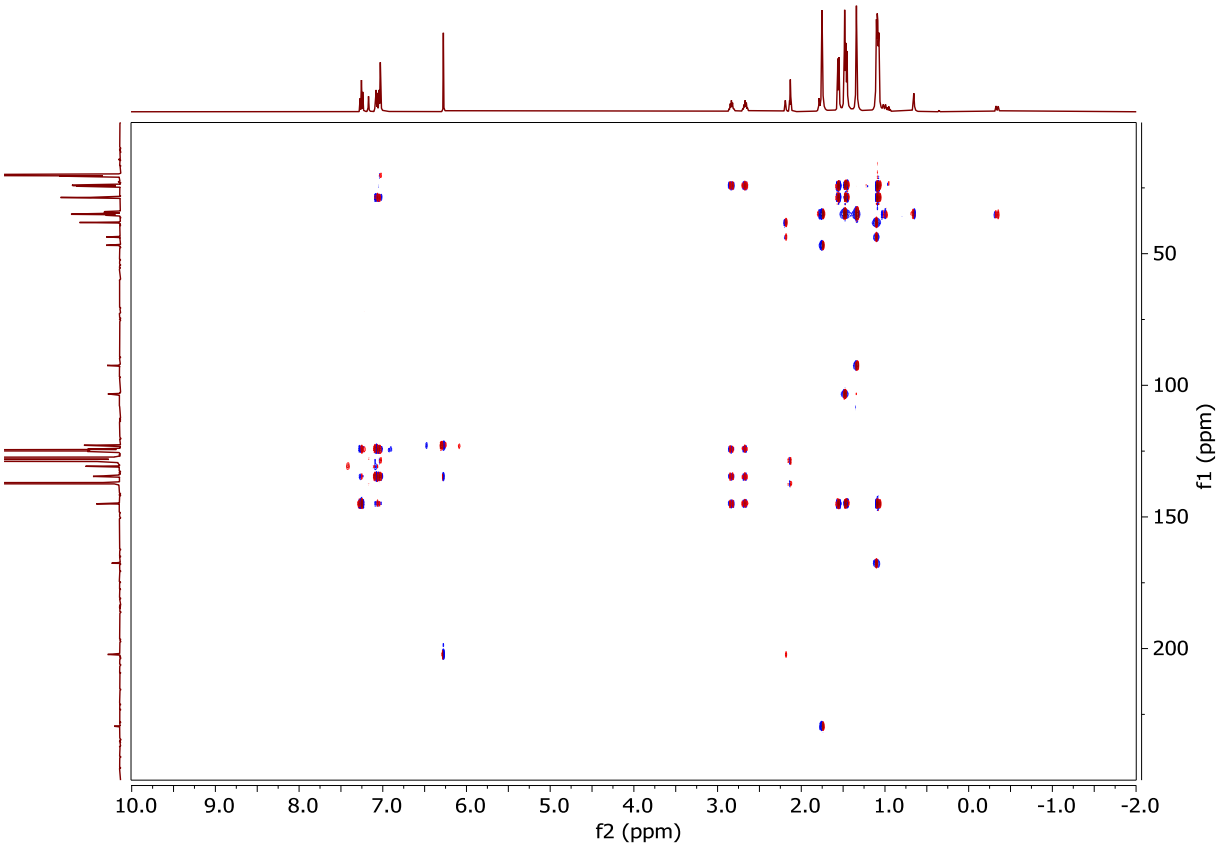


Figure S43. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, toluene-d_8, 253K) of compound **(3-Au)**.

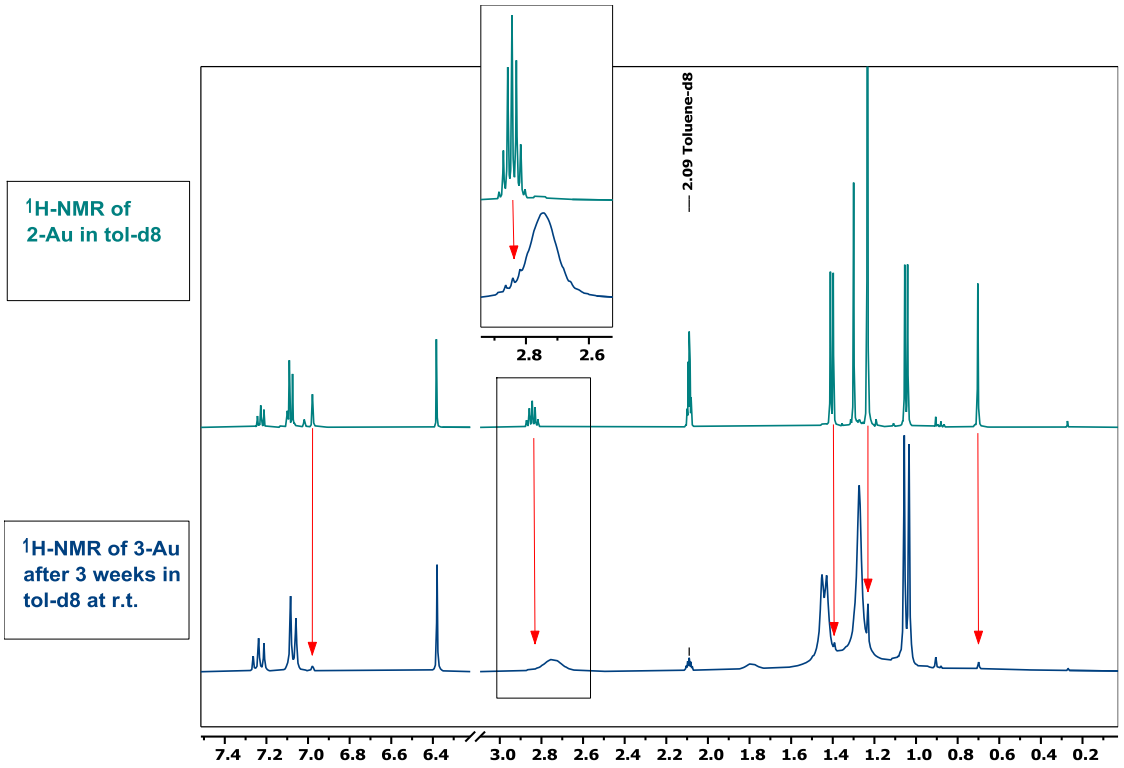


Figure S44. Top: ^{1}H-NMR spectrum (500 MHz, toluene-d_8, 298K) of compound **2-Au**. Bottom: ^{1}H-NMR spectrum (500 MHz, toluene-d_8, 298K) showing the formation of 6% **2-Au** from a solution of pure **3-Au** after 3 weeks in solution in toluene-d_8 at room temperature.

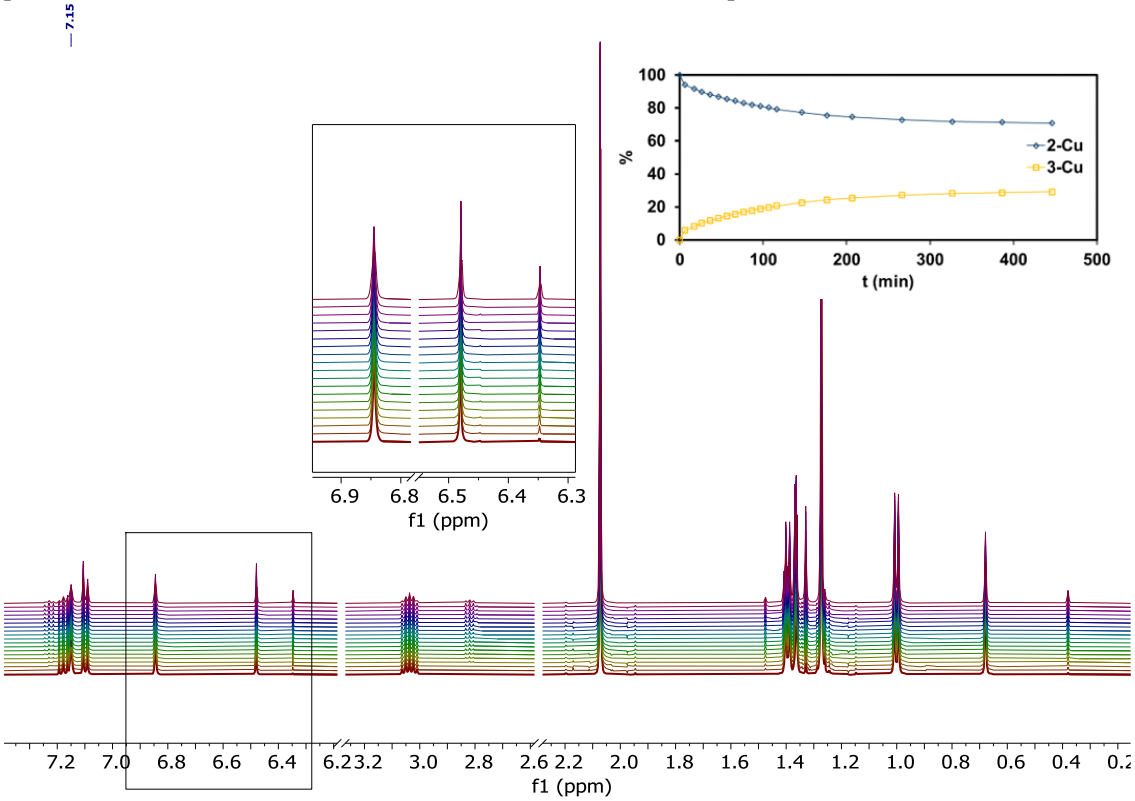


Figure S45. ^{1}H-NMR monitoring (500 MHz, C_6D_6, 303 K) of the establishment of the tautomeric equilibrium between **2-Cu** and **3-Cu**. This measurement was conducted using durene as an internal standard.

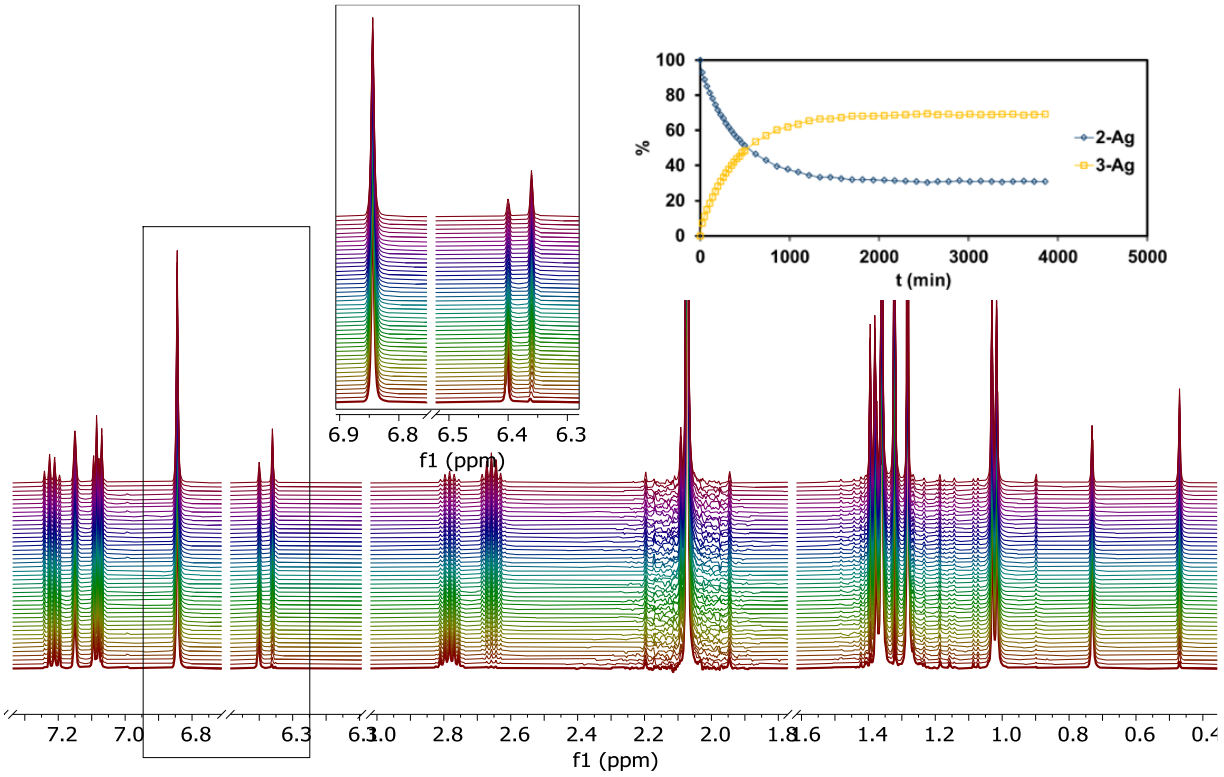


Figure S46. ^{1}H-NMR monitoring (500 MHz, C_6D_6, 303 K) of the establishment of the tautomeric equilibrium between **2-Ag** and **3-Ag**. This measurement was conducted using durene as an internal standard.

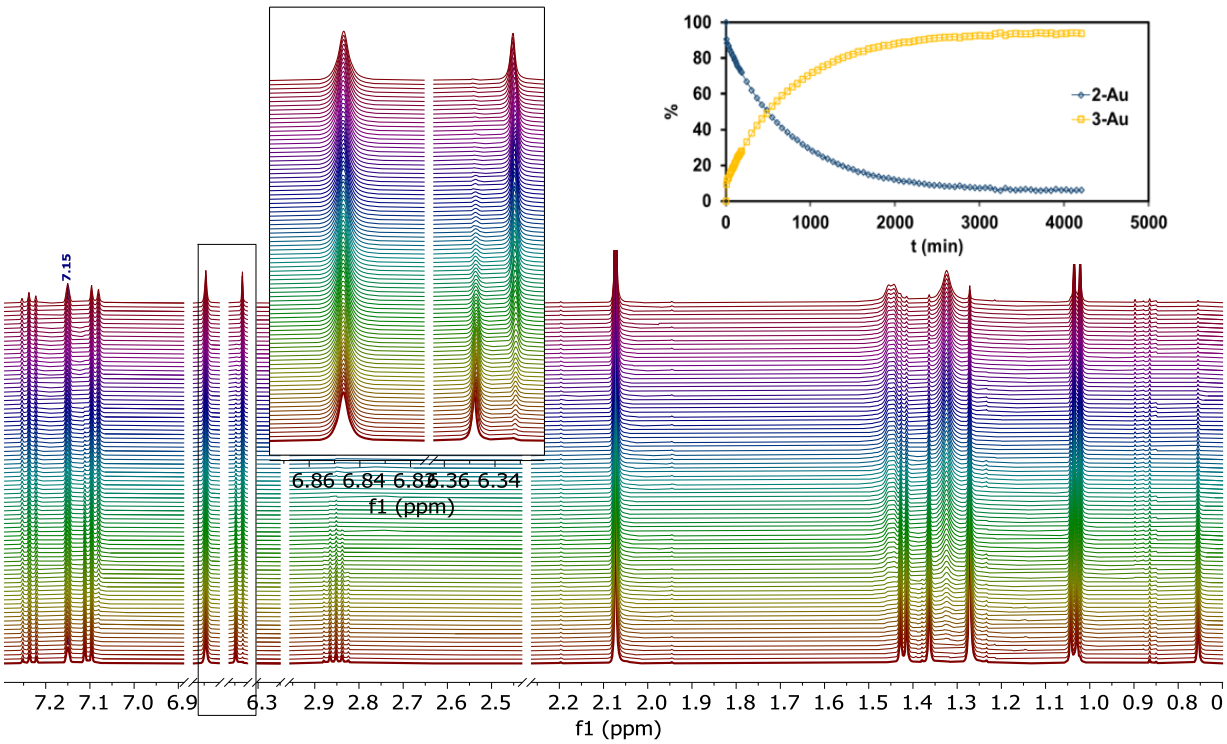


Figure S47. ^{1}H-NMR monitoring (500 MHz, C_6D_6, 303 K) of the conversion of **2-Au** to **3-Au**. This measurement was conducted using durene as an internal standard.

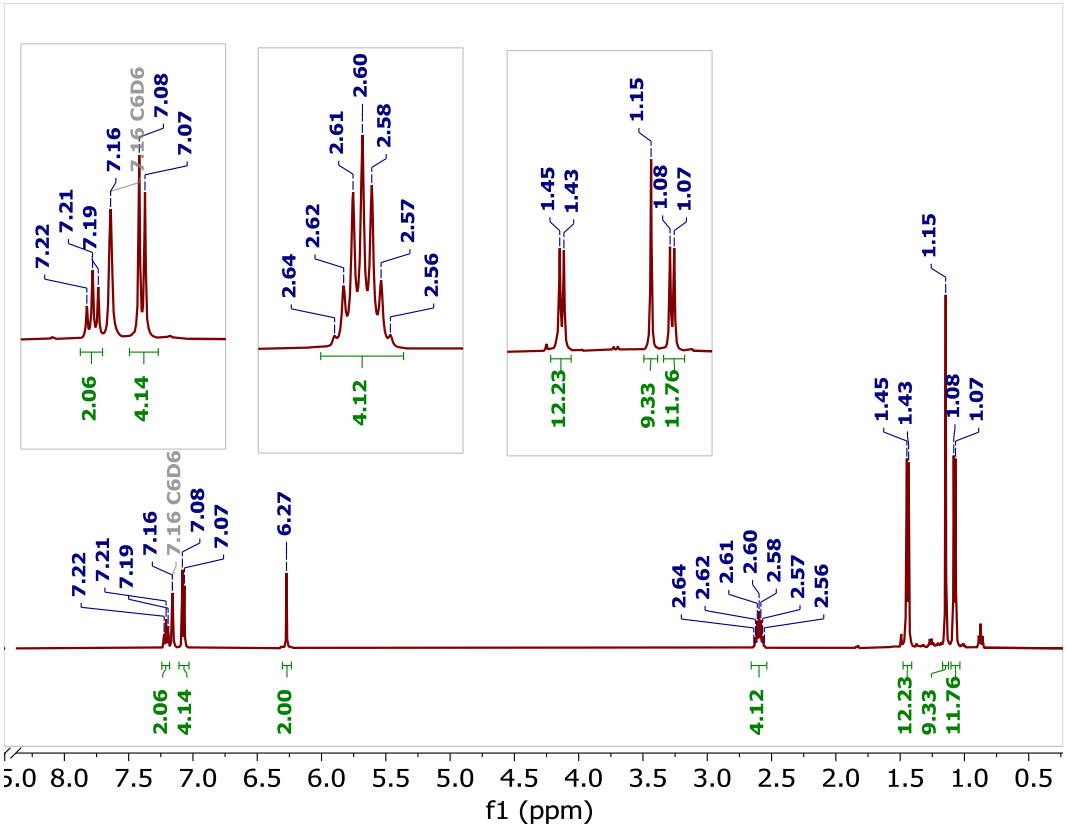


Figure S48. ^{1}H-NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(4-Cu)**.

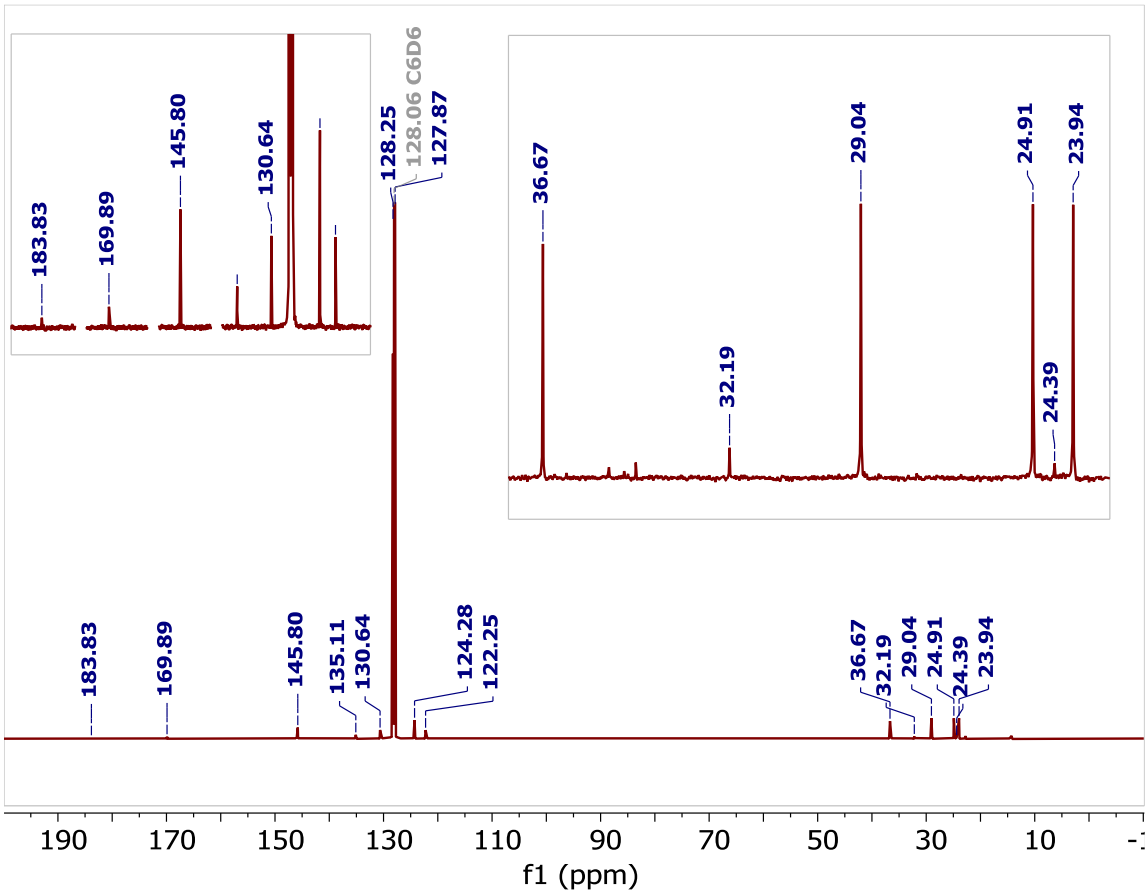


Figure S49. ^{13}C{^{1}H}-NMR spectrum (126 MHz, C_6D_6, 298K) of compound **(4-Cu)**.

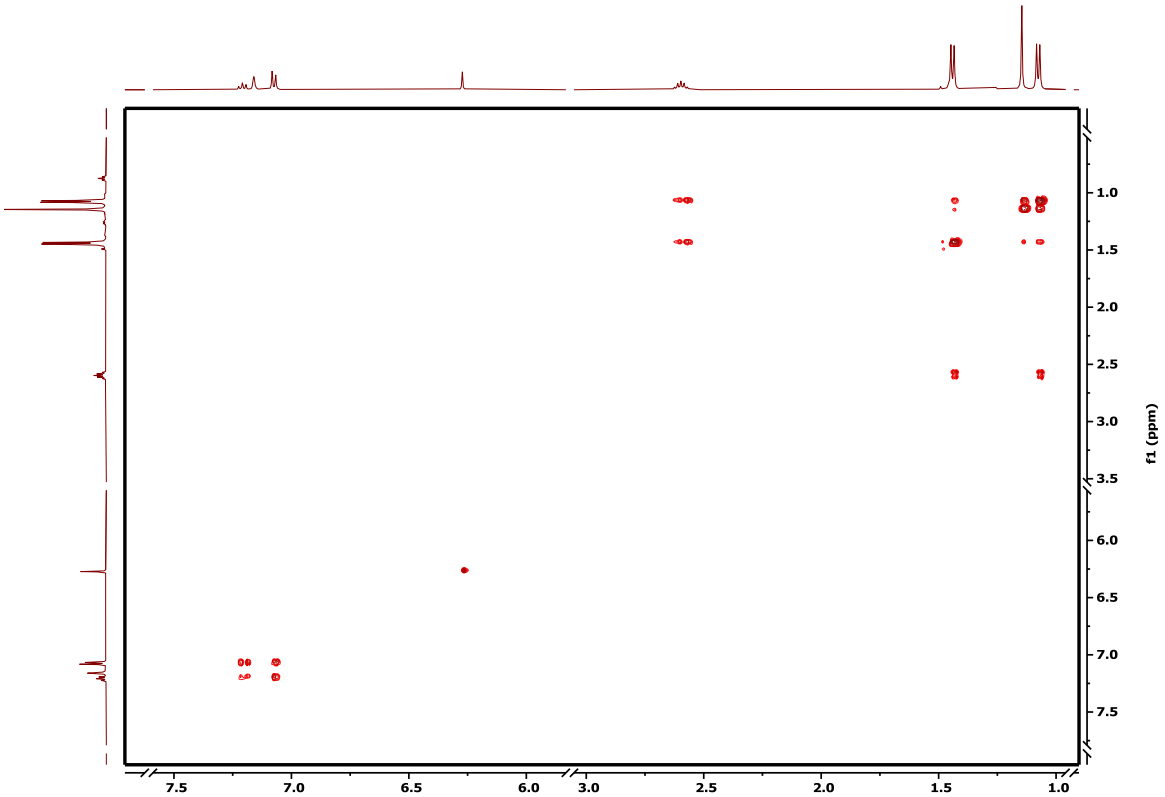


Figure S50. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(4-Cu)**.

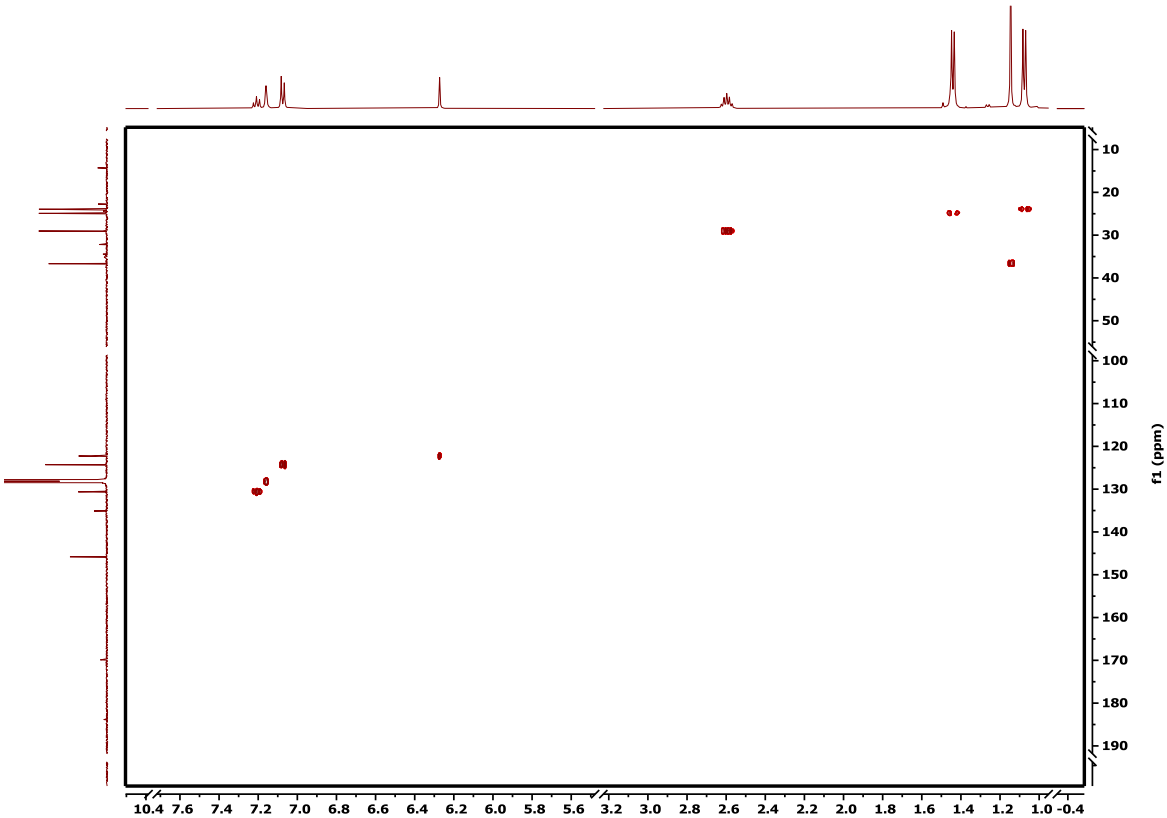


Figure S51. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(4-Cu)**.

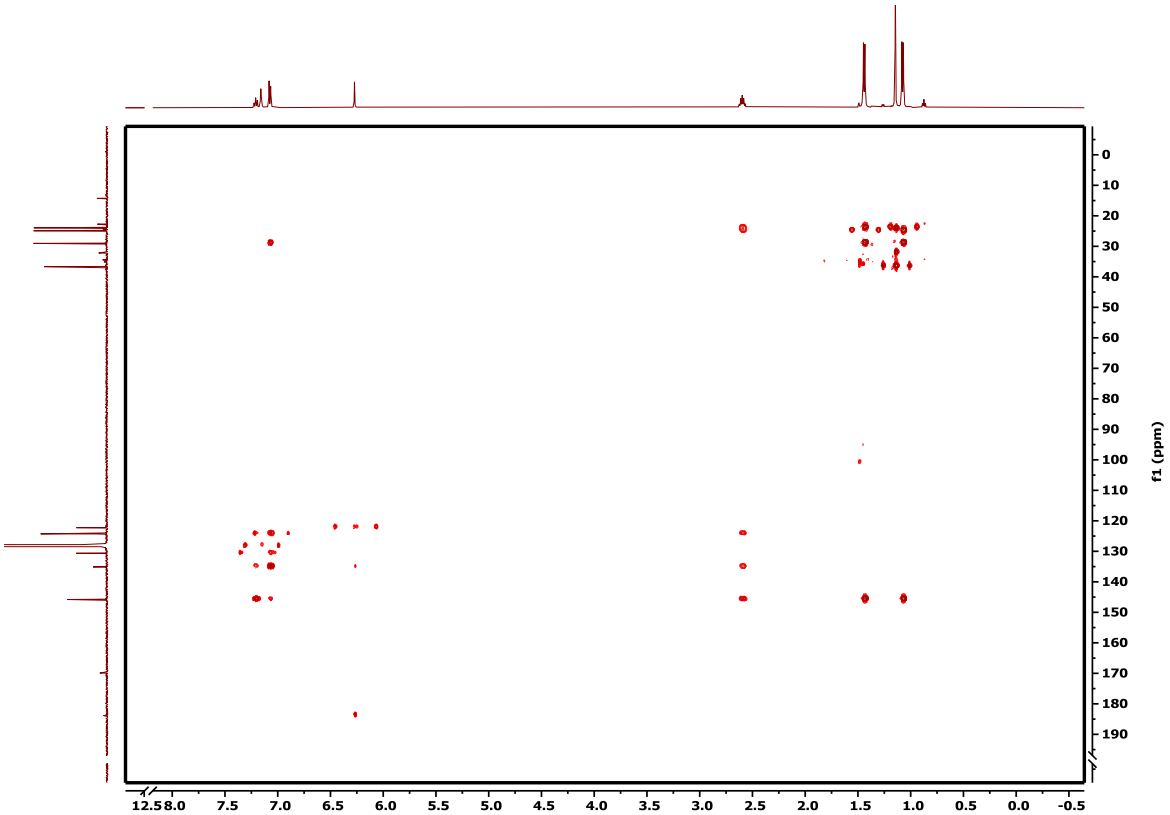


Figure S52. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, C_6D_6, 298K) of compound **(4-Cu)**.

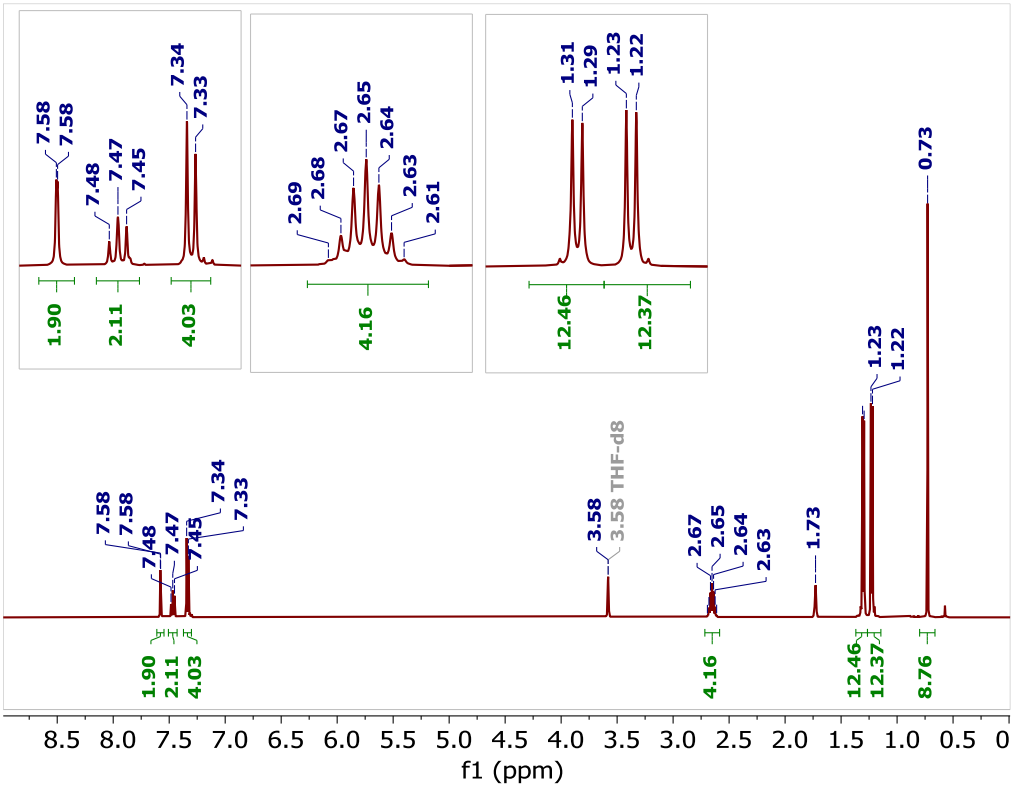


Figure S53. ^{1}H-NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Ag).**

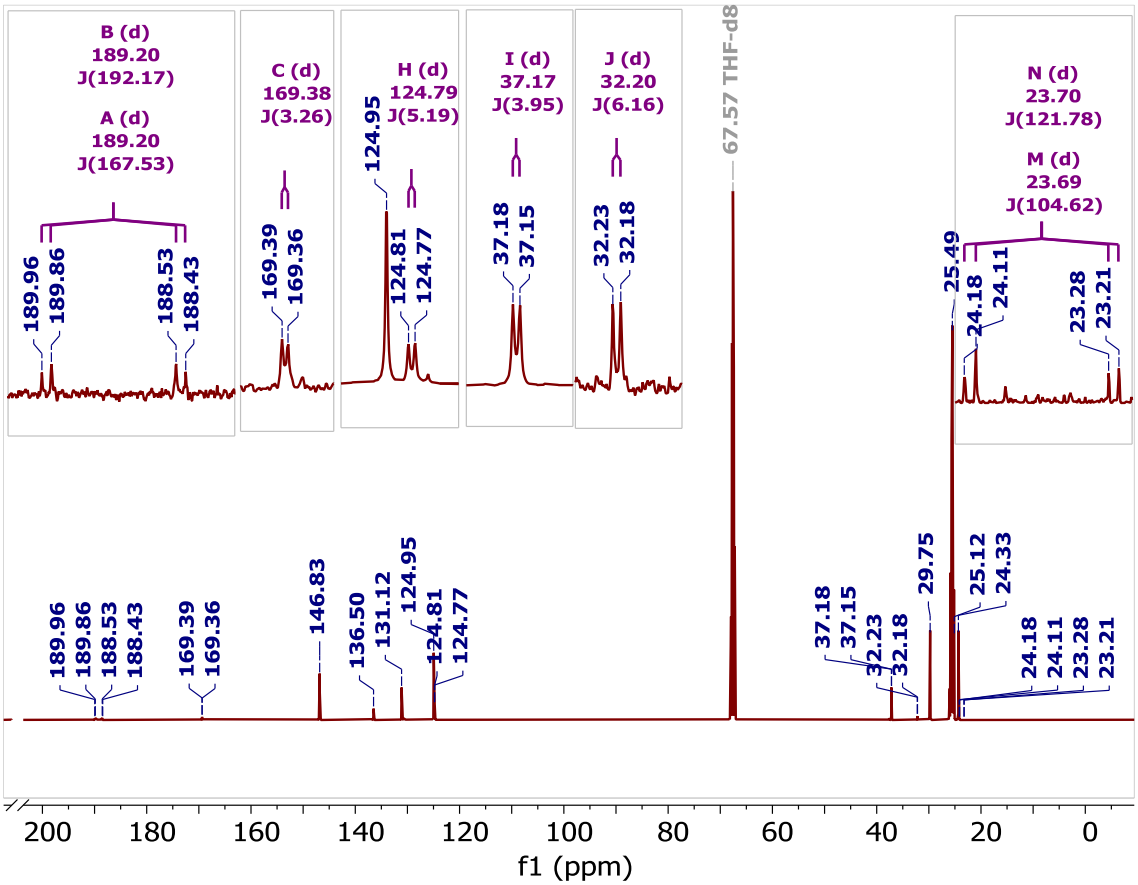


Figure S54. $^{13}C\{^{1}H\}$-NMR spectrum (126 MHz, THF-d_8, 298K) of compound **(4-Ag).**

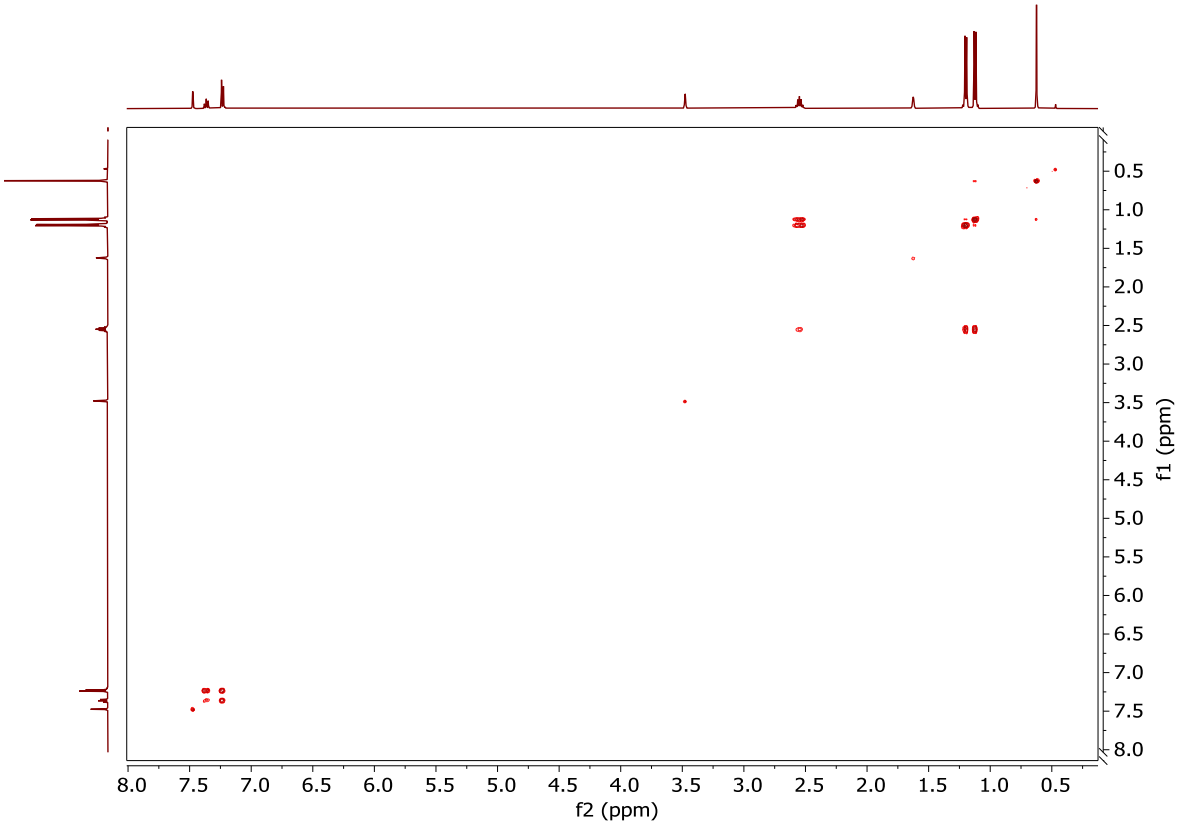


Figure S55. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Ag).**

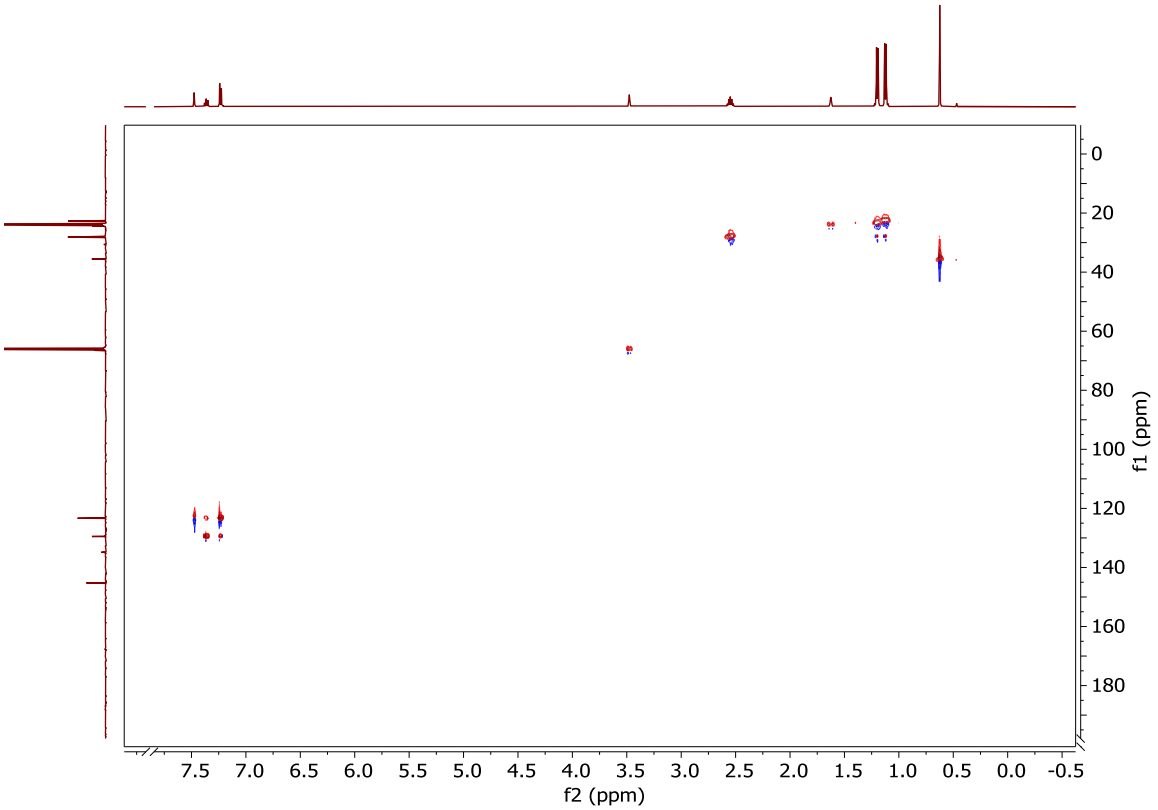


Figure S56. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Ag).**

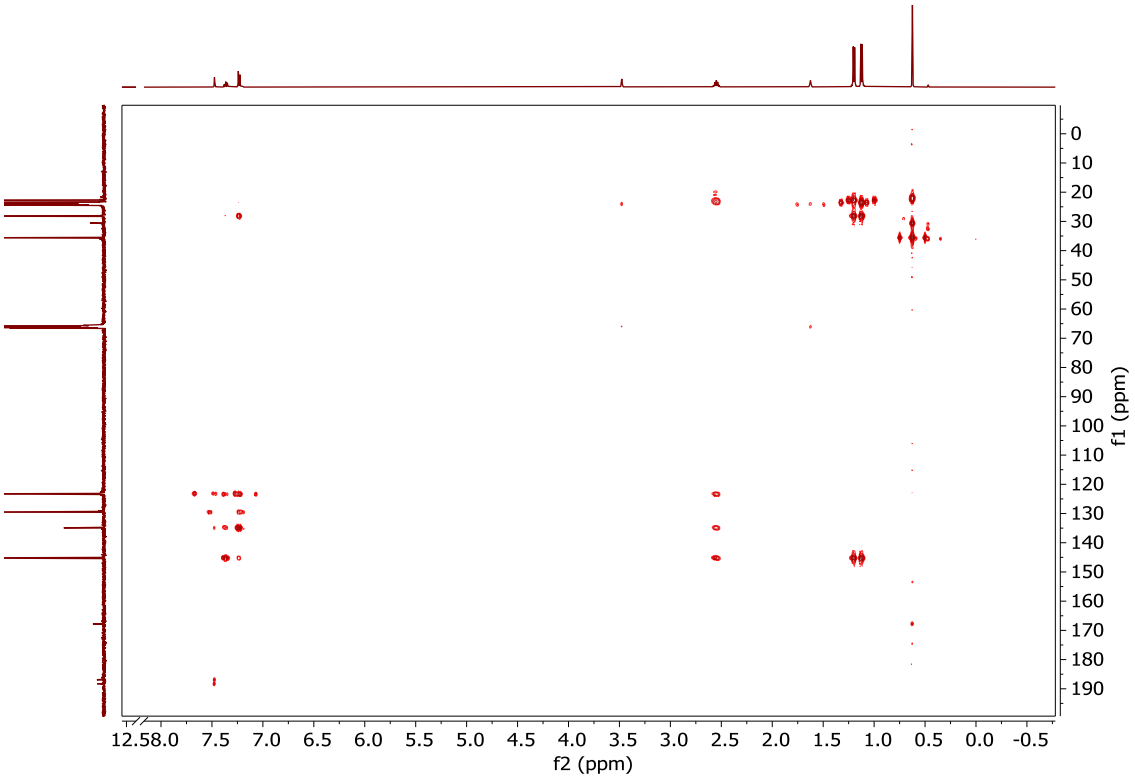


Figure S57. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Ag)**.

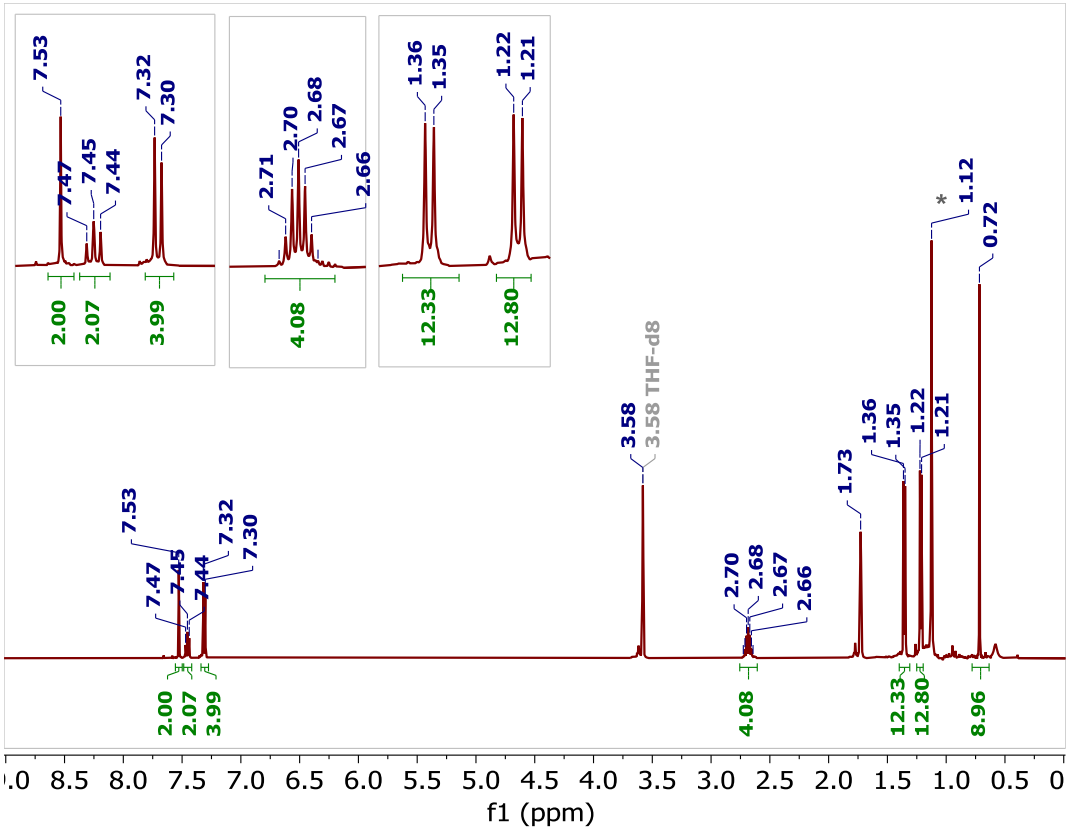


Figure S58. ^{1}H-NMR spectrum (500 MHz, THF-d$_8$, 298K) of compound **(4-Au).** *(*unidentified substance)*

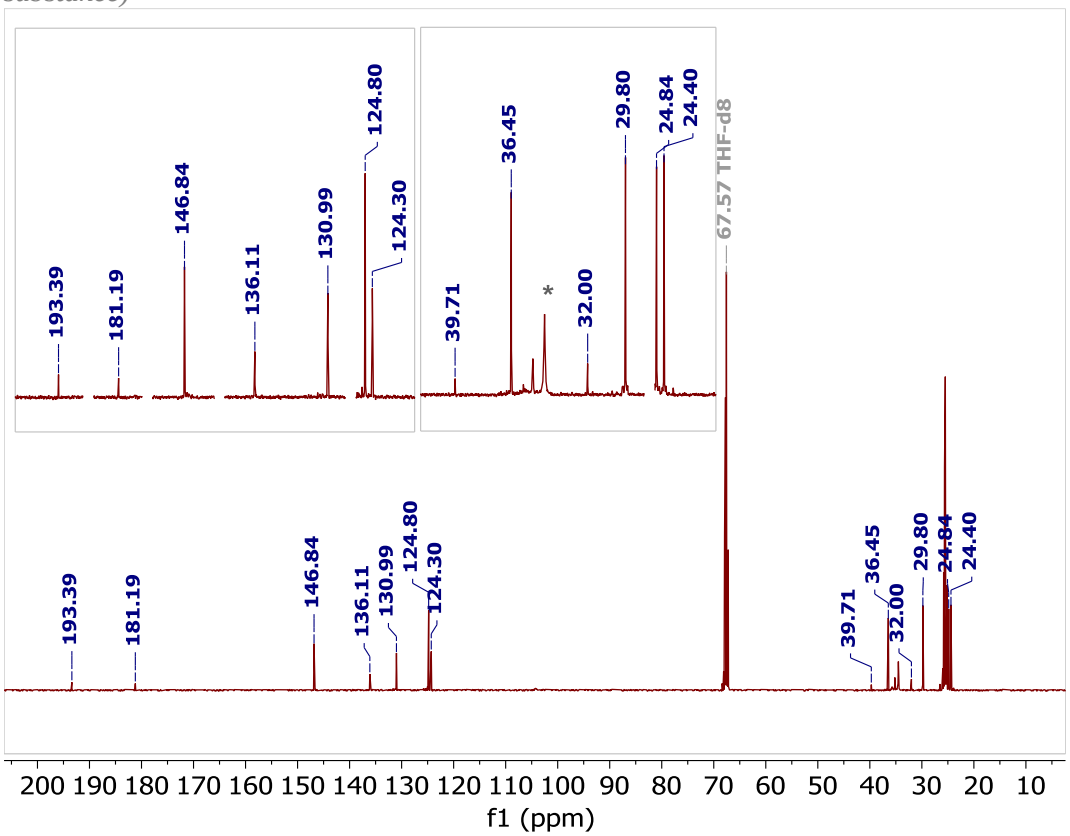


Figure S59. ^{13}C{^{1}H}-NMR spectrum (126 MHz, THF-d$_8$, 298K) of compound **(4-Au).** *(*unidentified substance)*

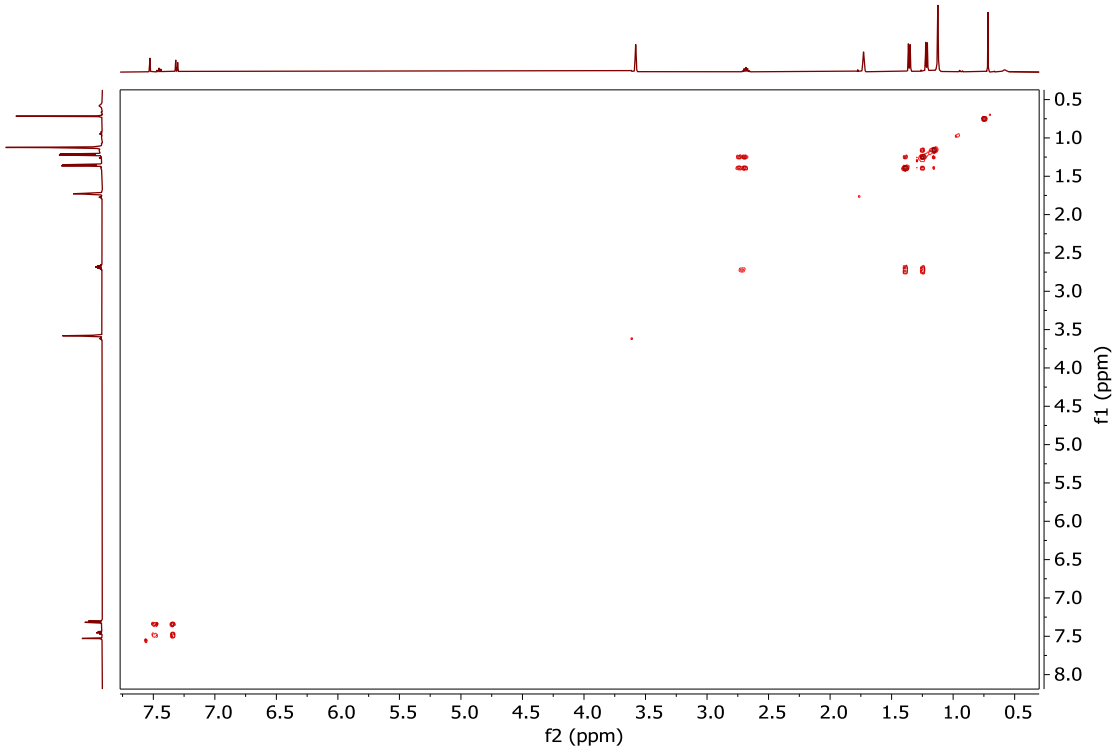


Figure S60. ^{1}H-^{1}H COSY NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Au).**

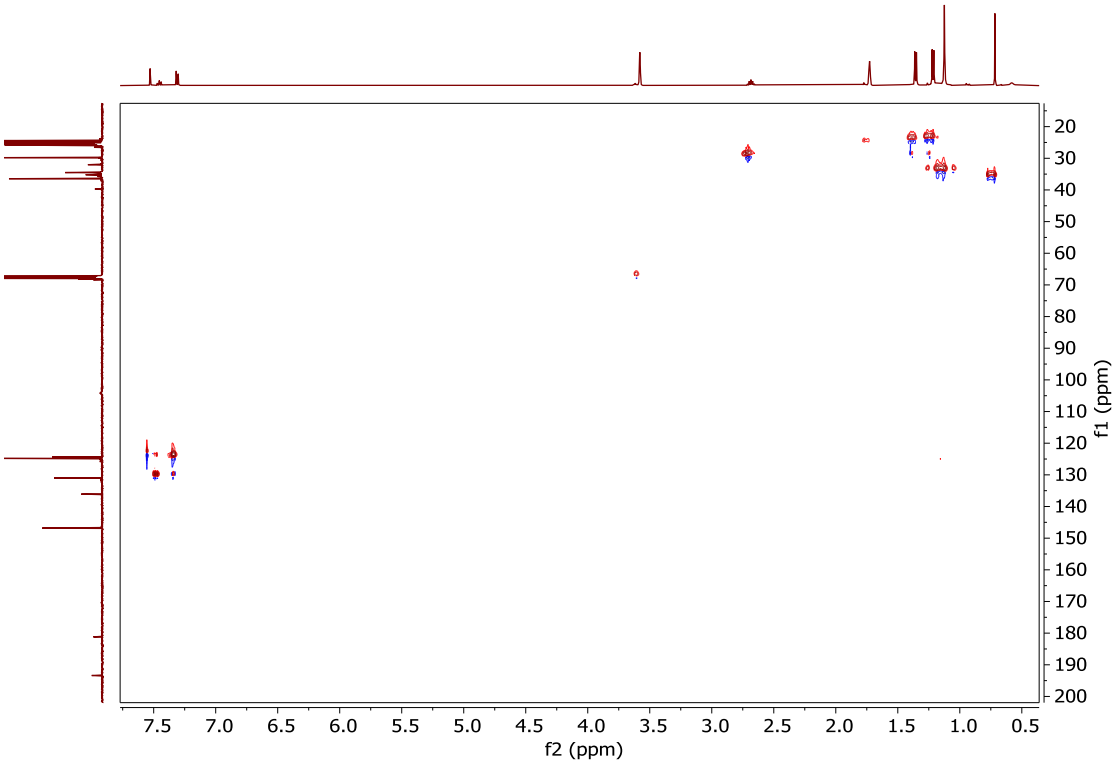


Figure S61. ^{1}H-^{13}C HSQC NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Au).**

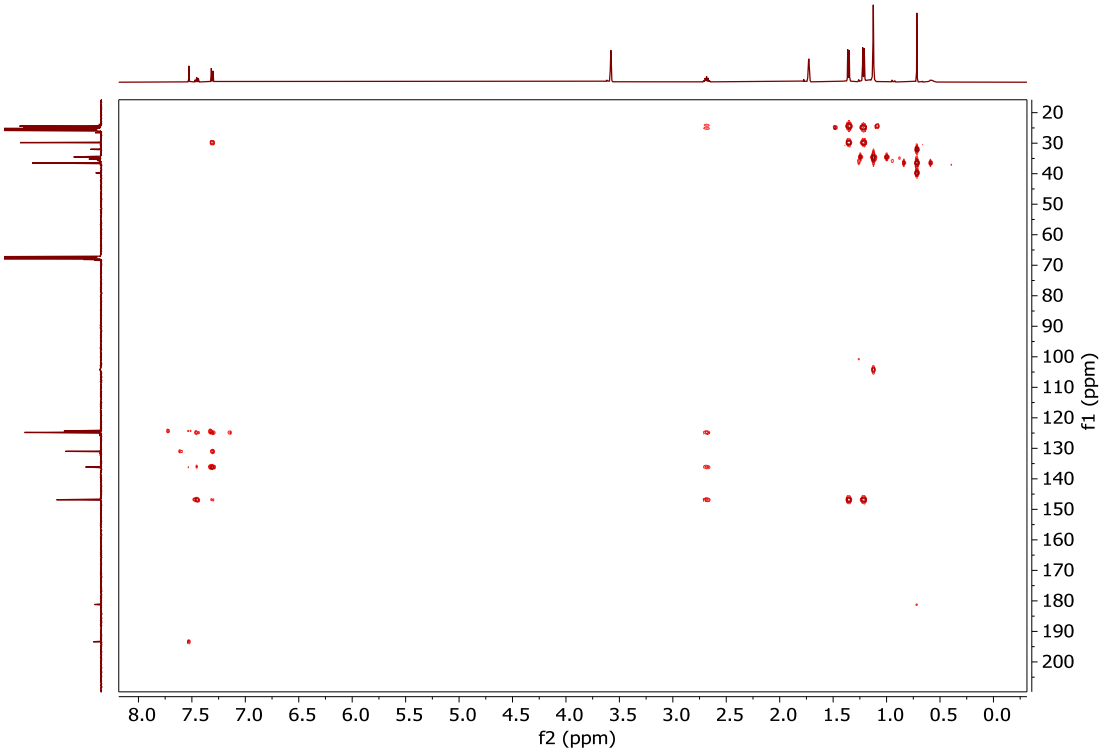


Figure S62. ^{1}H-^{13}C HMBC NMR spectrum (500 MHz, THF-d_8, 298K) of compound **(4-Au)**.

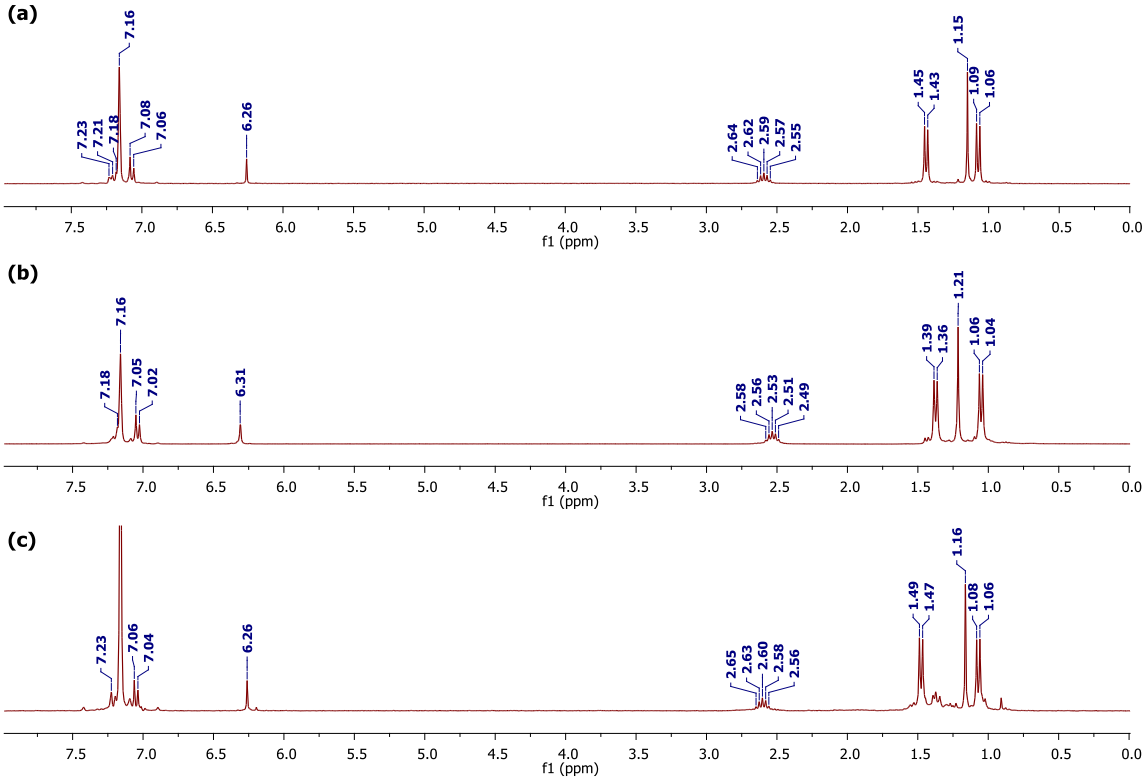


Figure S63. ^{1}H-NMR spectra (300 MHz, C_6D_6, 298K) of compounds **4-Cu** (a), **4-Ag** (b) and **4-Au** (c). Note that complex **4-Au** is not very soluble in C_6D_6.

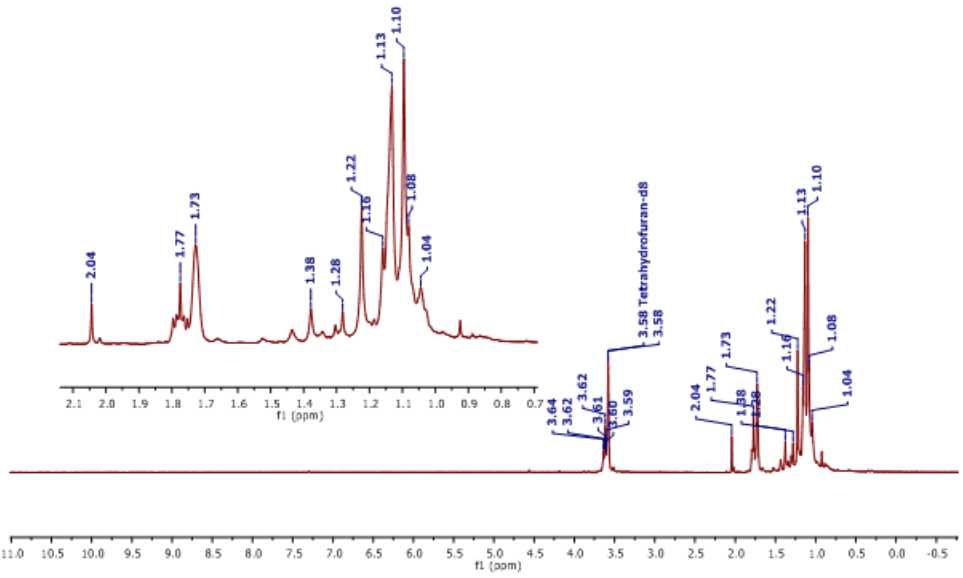


Figure S64. ^{1}H-NMR spectrum (300 MHz, THF-d_8, 298K) of the precipitate isolated from the reaction of **1** with 2 equivalents of CO_2 in pentane at room temperature.

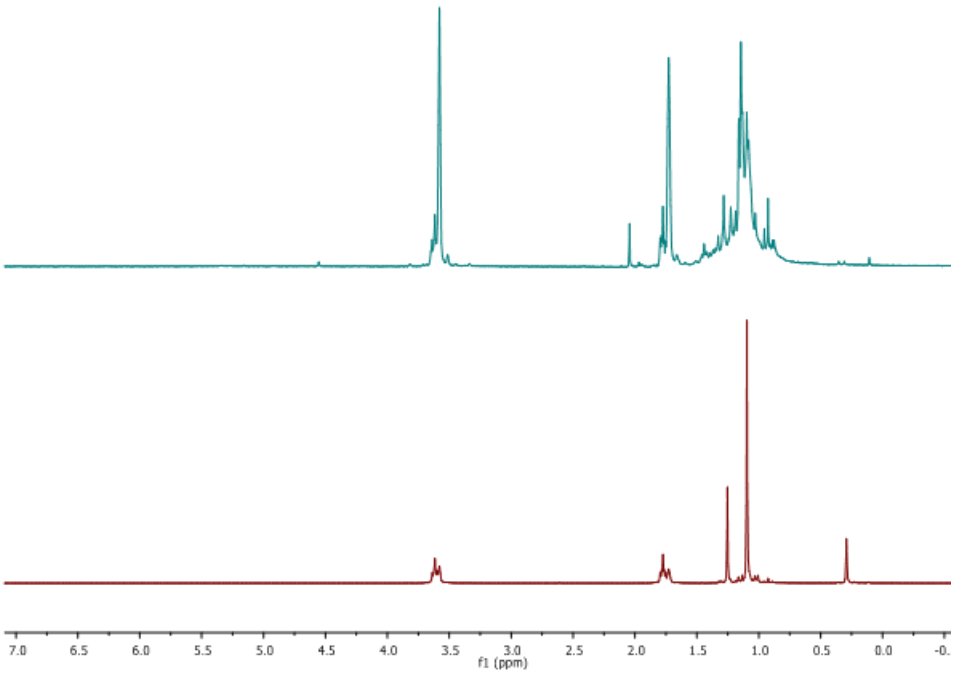


Figure S65. ^{1}H-NMR spectra (300 MHz, THF-d8, 298K) of complex **1** (bottom) and the reaction mixture supernatant of compound **1** with CO_2 after evaporation of all the volatiles (top).

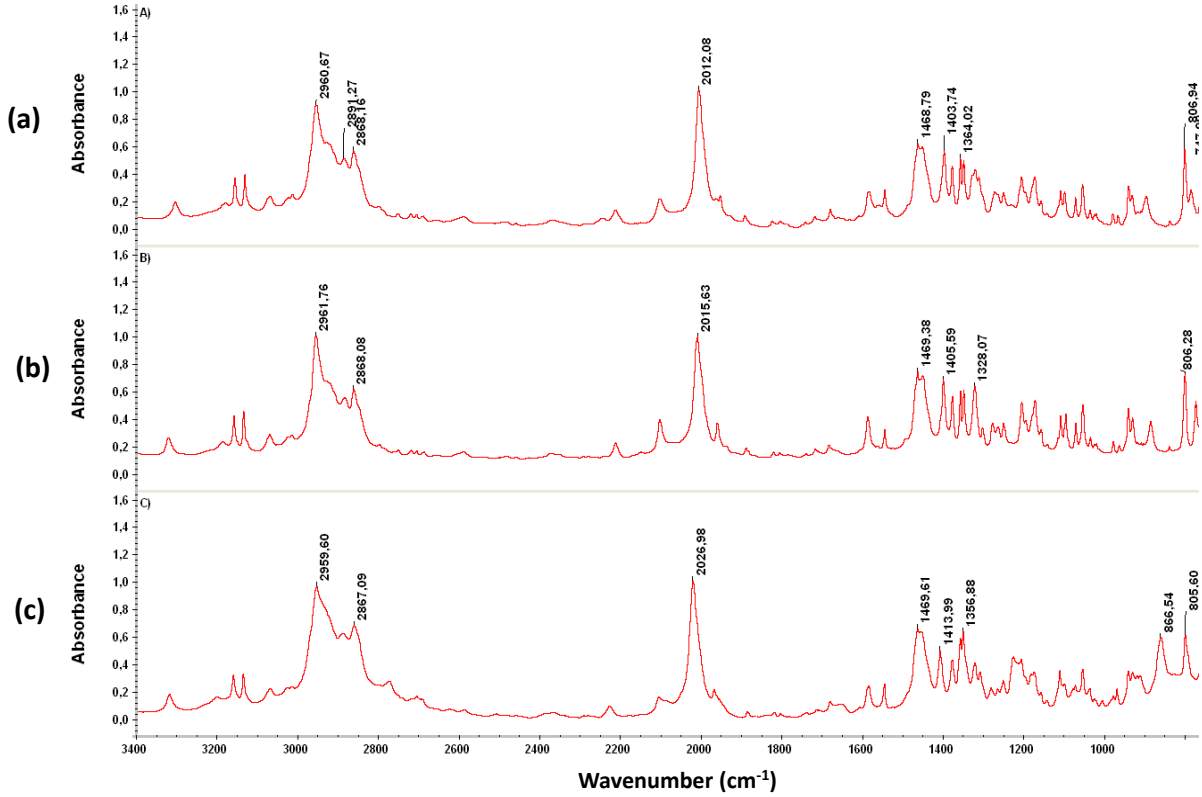


Figure S66. DRIFT (293 K, cm^{-1}) spectra of compounds **4-Cu** (a), **4-Ag** (b) and **4-Au** (c).

B. X-ray crystallography

Experimental. For each sample, several crystals were tested and they all showed multi-domain crystals (as shown on Figures S67-S71). Despite this feature, it was possible to determine the unit-cells of these compounds and to record X-ray diffraction data. Reflections with large overlap with other diffraction domains were omitted in the refinement. Samples were selected and mounted on a MITIGEN holder in perfluoroether oil on a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer. The crystal was kept at a steady T = 100.0(2) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015)[1] solution program using dual methods and by using **Olex2** 1.5-ac5-024 (Dolomanov et al., 2009)[2] as the graphical interface. The model was refined with **ShelXL** 2018/3 (Sheldrick, 2015)[3] using full matrix least squares minimisation on $\boldsymbol{F^2}$.

[1] Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), **C71**, 3-8.
[2] O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.
[3] Sheldrick, G.M., ShelXT-Integrated space-group and crystal-structure determination, *Acta Cryst.*, (2015), **A71**, 3-8.

Experimental details for 2-Cu

An orange plate-shaped-shaped crystal with dimensions 0.41 × 0.23 × 0.09 mm^3 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer operating at T = 100.0(3) K.

Data were measured using ω scans with Mo K_α radiation. The maximum resolution that was achieved was Θ = 28.58° (0.74 Å).

The unit cell was refined on 46684 reflections, 52% of the observed reflections.

Data reduction, scaling and absorption corrections were performed. The final completeness is 98.97 % out to 28.58° in Θ. A multi-scan absorption correction was performed using CrysAlisPro 1.171.42.86a (Rigaku Oxford Diffraction, 2023) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The absorption coefficient μ of this material is 2.833 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.358 and 1.000.

The structure was solved and the space group $P2_1/c$ (# 14) determined by the ShelXT (Sheldrick, 2015) structure solution program using dual methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of **ShelXL** 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

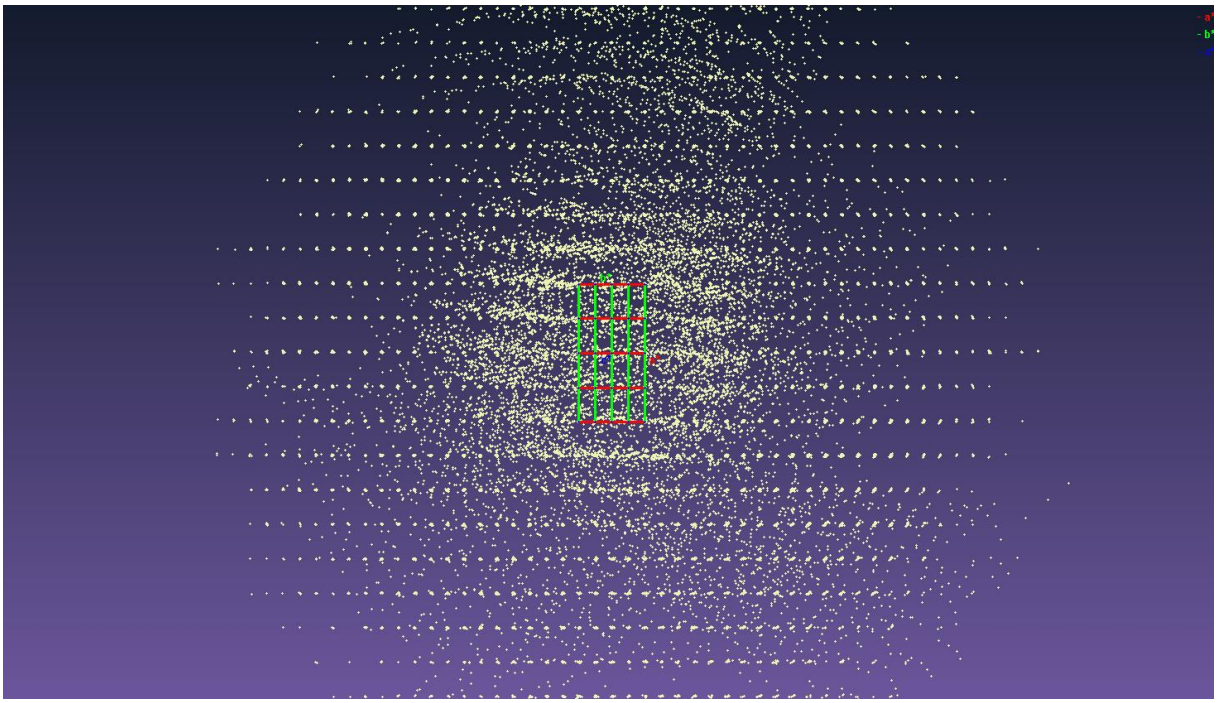


Figure S71. Projection of the reciprocical space for compound **2-Cu**. Additional diffraction spots clearly shows the presence of several diffraction domains.

Experimental details for 2-Ag

An orange block-shaped-shaped crystal with dimensions 0.76 × 0.56 × 0.40 mm^3 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer operating at T = 100.00(10) K.

Data were measured using ω scans with Mo K_α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The maximum resolution that was achieved was Θ= 30.020° (0.71 Å). The unit cell was refined using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022) on 75599 reflections, 44% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The final completeness is 98.90 % out to 30.020° in Θ. A multi-scan absorption correction was performed using CrysAlisPro 1.171.42.77a (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The absorption coefficient μ of this material is 2.737 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.189 and 1.000.

The structure was solved and the space group $P2_1/n$ (# 14) determined by the ShelXT (Sheldrick, 2015) structure solution program using dual methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of **ShelXL** 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model. The structure showed rotational disorder of a ter-butyl group. This disorder was modelled and refined using SADI, SIMU, RIGU and DFIX restraints.

_exptl_absorpt_process_details: CrysAlisPro 1.171.42.77a (Rigaku Oxford Diffraction, 2022) using spherical harmonics,implemented in SCALE3 ABSPACK scaling algorithm.

The value of Z' is 2. This means that there are two independent molecules in the asymmetric unit.

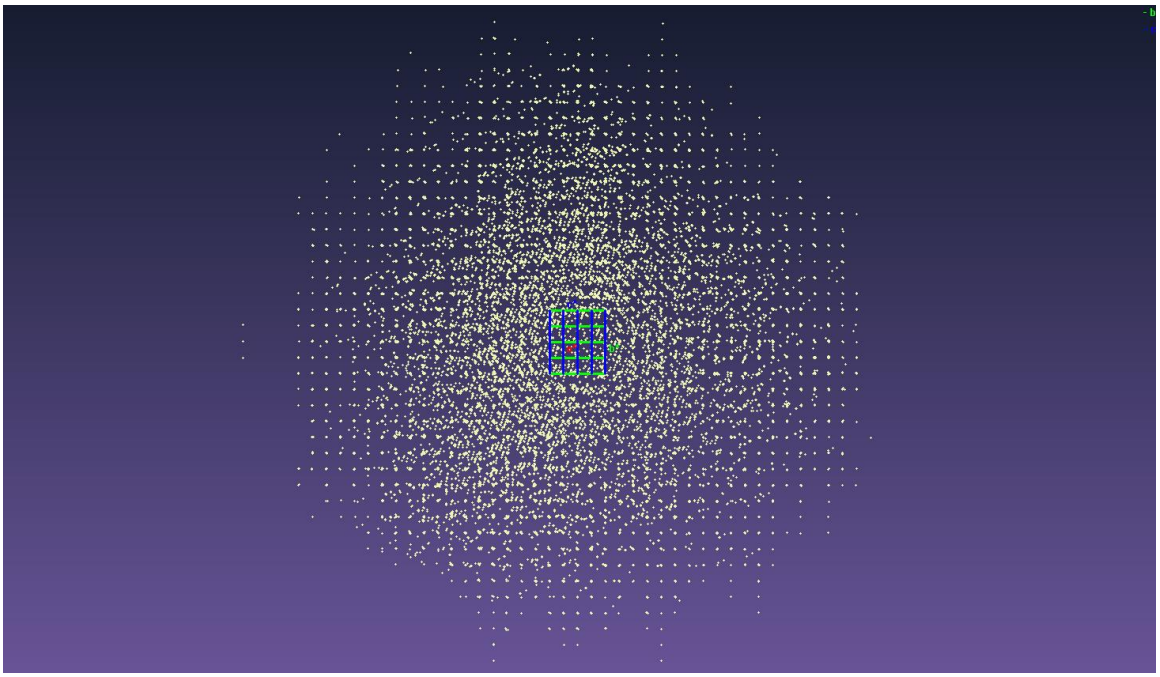


Figure S67. Projection of the reciprocical space for compounds **2-Ag**. Additional diffraction spots clearly shows the presence of several diffraction domains.

Experimental details for 2-Au

A red plate-shaped-shaped crystal with dimensions 0.45 × 0.28 × 0.08 mm^3 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer operating at T = 100.0(3) K.

Data were measured using ω scans with Mo K_α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro 1.171.42.93a (Rigaku OD, 2023). The maximum resolution that was achieved was Θ= 30.552° (0.70 Å).

The unit cell was refined using CrysAlisPro 1.171.42.93a (Rigaku OD, 2023) on 32315 reflections, 50% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.93a (Rigaku OD, 2023). The final completeness is 99.90 % out to 30.552° in Θ. A gaussian absorption correction was performed using CrysAlisPro 1.171.42.93a (Rigaku Oxford Diffraction, 2023) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The absorption coefficient μ of this material is 5.436 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.062 and 1.000.

The structure was solved and the space group P-1 (# 2) determined by the ShelXT (Sheldrick, 2015) structure solution program using dual methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of **ShelXL** 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

_exptl_absorpt_process_details: CrysAlisPro 1.171.42.93a (Rigaku Oxford Diffraction, 2023)Numerical absorption correction based on gaussian integration overa multifaceted crystal modelEmpirical absorption correction using spherical harmonics,implemented in SCALE3 ABSPACK scaling algorithm.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1.

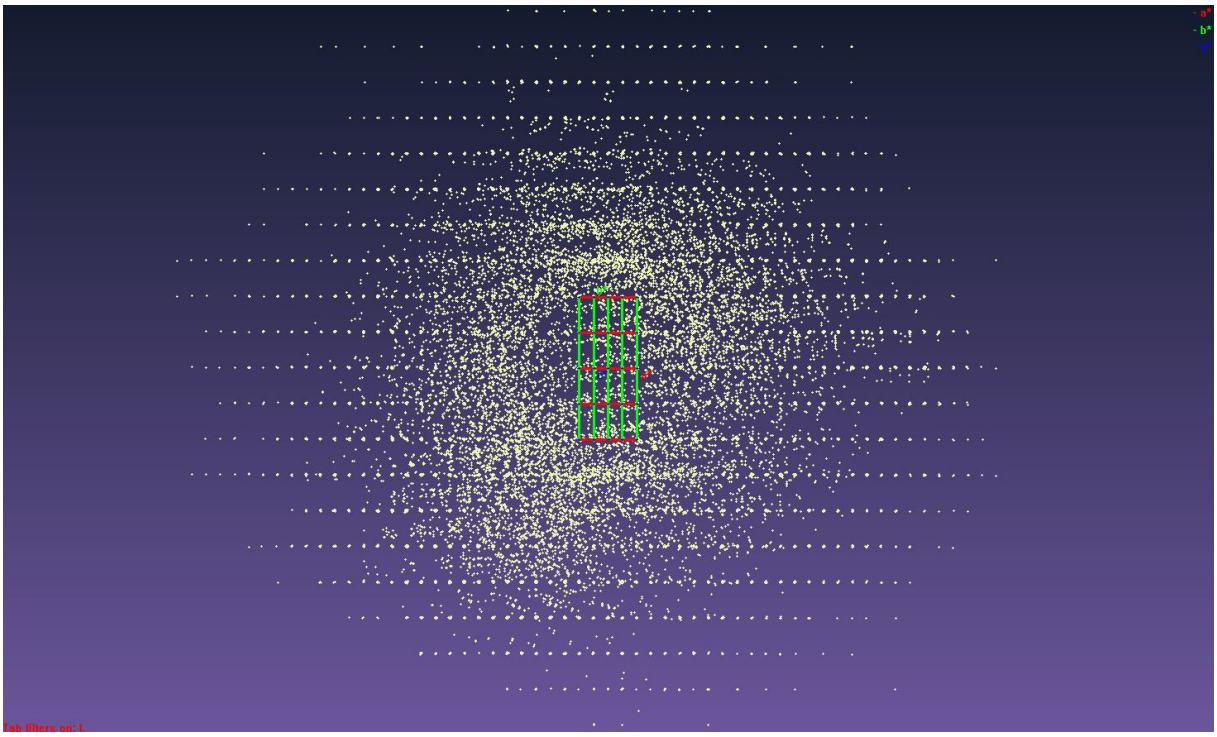


Figure S68. Projection of the reciprocical space for compounds **2-Au**. Additional diffraction spots clearly shows the presence of several diffraction domains.

Experimental details for 3-Au

A yellow plate-shaped-shaped crystal with dimensions 0.65 × 0.44 × 0.14 mm^3 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer operating at T = 100.0(2) K.

Data were measured using ω scans with Mo K_α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The maximum resolution that was achieved was Θ= 30.370° (0.70 Å).

The unit cell was refined using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022) on 41900 reflections, 67% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The final completeness is 99.20 % out to 30.370° in Θ. A gaussian absorption correction was performed using CrysAlisPro 1.171.42.77a (Rigaku Oxford Diffraction, 2022) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The absorption coefficient μ of this material is 5.351 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.230 and 1.000.

The structure was solved and the space group $P2_1/n$ (# 14) determined by the ShelXT (Sheldrick, 2015) structure solution program using dual methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of **ShelXL** 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

_exptl_absorpt_process_details: CrysAlisPro 1.171.42.77a (Rigaku Oxford Diffraction, 2022)Numerical absorption correction based on gaussian integration overa multifaceted crystal modelEmpirical absorption correction using spherical harmonics,implemented in SCALE3 ABSPACK scaling algorithm.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 4 and Z' is 1.

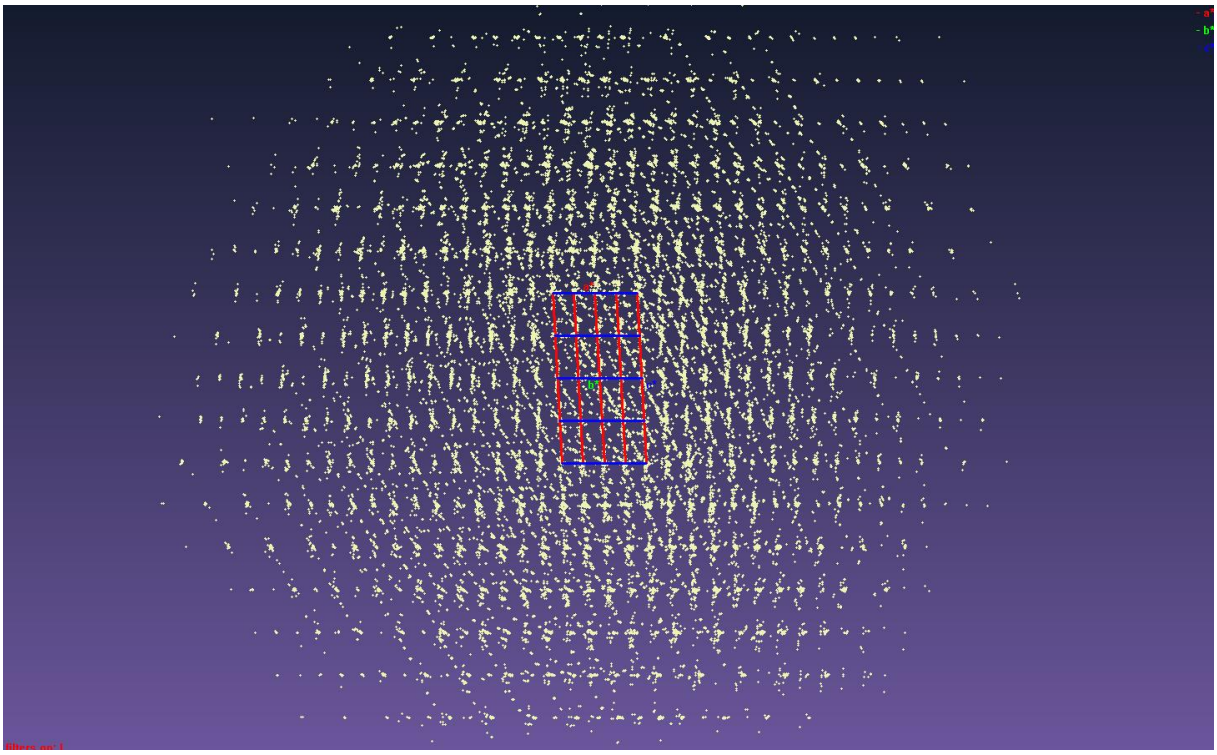


Figure S69. Projection of the reciprocical space for compounds **3-Au**. Additional diffraction spots clearly shoiws the presence of several diffraction domains.

Experimental details for 4-Cu

A colourless needle-shaped-shaped crystal with dimensions 0.66 × 0.15 × 0.06 mm^3 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer operating at T = 100.0(3) K.

Data were measured using ω scans with Mo K_α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The maximum resolution that was achieved was Θ= 30.504° (0.70 Å).

The unit cell was refined using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022) on 13647 reflections, 50.9 % of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.77a (Rigaku OD, 2022). The final completeness is 99.30 % out to 30.504° in Θ. A multi-scan absorption correction was performed using CrysAlisPro 1.171.42.77a (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The absorption coefficient μ of this material is 0.707 mm^{-1} at this wavelength (λ = 0.71073Å) and the minimum and maximum transmissions are 0.860 and 1.000.

The structure was solved and the space group P-1 (# 2) determined by the ShelXT (Sheldrick, 2015) structure solution program using dual methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of **ShelXL** 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model. The analysis of the Fobs vs Fcalc graph showed the presence of a twin law (rotation of 118° around the 0.78 0.33 -0.54 reciprocical vector). The twin fraction was refined to 75% for the first twin individual and to 25% for the second one.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1.

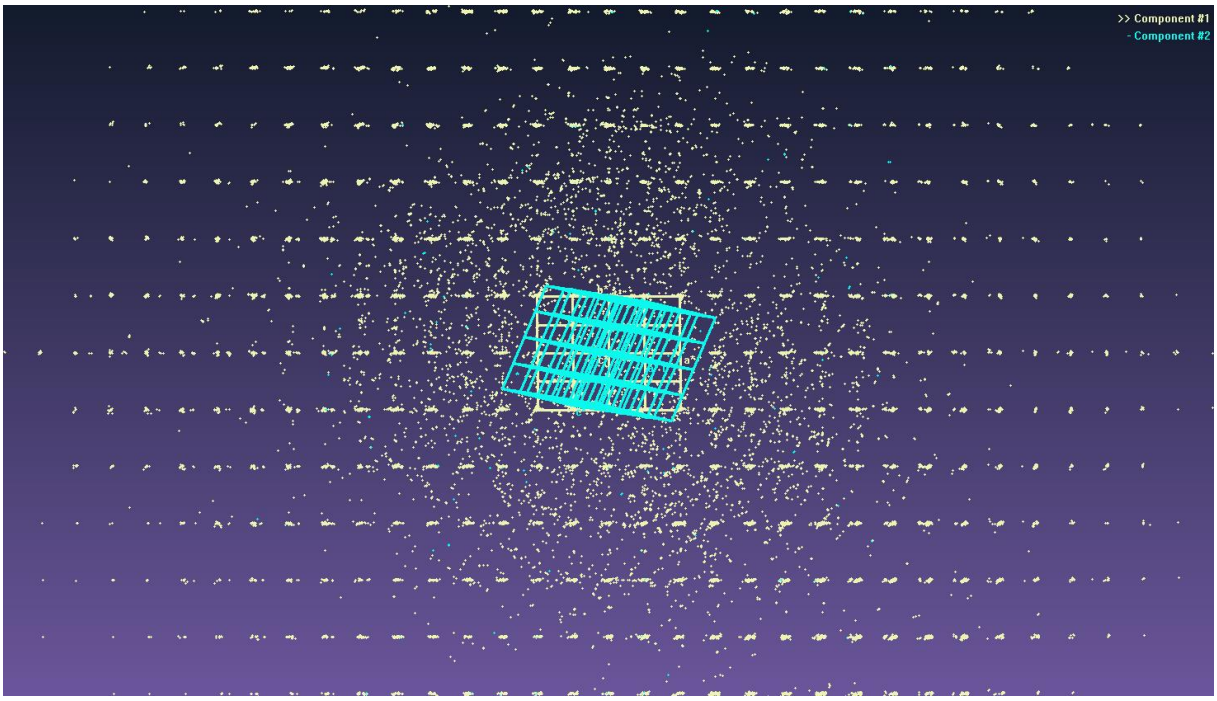


Figure S70. Projection of the reciprocical space for compound **4-Cu**. Additional diffraction spots clearly shows the presence of several diffraction domains.

Table S1. Crystallographic parameters for compounds **1**, **2-Cu** and **2-Ag**.

Compound	**1**	**2-Cu**	**2-Ag**
Formula	$C_{28}H_{58}LiO_2Ta$	$C_{47}H_{78}CuN_2Ta$	$C_{47}H_{78}AgN_2Ta$
$D_{calc.}$/ g cm^{-3}	1.323	1.305	1.339
□/mm^{-1}	3.581	2.833	2.737
Formula Weight	614.63	915.650	959.93
Colour	yellow	orange	orange
Shape	block-shaped	plate-shaped	block-shaped
Size/mm^3	0.40×0.32×0.19	0.41×0.23×0.09	0.76×0.56×0.40
T/K	100.0(2)	100.0(3)	100.00(10)
Crystal System	monoclinic	monoclinic	monoclinic
Space Group	$P2_1/n$	$P2_1/c$	$P2_1/n$
a/Å	11.41010(10)	21.7416(3)	26.0205(4)
b/Å	18.0194(2)	10.3899(1)	10.4785(2)
c/Å	15.0071(2)	22.2686(3)	35.0450(5)
α/°	90	90	90
β/°	90.5350(10)	112.111(2)	94.4430(10)
γ/°	90	90	90
V/Å^3	3085.37(6)	4660.37(12)	9526.5(3)
Z	4	4	8
Z'	1	1	2
Wavelength/Å	0.71073	0.71073	0.71073
Radiation type	Mo K$_\alpha$	Mo K$_\alpha$	Mo K$_\alpha$
Θ_{min}/°	3.428	5.39	5.381
Θ_{max}/°	29.639	28.58	30.020
Measured Refl's.	42436	89105	170147
Indep't Refl's	7740	11092	24745
Refl's I≥2 □(I)	6491	9782	20750
R_{int}	0.0442	0.0438	0.0613
Parameters	309	561	991
Restraints	0	66	131
Largest Peak	1.702	1.0937	1.688
Deepest Hole	-1.234	-0.6173	-1.037
GooF	1.113	1.0400	1.026
wR_2 (all data)	0.0532	0.0547	0.0722
wR_2	0.0478	0.0526	0.0688
R_1 (all data)	0.0374	0.0305	0.0458
R_1	0.0259	0.0243	0.0336

Table S2. Crystallographic parameters for compounds **2-Au**, **3-Au** and **4**.

Compound	**2-Au**	**3-Au**	**4-Cu**
Formula	$C_{47}H_{78}AuN_2Ta$	$C_{47}H_{78}AuN_2Ta$	$C_{33}H_{45}CuN_2O$
$D_{calc.}$/ g cm^{-3}	1.472	1.449	1.140
□/mm^{-1}	5.436	5.351	0.707
Formula Weight	1049.03	1049.03	549.25
Colour	red	yellow	colourless
Shape	plate-shaped	plate-shaped	needle-shaped
Size/mm^3	0.45×0.28×0.08	0.65×0.44×0.14	0.66×0.15×0.06
T/K	100.0(3)	100.0(2)	100.0(3)
Crystal System	triclinic	monoclinic	triclinic
Space Group	*P*-1	$P2_1/n$	*P*-1
a/Å	10.5643(2)	12.9354(3)	9.9345(3)
b/Å	11.9712(3)	21.1316(4)	10.4532(6)
c/Å	21.2897(3)	18.4661(4)	15.9016(5)
α/°	75.108(2)	90	91.683(4)
β/°	86.715(2)	107.709(2)	90.314(3)
γ/°	65.642(2)	90	104.110(4)
V/Å^3	2366.78(9)	4808.44(18)	1600.69(12)
Z	2	4	2
Z'	1	1	1
Wavelength/Å	0.71073	0.71073	0.71073
Radiation type	Mo K$_\alpha$	Mo K$_\alpha$	Mo K$_\alpha$
Θ_{min}/°	2.387	2.508	2.418
Θ_{max}/°	30.552	30.370	30.504
Measured Refl's.	64724	62518	7848
Indep't Refl's	12200	12114	7848
Refl's I≥2 □(I)	9265	9207	6396
R_{int}	0.0618	0.0839	.
Parameters	480	480	346
Restraints	0	0	0
Largest Peak	3.018	4.567	1.799
Deepest Hole	-1.806	-5.908	-1.033
GooF	1.065	1.118	1.086
wR_2 (all data)	0.1198	0.1688	0.2360
wR_2	0.1082	0.1565	0.2147
R_1 (all data)	0.0650	0.0843	0.0931
R_1	0.0428	0.0600	0.0757

C. Computational data

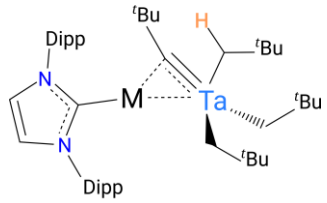
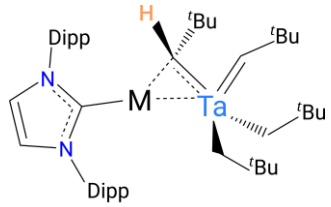
Computational Details

All DFT calculations were carried out with the Gaussian 09 suite of programs.[6a] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[6b-c] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Silver, gold, tantalum and copper atoms were treated with a Stuttgart effective core potential, augmented with a polarization function (ζ_f = 0,790 for Ta, ζ_f = 1,611 for Ag, ζ_f = 1,050 for Au and ζ_f = 3,525 for Cu)[6d], associated with its adapted basis set. [6e-f] H, C, N and O atoms were treated with Pople's double-ζ basis set 6-31G(d,p).[6g-i] Dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping[6j] for the B3PW91 functional. The comparison of the stability of **2-Cu**, **2-Ag** and **2-Au** vs. **3-Cu**, **3-Ag** and **3-Au** including or not the dispersion corrections are given in Table **S3**.

Interestingly, the inclusion of dispersion correction induces a destabilization of the **3-M** complexes, independently of the considered metal. Thus, the formation of these complexes becomes endothermic for all 3 systems, which is completely in disagreement with the experimental data.

[6] a) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian, Inc.*, Wallingford CT, **2016**.; b) J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B*, **1992**, 46, 6671-6687; c) A. D. Becke, *J. Chem. Phys.,* **1993**, 98, 5648-5652; d) M. J. Frisch, J. A. Pople, J. S. Binkley, *J. Chem. Phys.* **1984**, 80, 3265-3269; e) M. Dolg, U. Wedig, H. Stoll, H. Preuss, J. Chem. Phys. **1987**, 86, 866 – 872 ; f) D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, Theoretica chimica acta **1990**, 77, 123-141 ; g) R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.*, **1971**, 54, 724-728; h) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, **1972**, 56, 2257-2261; i) C. Hariharan and J. A. Pople, *Theor. Chim. Acta,* **1973**, 28, 213-222; j) S. Grimme, S. Ehrlich, L. Goerigk, J. Comp. Chem. 2011, 32, 1456-1465.

Table S3. Relative stability, Δ_rH (Δ_rG) in kcal/mol, of **2-M** *vs.* **3-M** complexes (M = Cu, Ag or Au) with or without dispersion corrections.

	Without dispersion corrections			*With dispersion corrections*		
M	**Cu**	**Ag**	**Au**	**Cu**	**Ag**	**Au**
 **2-M** M = Cu, Ag or Au	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
 **3-M** M = Cu, Ag or Au	0.8 (-0.4)	-0.1 (0.1)	-1.4 (-3.2)	5.2 (4.5)	1.8 (1.7)	2.1 (3.9)

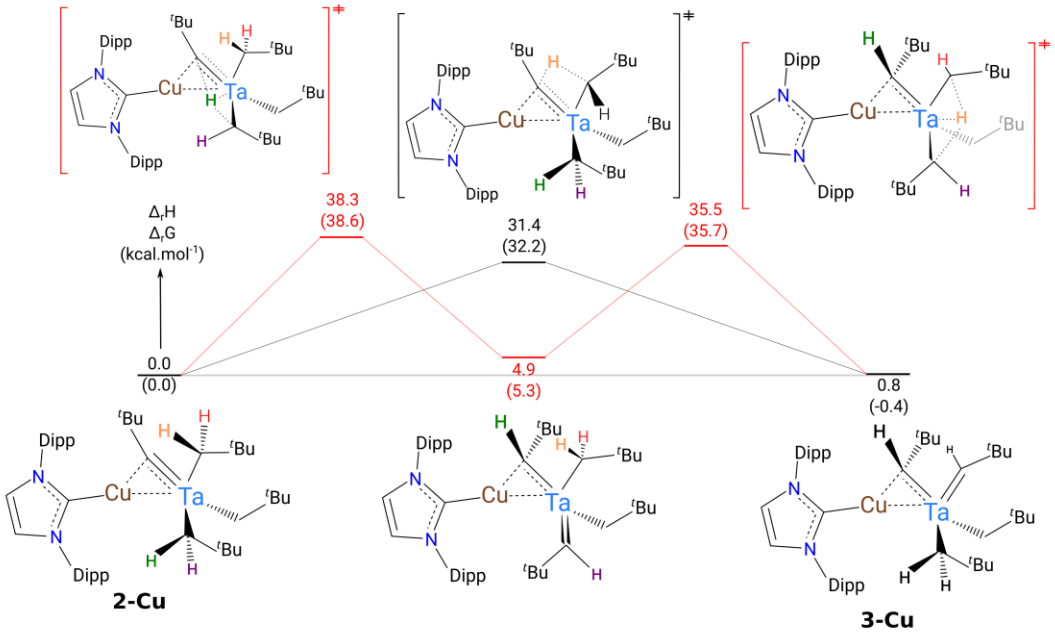


Figure DFT-1. Computed energy profile at room temperature for the one-step (black pathway) and two-steps (red pathway) **2-Cu** ⇌ **3-Cu** tautomerism reaction. The energies are given in kcal.mol^{-1}. The two-step reaction begins by a Ta-assisted hydrogen transfer from the neopentyl, which are not in the same plane as Cu, Ta and $C_{alkylidyne}$, to the alkylidyne leading to the formation of an endothermic intermediate locate at +4.9 kcal/mol with respect to the alkylidyne-bridged **2-Cu**. The final **3-Cu** complex is then formed by a second Ta-assisted hydrogen transfer between the neopentyl ligand in the Cu, Ta and $C_{alkylidyne}$ plane to the terminal alkylidene. The rate-determing step of this two-steps mechanism is the first hydrogen transfer with a high activation barrier of +38.3 kcal/mol. This reaction is therefore not competitive with respect to the one-step hydrogen transfer.

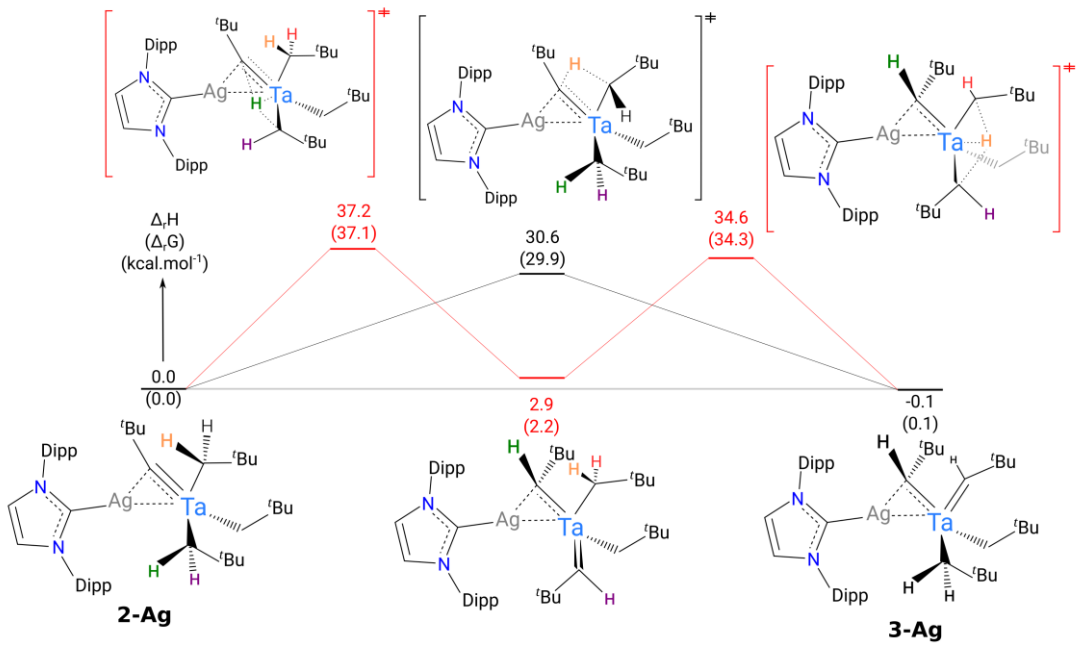


Figure DFT-2. Computed energy profile at room temperature for the one-step (black pathway) and two-steps (red pathway) **2-Ag** ⇌ **3-Ag** tautomerism reaction. The energies are given in kcal.mol^{-1}. The two-step reaction begins by a Ta-assisted hydrogen transfer from the neopentyl, which are not in the same plane as Ag, Ta and $C_{alkylidyne}$, to the alkylidyne leading to the formation of an endothermic intermediate locate at +2.9 kcal/mol with respect to the alkylidyne-bridged **2-Ag**. The final **3-Ag** complex is then formed by a second Ta-assisted hydrogen transfer between the neopentyl ligand in the Ag, Ta and $C_{alkylidyne}$ plane to the terminal alkylidene. The rate-determing step of this two-steps mechanism is the first hydrogen transfer with a high activation barrier of +37.2 kcal/mol. This reaction is therefore not competitive with respect to the one-step hydrogen transfer.

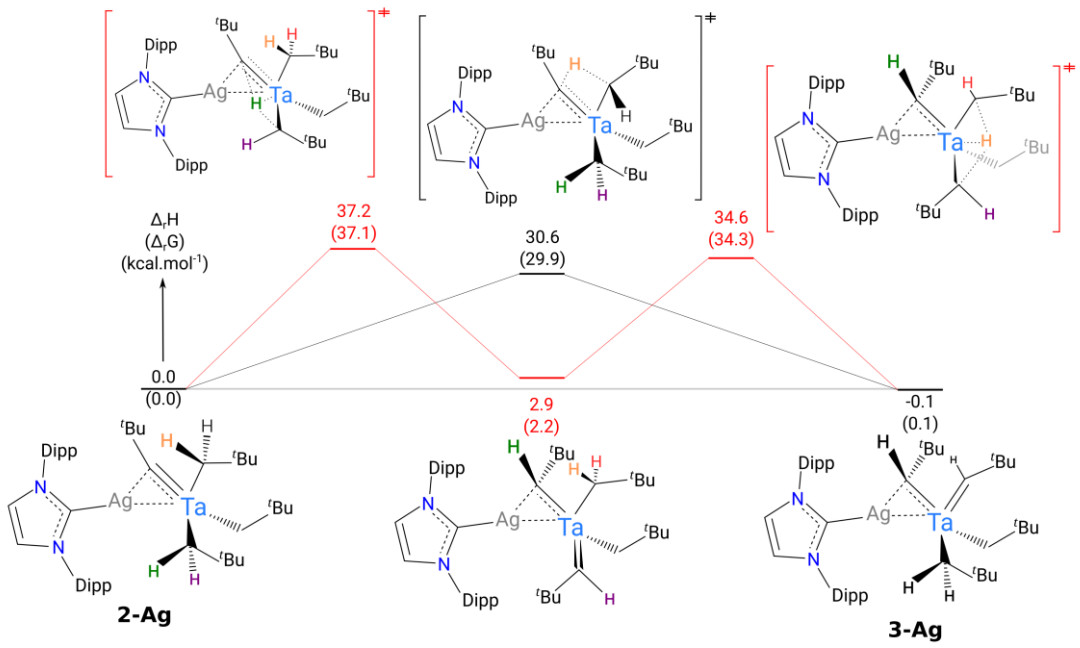


Figure DFT-3. Computed energy profile at room temperature for the one-step (black pathway) and two-steps (red pathway) **2-Au** ⇌ **3-Au** tautomerism reaction. The energies are given in kcal.mol^{-1}. The two-step reaction begins by a Ta-assisted hydrogen transfer from the neopentyl, which are not in the same plane as Au, Ta and $C_{alkylidyne}$, to the alkylidyne leading to the formation of an endothermic intermediate locate at +1.4 kcal/mol with respect to the alkylidyne-bridged **2-Au**. The final **3-Au** complex is then formed by a second Ta-assisted hydrogen transfer between the neopentyl ligand in the Au, Ta and $C_{alkylidyne}$ plane to the terminal alkylidene. The rate-determing step of this two-steps mechanism is the first hydrogen transfer with a high activation barrier of +37.5 kcal/mol. This reaction is therefore not competitive with respect to the one-step hydrogen transfer.

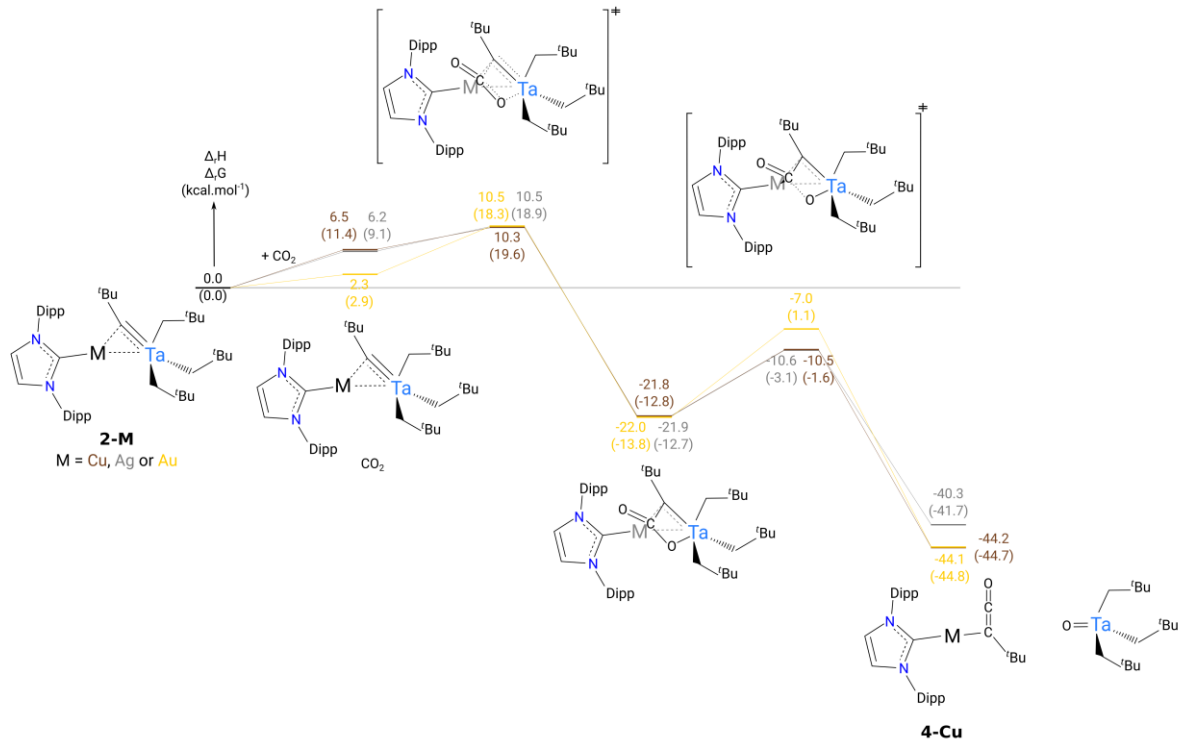


Figure DFT-4. Computed reaction pathway of the formation of **4-Cu**, **4-Au** and **4-Ag** at room temperature. The energies are given in kcal.mol^{-1}.

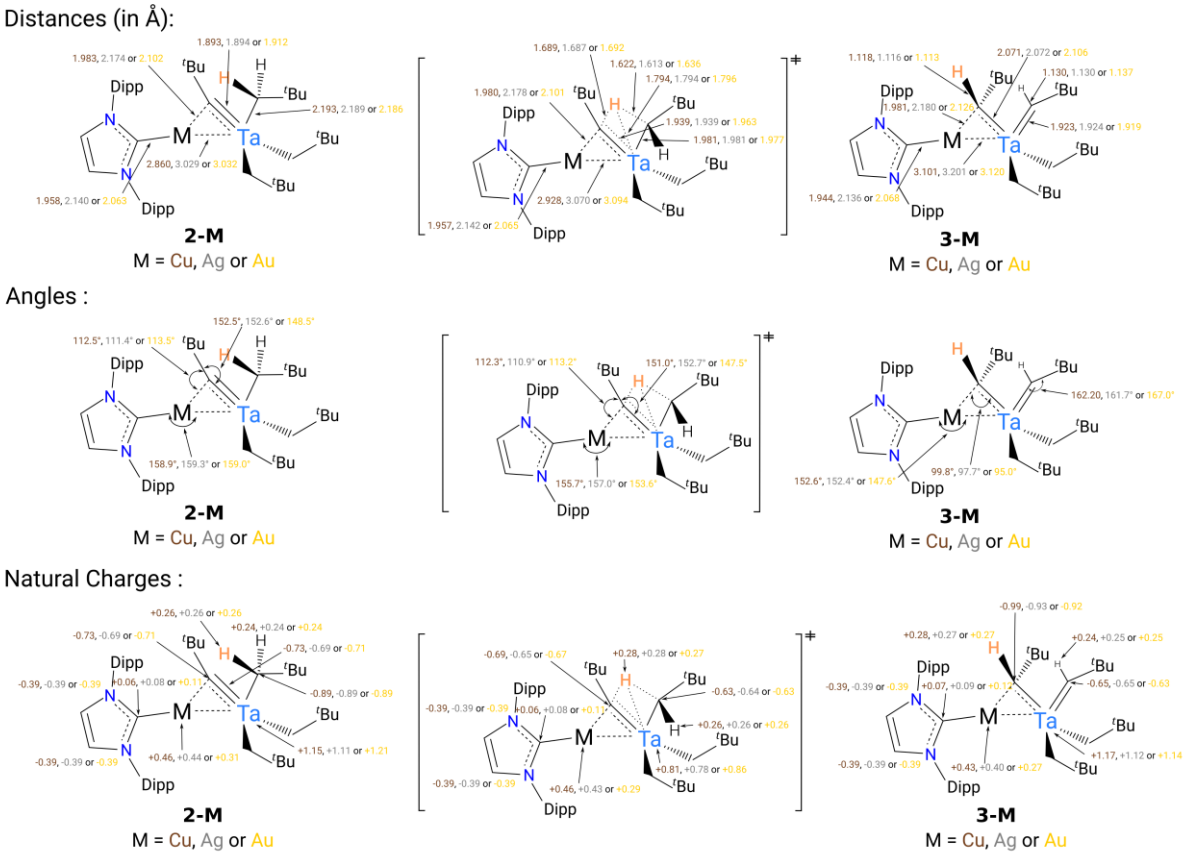


Figure DFT-5. Computed metrical parameters and charges for compounds **2-M** and **3-M** (M = Cu, Ag, Au) and in the corresponding transition state.

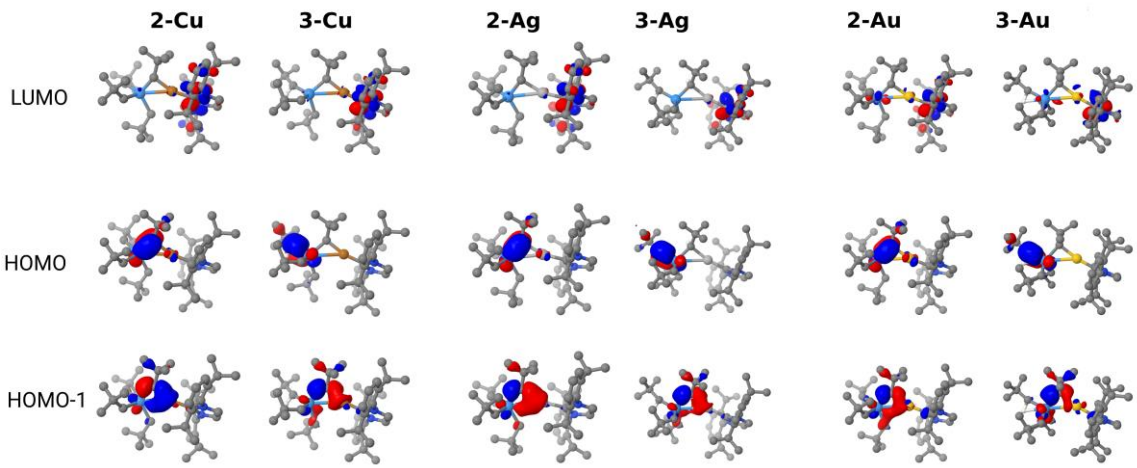


Figure DFT-6. Computed frontier orbitals for compounds **2-M** and **3-M** (M = Cu, Ag, Au).

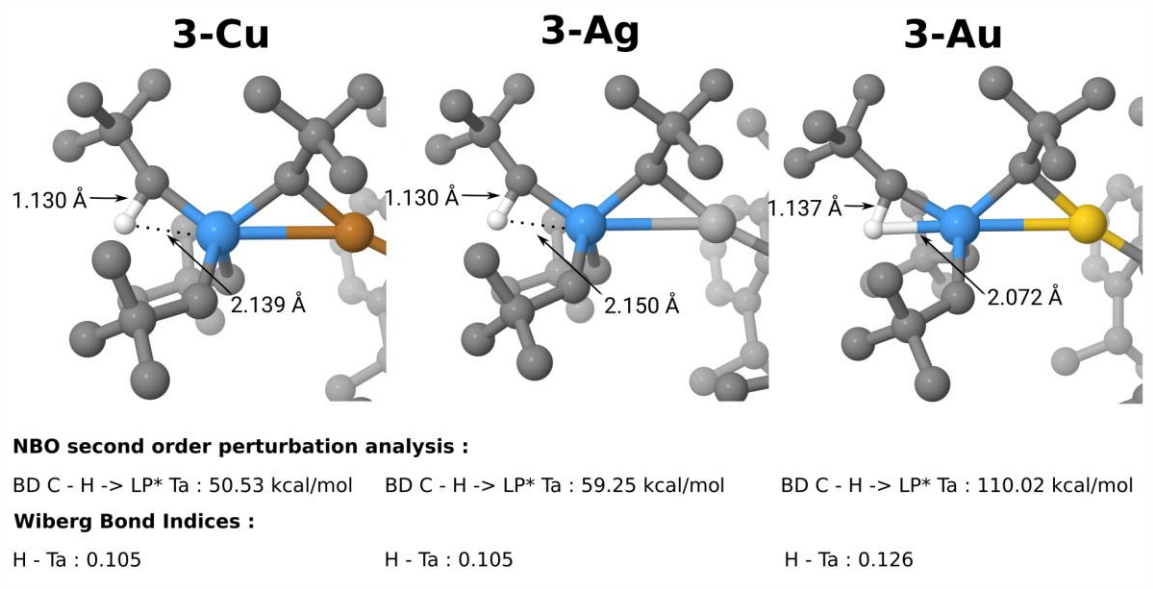


Figure DFT-7. Top: computed metrical parameters for compounds **3-Cu**, **3-Ag** and **3-Au**. Bottom: corresponding NBO data and Wiberg Bond Indices.

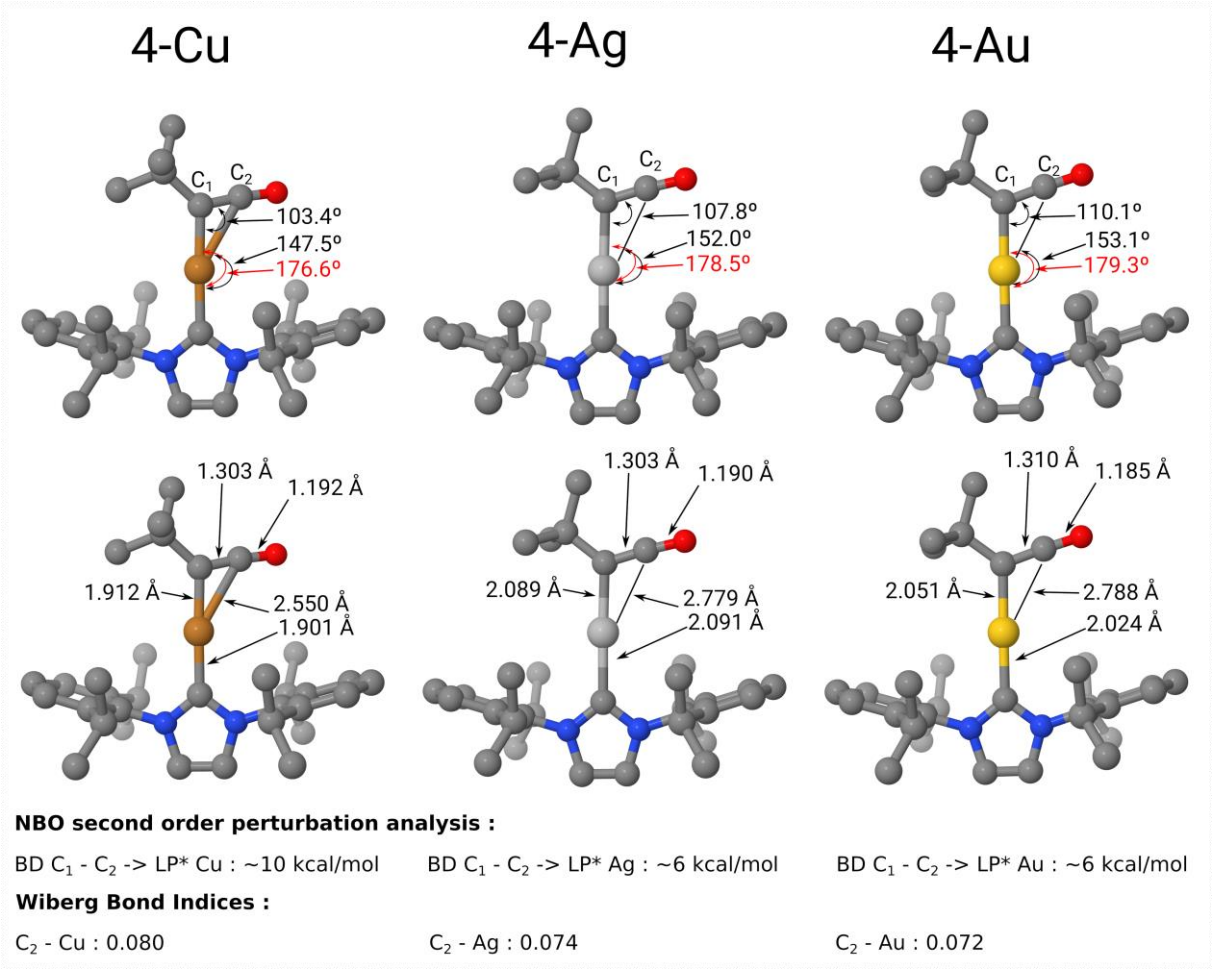


Figure DFT-8. Computed metrical parameters (top: angles; middle: distances) for compounds **4-Cu**, **4-Ag** and **4-Au**. Bottom: corresponding NBO data and Wiberg Bond Indices.

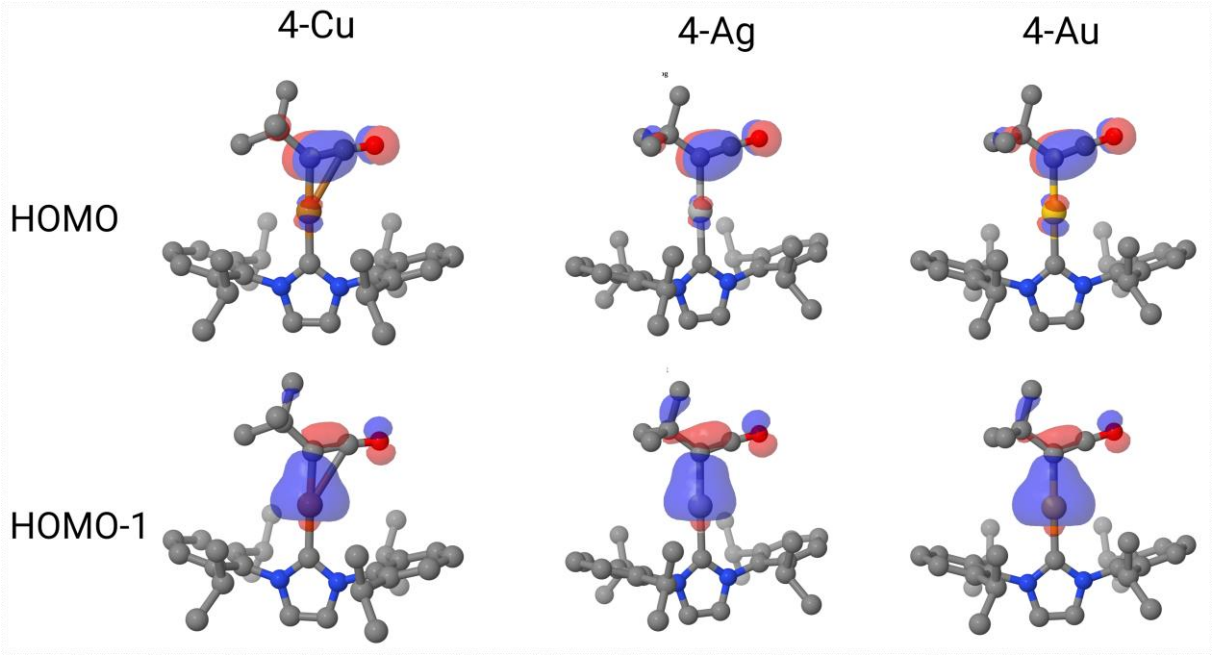


Figure DFT-9. Computed frontier orbitals for compounds **4-M** (M = Cu, Ag, Au).

Cartesian Coordinates :

129
2 - Cu

Ta	9.38649	4.11468	17.71641
Cu	10.36375	4.69719	15.09276
N	11.74526	4.55366	12.44704
N	9.62056	4.61730	12.16249
C	10.59761	5.35180	16.95002
C	11.57274	6.52073	17.03774
C	11.08593	7.70883	16.18459
H	11.00339	7.42218	15.12959
H	10.10010	8.04832	16.51407
H	11.78065	8.55721	16.25802
C	12.97773	6.11861	16.55327
H	13.38058	5.29837	17.15301
H	12.95455	5.78078	15.51279
H	13.67468	6.96511	16.62349
C	11.68791	7.00356	18.49624
H	10.71404	7.32275	18.87660
H	12.06123	6.20419	19.14302
H	12.38152	7.85168	18.57249
C	10.45945	2.64331	18.92887
H	9.59762	2.19016	19.46497
H	10.67992	1.92031	18.11410
C	11.64727	2.65183	19.91077
C	11.83355	1.24897	20.51883
H	10.93419	0.93004	21.05937
H	12.03418	0.50585	19.73788
H	12.67320	1.22757	21.22539
C	11.37032	3.64301	21.05009
H	11.27287	4.66417	20.66812
H	10.43990	3.39098	21.57342
H	12.18185	3.63323	21.78814
C	12.93664	3.04759	19.18584
H	13.18157	2.32260	18.40059
H	12.82114	4.02338	18.70908
H	13.78464	3.09047	19.88057
C	8.16868	5.21104	19.17426
H	7.69472	4.35017	19.69303
H	8.96777	5.54178	19.86758
C	7.11489	6.33437	19.07338
C	6.48158	6.58150	20.45535
H	5.98175	5.67892	20.82681
H	7.24386	6.86649	21.18963
H	5.73558	7.38579	20.41637
C	7.76682	7.63592	18.59342
H	8.51802	7.98591	19.31059
H	8.26841	7.48369	17.63342
H	7.02009	8.43192	18.47992
C	6.00049	5.94286	18.09244
H	6.39621	5.79497	17.08151
H	5.50957	5.01271	18.40142
H	5.22991	6.72231	18.04251
C	8.13229	3.07133	16.21761
H	7.41595	3.91011	16.07241
H	8.53650	2.90065	15.20727
C	7.31547	1.80822	16.62186
C	8.19836	0.55594	16.52591
H	8.60034	0.43183	15.51391
H	9.04681	0.61232	17.21546
H	7.62788	-0.34840	16.77079
C	6.75619	1.91090	18.04979
H	7.54888	1.93386	18.80598
H	6.14399	2.81047	18.17257
H	6.12371	1.04459	18.27990
C	6.11628	1.64529	15.67080
H	5.42997	2.49512	15.76114
H	6.44115	1.59795	14.62757
H	5.55023	0.73099	15.89373
C	10.56886	4.56918	13.14980
C	10.19049	4.63943	10.90022
H	9.59315	4.68229	10.00388
C	11.52979	4.58806	11.07950
H	12.34264	4.56758	10.37214
C	13.07417	4.48198	12.99602
C	13.51454	3.26931	13.56026
C	14.82706	3.22248	14.04019
H	15.19416	2.30332	14.48726
C	15.67254	4.32040	13.94284

H 16.68934 4.25817 14.32050
C 15.21960 5.49598 13.35696
H 15.88953 6.34729 13.27969
C 13.91295 5.60886 12.87335
C 12.65905 2.01343 13.61118
H 11.64494 2.27874 13.29973
C 12.55486 1.44309 15.03101
H 13.52527 1.09640 15.40283
H 12.17185 2.19429 15.72822
H 11.87453 0.58503 15.04277
C 13.18912 0.96074 12.62502
H 13.22496 1.34959 11.60199
H 14.20098 0.63842 12.89403
H 12.54503 0.07477 12.62984
C 13.46852 6.91375 12.22603
H 12.38954 6.85685 12.04955
C 13.71305 8.12868 13.13130
H 13.23359 8.00521 14.10464
H 14.78125 8.30072 13.30045
H 13.30822 9.03158 12.66166
C 14.15761 7.11660 10.86700
H 15.24282 7.20430 10.98790
H 13.97177 6.28456 10.18042
H 13.79938 8.03473 10.38927
C 8.19348 4.55978 12.34518
C 7.51021 5.70916 12.78683
C 6.12206 5.61608 12.92405
H 5.56312 6.48000 13.26884
C 5.44230 4.44351 12.61338
H 4.36278 4.39682 12.72691
C 6.13924 3.33714 12.14485
H 5.59665 2.43171 11.88851
C 7.52975 3.36645 11.99859
C 8.21829 7.03615 13.01027
H 9.26760 6.82214 13.23526
C 7.66314 7.83050 14.19553
H 6.63988 8.17928 14.01841
H 7.67258 7.23386 15.11152
H 8.28031 8.71778 14.36677
C 8.17365 7.87558 11.72194
H 8.62901 7.34763 10.87783
H 7.13969 8.11426 11.44844
H 8.71244 8.81911 11.86099
C 8.24655 2.14931 11.42725
H 9.32428 2.33151 11.47556
C 7.87611 1.94692 9.94907
H 6.80901 1.72661 9.83714
H 8.09061 2.83600 9.34758
H 8.43673 1.10725 9.52459
C 7.97510 0.86871 12.22512
H 8.27419 0.98053 13.27004
H 6.91584 0.59187 12.20634
H 8.53947 0.03313 11.79722
129
2 - Cu with dispersion
Ta 9.35480 4.06500 17.54111
Cu 10.33564 4.65275 15.04076
N 11.71047 4.57242 12.42806
N 9.58874 4.62396 12.16179
C 10.63162 5.28314 16.88772
C 11.66663 6.38823 16.96761
C 11.21461 7.61727 16.16260
H 11.04548 7.34723 15.11368
H 10.28132 8.02327 16.55784
H 11.97331 8.41016 16.20126
C 13.01763 5.92553 16.40233
H 13.39844 5.05336 16.93706
H 12.91476 5.64348 15.35262
H 13.76783 6.72425 16.46911
C 11.85555 6.81380 18.43228
H 10.90018 7.11518 18.87034
H 12.25738 5.98881 19.02578
H 12.55475 7.65665 18.50684
C 10.39258 2.50966 18.65984
H 9.54793 2.00150 19.17044
H 10.67663 1.82362 17.83854
C 11.55614 2.59677 19.65812
C 11.77289 1.23501 20.33460
H 10.87879 0.92629 20.88905
H 11.98796 0.46100 19.58876

H	12.61233	1.26695	21.04039
C	11.22699	3.63736	20.73418
H	11.11763	4.63181	20.29176
H	10.28591	3.39034	21.23996
H	12.01572	3.68779	21.49444
C	12.83353	2.99802	18.92198
H	13.13026	2.21980	18.20962
H	12.65870	3.91312	18.35453
H	13.66509	3.15667	19.61881
C	8.16020	5.15348	19.00384
H	7.60301	4.32067	19.48078
H	8.92565	5.44353	19.74702
C	7.19289	6.33114	18.80098
C	6.40885	6.59881	20.09432
H	5.80998	5.72486	20.37605
H	7.09202	6.81763	20.92250
H	5.72842	7.45236	19.98193
C	7.98552	7.58547	18.42961
H	8.64707	7.88310	19.25084
H	8.61022	7.38761	17.55652
H	7.31859	8.42791	18.21034
C	6.19531	6.01307	17.68078
H	6.70819	5.86055	16.72654
H	5.62725	5.10377	17.90697
H	5.47697	6.83156	17.54925
C	8.14680	3.16577	15.92637
H	7.42860	3.99392	15.76214
H	8.57865	2.99631	14.92836
C	7.34281	1.89641	16.32007
C	8.25211	0.66356	16.27759
H	8.71395	0.55398	15.29154
H	9.05676	0.73559	17.01431
H	7.68527	-0.25076	16.48977
C	6.74076	2.02699	17.72584
H	7.50951	2.07964	18.50491
H	6.11646	2.92246	17.80607
H	6.11522	1.15797	17.96155
C	6.18210	1.69214	15.33857
H	5.50093	2.54930	15.36110
H	6.54833	1.59935	14.31359
H	5.60726	0.78940	15.58243
C	10.54306	4.56311	13.13361
C	10.14420	4.68956	10.89387
H	9.53655	4.76744	10.00686
C	11.48805	4.64416	11.06189
H	12.29835	4.65660	10.35215
C	13.01369	4.51550	13.01891
C	13.41219	3.33627	13.66854
C	14.68194	3.32126	14.24985
H	15.01092	2.43066	14.77643
C	15.52688	4.42053	14.16064
H	16.51146	4.38577	14.61747
C	15.11088	5.56815	13.49639
H	15.77218	6.42719	13.44268
C	13.83899	5.64849	12.92628
C	12.53312	2.10575	13.75068
H	11.60626	2.31999	13.21528
C	12.16038	1.78892	15.20156
H	13.03974	1.49211	15.78276
H	11.71840	2.66354	15.69318
H	11.43590	0.96923	15.24097
C	13.19036	0.90597	13.06131
H	13.43070	1.12910	12.01695
H	14.11829	0.61324	13.56361
H	12.51611	0.04356	13.08198
C	13.38659	6.93543	12.26269
H	12.31286	6.85569	12.06522
C	13.58779	8.14753	13.17737
H	13.10671	7.99461	14.14477
H	14.64939	8.34731	13.35470
H	13.15824	9.04225	12.71520
C	14.10320	7.14223	10.92289
H	15.18322	7.24283	11.07408
H	13.94597	6.30087	10.24108
H	13.74571	8.05193	10.42970
C	8.18104	4.57180	12.42109
C	7.56319	5.68004	13.01386
C	6.19395	5.58247	13.28244
H	5.68347	6.41906	13.74815
C	5.47822	4.44334	12.94258

H 4.41465 4.38833 13.15504
C 6.11447 3.37226 12.32205
H 5.53797 2.49373 12.05599
C 7.48320 3.40487 12.05738
C 8.29737 6.98054 13.27216
H 9.37157 6.78713 13.20293
C 8.03433 7.52443 14.67378
H 6.97551 7.74256 14.84301
H 8.36871 6.80500 15.42637
H 8.59115 8.45270 14.82857
C 7.93430 8.00104 12.18590
H 8.16439 7.61697 11.18672
H 6.86564 8.23975 12.21421
H 8.49288 8.93118 12.33324
C 8.19984 2.21791 11.43338
H 8.97386 2.60853 10.76483
C 7.28668 1.33192 10.58662
H 6.55910 0.79414 11.20342
H 6.73735 1.91213 9.83881
H 7.88308 0.57816 10.06376
C 8.91493 1.38289 12.50249
H 9.53037 2.00554 13.15571
H 8.18735 0.86382 13.13180
H 9.55799 0.62974 12.03545
129
2 - Cu 1 step tautomerisation TS
C 13.60776 3.45845 13.43230
C 13.10915 4.68448 12.95239
C 13.89050 5.85758 12.91283
C 15.20113 5.77588 13.39127
C 15.71188 4.58498 13.89331
C 14.92161 3.44263 13.91097
N 11.77676 4.73122 12.40907
C 10.60258 4.65703 13.11157
N 9.65073 4.72067 12.13030
C 10.21537 4.84106 10.87145
C 11.55628 4.83646 11.04620
C 8.22715 4.58405 12.29855
C 7.48165 5.67214 12.78750
C 6.09522 5.51026 12.87811
C 5.47825 4.32940 12.48312
C 6.23888 3.28012 11.98155
C 7.62904 3.37929 11.87713
C 8.10905 7.01400 13.13090
C 7.64526 7.54957 14.48978
C 8.41843 2.22127 11.27911
C 8.07237 2.03270 9.79367
Cu 10.40447 4.68825 15.05784
Ta 9.34935 3.81925 17.64737
C 8.16222 4.93838 18.77015
C 7.48869 6.06076 19.53437
C 6.44537 6.77125 18.64908
C 13.37673 7.18267 12.36576
C 13.54837 8.33244 13.36792
C 12.81185 2.16342 13.40113
C 12.69421 1.52806 14.79258
C 14.05822 7.52924 11.03257
C 13.41769 1.17939 12.38835
C 10.61276 5.12828 16.97695
C 11.59021 6.27893 17.20393
C 11.05557 7.59395 16.60696
C 12.93551 5.93622 16.53878
C 11.87168 6.49756 18.70216
C 8.21753 0.90994 12.04820
C 7.83343 8.03134 12.01172
C 8.03276 2.88918 16.06886
C 7.12411 1.66714 16.41626
C 6.40309 1.83602 17.76344
C 10.23490 2.17936 18.86614
C 11.35798 2.17638 19.92269
C 11.03391 3.18082 21.03809
C 6.04076 1.50658 15.33544
C 7.95755 0.37786 16.46187
C 12.69942 2.53665 19.27167
C 11.48688 0.77586 20.55142
C 6.76588 5.43494 20.74505
C 8.48743 7.10063 20.05281
H 10.95964 6.73009 19.25229
H 12.31232 5.60195 19.14738
H 12.57571 7.32819 18.84440

H 10.88053 7.48956 15.52988
H 10.10245 7.87339 17.06865
H 11.76261 8.41915 16.76641
H 13.34059 5.00406 16.94358
H 12.83045 5.80685 15.45754
H 13.66875 6.73386 16.71625
H 9.34943 1.69915 19.32344
H 10.54044 1.48923 18.05074
H 10.55465 0.48109 21.04778
H 11.71102 0.02163 19.78749
H 12.28958 0.74374 21.29982
H 10.97178 4.19987 20.64489
H 10.06702 2.94900 21.49954
H 11.79916 3.15720 21.82473
H 12.97968 1.78685 18.52149
H 12.63785 3.50318 18.76430
H 13.50381 2.58071 20.01672
H 7.37463 4.20225 18.45435
H 9.14266 5.60162 17.66129
H 9.24427 6.63271 20.68984
H 8.99670 7.60927 19.22786
H 7.97081 7.86622 20.64389
H 6.92591 7.24449 17.78624
H 5.70274 6.05989 18.27017
H 5.91168 7.54888 19.21096
H 6.02122 4.69877 20.42155
H 7.47978 4.92461 21.39875
H 6.24708 6.20476 21.33017
H 7.38230 3.71111 15.72531
H 8.61467 2.61818 15.17048
H 8.45921 0.20098 15.50290
H 8.72747 0.42171 17.23826
H 7.32390 -0.49304 16.67069
H 7.10217 1.88659 18.60608
H 5.79227 2.74666 17.77414
H 5.73227 0.98806 17.95089
H 5.39052 2.38807 15.30208
H 6.48689 1.38985 14.34386
H 5.41009 0.62883 15.53007
H 9.61293 4.91043 9.98013
H 12.36730 4.89202 10.33844
H 15.33348 2.51348 14.29382
H 16.73082 4.54614 14.26834
H 15.82770 6.66295 13.37717
H 11.79614 2.39612 13.06922
H 13.67021 1.21825 15.18178
H 12.25083 2.22649 15.50867
H 12.06103 0.63573 14.74717
H 13.46809 1.61461 11.38488
H 14.43356 0.88708 12.67560
H 12.81258 0.26808 12.33386
H 12.30351 7.07986 12.17585
H 13.07509 8.10273 14.32527
H 14.60444 8.55082 13.55822
H 13.09284 9.24602 12.97118
H 15.13686 7.66451 11.16740
H 13.91851 6.74432 10.28259
H 13.65307 8.46159 10.62494
H 5.48891 6.32983 13.25169
H 4.39921 4.22899 12.55997
H 5.74599 2.36482 11.66632
H 9.19251 6.87480 13.19476
H 6.57363 7.77562 14.49782
H 7.85129 6.83009 15.28716
H 8.17528 8.47793 14.72591
H 8.20846 7.67963 11.04500
H 6.75893 8.21675 11.90440
H 8.31789 8.98777 12.23624
H 9.48357 2.46361 11.34036
H 7.02060 1.75551 9.66507
H 8.24308 2.94621 9.21503
H 8.68283 1.23560 9.35611
H 8.49460 1.02005 13.09969
H 7.17795 0.56820 12.00750
H 8.83909 0.12022 11.61234
129
3 - Cu
C 3.67365 -0.90562 -2.12396
C 3.21083 0.34476 -2.57532
C 3.99862 1.51177 -2.51991

C	5.27803	1.39767	-1.96841
C	5.75260	0.18067	-1.49335
C	4.95842	-0.95641	-1.57378
N	1.90743	0.41642	-3.18470
C	0.70846	0.43337	-2.52535
N	-0.20744	0.45100	-3.53953
C	0.40157	0.44569	-4.78265
C	1.73643	0.41501	-4.55878
C	-1.63843	0.38723	-3.38768
C	-2.34926	1.55836	-3.06443
C	-3.74051	1.45694	-2.96910
C	-4.39378	0.25125	-3.19841
C	-3.66604	-0.88434	-3.53273
C	-2.27195	-0.84600	-3.63321
C	-1.66821	2.90795	-2.90096
C	-2.19936	3.70653	-1.70538
C	-1.51132	-2.10483	-4.02566
C	-1.82937	-2.51056	-5.47312
Cu	0.37981	0.65785	-0.62254
Ta	-0.53490	-0.37402	2.15462
C	-1.53304	0.20400	3.69291
C	-2.26576	1.07307	4.69059
C	-3.48968	0.33124	5.26201
C	3.52603	2.85161	-3.06613
C	3.81974	4.01750	-2.11328
C	2.86633	-2.18621	-2.26537
C	2.72279	-2.93216	-0.93384
C	4.14875	3.12991	-4.44428
C	3.47823	-3.09199	-3.34561
C	0.18103	1.33444	1.22846
C	1.29869	2.35123	1.56454
C	1.12910	3.62961	0.72371
C	2.68627	1.75481	1.28675
C	1.24699	2.75535	3.05001
C	-1.77789	-3.26772	-3.06175
C	-1.78785	3.72160	-4.20029
C	-1.97809	-1.44173	0.84528
C	-3.40587	-1.93650	1.18225
C	-4.33630	-0.73220	1.37181
C	1.03607	-1.78070	2.73832
C	1.38190	-2.47124	4.07413
C	0.21533	-3.35219	4.54293
C	-3.95009	-2.79740	0.02820
C	-3.40718	-2.79411	2.45400
C	1.69192	-1.41603	5.14390
C	2.62140	-3.36665	3.88923
C	-1.33857	1.45075	5.86335
C	-2.74550	2.35879	3.99750
H	0.27390	3.18453	3.30563
H	1.40335	1.88653	3.69692
H	2.01898	3.50234	3.28099
H	1.16434	3.40159	-0.34837
H	0.16182	4.10296	0.92780
H	1.91400	4.36488	0.94653
H	2.84842	0.84541	1.87528
H	2.80423	1.48964	0.22969
H	3.48004	2.46595	1.54958
H	0.95295	-2.55865	1.95219
H	1.91429	-1.17613	2.42493
H	2.43367	-4.15165	3.14672
H	3.48159	-2.77981	3.54581
H	2.90528	-3.85741	4.82900
H	-0.68065	-2.75603	4.74498
H	-0.04332	-4.10015	3.78374
H	0.47410	-3.88753	5.46470
H	2.56064	-0.81105	4.85603
H	0.84354	-0.73756	5.27634
H	1.91887	-1.88580	6.10896
H	-1.48003	-0.88014	4.00545
H	-0.80252	1.86415	1.18304
H	-1.90106	2.91126	3.57484
H	-3.43615	2.12617	3.18026
H	-3.26265	3.01543	4.70826
H	-4.19059	0.05302	4.46913
H	-3.18455	-0.58642	5.77859
H	-4.02525	0.95971	5.98504
H	-0.99876	0.55500	6.39486
H	-0.45432	1.98465	5.50443
H	-1.86105	2.09207	6.58575
H	-2.03678	-0.86728	-0.09715

H -1.36440 -2.33051 0.57873
H -2.72750 -3.64922 2.35081
H -3.09099 -2.20906 3.32174
H -4.40991 -3.18872 2.66071
H -3.95815 -0.08670 2.16993
H -4.39313 -0.13622 0.45236
H -5.35456 -1.05171 1.62798
H -3.96057 -2.23185 -0.90996
H -3.33089 -3.69019 -0.12260
H -4.97522 -3.13499 0.23020
H -0.16768 0.45531 -5.69827
H 2.57158 0.38157 -5.23940
H 5.34388 -1.90499 -1.21156
H 6.74829 0.11781 -1.06313
H 5.91068 2.27783 -1.90657
H 1.85708 -1.91751 -2.59047
H 3.68773 -3.28852 -0.55815
H 2.27952 -2.29146 -0.16687
H 2.07798 -3.80803 -1.06117
H 3.53376 -2.58336 -4.31354
H 4.49322 -3.40199 -3.07409
H 2.87511 -3.99743 -3.47177
H 2.43885 2.79882 -3.19135
H 3.43791 3.82292 -1.10881
H 4.89348 4.21903 -2.03616
H 3.34703 4.93183 -2.48674
H 5.24007 3.19093 -4.37040
H 3.91021 2.34800 -5.17109
H 3.78504 4.08248 -4.84426
H -4.32194 2.33893 -2.71940
H -5.47593 0.19789 -3.11911
H -4.18675 -1.82007 -3.71435
H -0.60424 2.72743 -2.71644
H -3.24155 4.01302 -1.84458
H -2.13234 3.12788 -0.78002
H -1.60877 4.61913 -1.57686
H -1.35680 3.18733 -5.05315
H -2.83767 3.93065 -4.43419
H -1.26717 4.68039 -4.10268
H -0.44023 -1.88598 -3.97459
H -2.88896 -2.76174 -5.59046
H -1.60145 -1.70670 -6.18064
H -1.24495 -3.39096 -5.76092
H -1.55078 -2.98895 -2.02962
H -2.82308 -3.59189 -3.09513
H -1.15831 -4.12943 -3.33312
129
3 - Cu with dispersion
C 3.56753 -0.84029 -2.06064
C 3.12298 0.37508 -2.60032
C 3.85255 1.57103 -2.49995
C 5.08151 1.51692 -1.84002
C 5.54310 0.32959 -1.28202
C 4.79156 -0.83432 -1.38706
N 1.84188 0.40391 -3.24216
C 0.67058 0.41154 -2.55259
N -0.27910 0.45474 -3.52344
C 0.28428 0.46862 -4.78977
C 1.62905 0.42682 -4.61162
C -1.68548 0.43808 -3.24163
C -2.26808 1.57121 -2.64989
C -3.63731 1.51233 -2.37953
C -4.38448 0.38643 -2.70463
C -3.77635 -0.71885 -3.28879
C -2.40524 -0.72743 -3.55213
C -1.45830 2.82204 -2.35976
C -2.05343 3.68825 -1.25288
C -1.70298 -1.96515 -4.08585
C -2.63675 -2.93492 -4.80805
Cu 0.38574 0.60562 -0.67613
Ta -0.46499 -0.45384 1.91904
C -1.56729 0.08951 3.38832
C -2.33257 1.03073 4.27742
C -3.62624 0.36668 4.77684
C 3.33520 2.87433 -3.07814
C 3.65330 4.07958 -2.18973
C 2.75067 -2.11206 -2.16169
C 2.09791 -2.43098 -0.81414
C 3.89153 3.10529 -4.48979
C 3.57951 -3.29299 -2.67413

C	0.26060	1.29274	1.14913
C	1.43303	2.22661	1.46992
C	1.30061	3.52834	0.66733
C	2.76506	1.55339	1.11971
C	1.43030	2.57119	2.96747
C	-0.95807	-2.68303	-2.95173
C	-1.24191	3.63066	-3.64521
C	-1.80521	-1.46144	0.47590
C	-3.19329	-2.04286	0.81694
C	-4.17498	-0.88791	1.02595
C	1.05095	-1.87191	2.56621
C	1.33714	-2.43994	3.96441
C	0.15187	-3.28302	4.44553
C	-3.69537	-2.92313	-0.33642
C	-3.13160	-2.90485	2.08168
C	1.58642	-1.29081	4.94669
C	2.58565	-3.33428	3.91112
C	-1.47581	1.42284	5.49378
C	-2.68558	2.29412	3.48149
H	0.48754	3.04814	3.25123
H	1.53073	1.66372	3.57043
H	2.25123	3.25522	3.22066
H	1.28503	3.31643	-0.40814
H	0.36456	4.03940	0.91738
H	2.12831	4.21885	0.87450
H	2.88854	0.62074	1.67968
H	2.81450	1.30544	0.05379
H	3.61485	2.20508	1.35627
H	0.95940	-2.70829	1.84740
H	1.94838	-1.31413	2.22348
H	2.43333	-4.17559	3.22478
H	3.45453	-2.76627	3.55870
H	2.82962	-3.74492	4.89879
H	-0.74891	-2.67240	4.55753
H	-0.07325	-4.08429	3.73220
H	0.36625	-3.74435	5.41665
H	2.44825	-0.69075	4.62980
H	0.71684	-0.62819	4.99038
H	1.79321	-1.66887	5.95515
H	-1.53696	-0.97065	3.75757
H	-0.70314	1.85293	1.14720
H	-1.77672	2.77940	3.11342
H	-3.30624	2.04220	2.61497
H	-3.23270	3.01201	4.10433
H	-4.26998	0.08078	3.93998
H	-3.39785	-0.54020	5.34860
H	-4.19077	1.04415	5.42967
H	-1.21139	0.53657	6.08071
H	-0.54690	1.89945	5.16909
H	-2.01525	2.11722	6.15125
H	-1.91039	-0.85295	-0.43965
H	-1.14508	-2.29991	0.16684
H	-2.36622	-3.68523	1.98820
H	-2.89212	-2.29422	2.95479
H	-4.09326	-3.39782	2.26873
H	-3.79820	-0.23088	1.81487
H	-4.27243	-0.29733	0.10784
H	-5.17059	-1.25268	1.30731
H	-3.72604	-2.35346	-1.26964
H	-3.03523	-3.78702	-0.48265
H	-4.70468	-3.30676	-0.13954
H	-0.31696	0.50953	-5.68370
H	2.44173	0.39967	-5.31790
H	5.15700	-1.75300	-0.93911
H	6.49230	0.31458	-0.75461
H	5.67233	2.42086	-1.73786
H	1.94895	-1.94022	-2.88619
H	2.85060	-2.60573	-0.03942
H	1.47178	-1.59446	-0.48118
H	1.46480	-3.32088	-0.88675
H	4.05792	-3.06046	-3.63051
H	4.36374	-3.57697	-1.96522
H	2.93625	-4.16721	-2.81546
H	2.24402	2.79419	-3.14811
H	3.36906	3.89860	-1.15192
H	4.71936	4.32825	-2.21528
H	3.10864	4.95915	-2.54641
H	4.98370	3.18087	-4.45913
H	3.63442	2.29184	-5.17250
H	3.49804	4.03627	-4.91062

H -4.12566 2.35914 -1.91156
H -5.44851 0.36478 -2.48950
H -4.37298 -1.59218 -3.52510
H -0.47384 2.49893 -2.00074
H -2.99711 4.15522 -1.55479
H -2.22735 3.10322 -0.34519
H -1.35618 4.49305 -1.00448
H -0.73519 3.03810 -4.41266
H -2.19974 3.96777 -4.05602
H -0.62873 4.51460 -3.44107
H -0.95140 -1.64026 -4.81414
H -3.34303 -3.40462 -4.11563
H -3.20900 -2.43875 -5.59820
H -2.05176 -3.73890 -5.26448
H -0.29872 -2.00416 -2.40754
H -1.66803 -3.09017 -2.22908
H -0.35751 -3.50701 -3.35179
129
2 - Cu 2 steps tautomerisation TS - First H trans.
C 4.11074 2.73523 -1.94274
C 3.87986 1.34500 -1.96145
C 4.76532 0.42160 -1.36815
C 5.87959 0.93953 -0.70128
C 6.11826 2.30778 -0.64633
C 5.24729 3.19223 -1.26782
N 2.75188 0.84915 -2.71423
C 1.49417 0.56316 -2.24487
N 0.81909 0.19206 -3.37680
C 1.62326 0.25432 -4.50187
C 2.84100 0.66717 -4.08434
C -0.57417 -0.15904 -3.50730
C -0.93072 -1.52074 -3.50968
C -2.26171 -1.83563 -3.79850
C -3.19436 -0.84255 -4.07396
C -2.81587 0.49376 -4.05348
C -1.49834 0.86843 -3.77315
C 0.07967 -2.63129 -3.26602
C 0.55624 -3.23804 -4.59620
C -1.11111 2.33802 -3.81202
C -1.99197 3.18920 -2.88866
Cu 0.77078 0.80355 -0.45345
C 0.16532 1.50553 1.30165
C 0.64770 2.93063 1.56204
C 2.18636 2.93737 1.59709
C 4.57477 -1.08437 -1.48974
C 5.18446 -1.86964 -0.32390
C 3.21681 3.73047 -2.66936
C 2.96807 5.01307 -1.86596
C 5.16279 -1.60770 -2.81271
C 3.80634 4.08741 -4.04490
C -2.39578 0.30993 0.57000
Ta -0.86853 -0.01516 1.88968
C -1.72147 0.43193 3.90646
C -1.36740 -0.17273 5.28507
C -1.86001 -1.62540 5.36449
C -3.82062 -0.24444 0.79636
C -3.83079 -1.50376 1.67982
C -4.72551 0.83323 1.42326
C -4.40781 -0.63193 -0.57131
C -1.14080 2.87629 -5.25089
C -0.46180 -3.72980 -2.34352
C 0.01906 -2.00035 1.30310
C 1.30446 -2.65186 1.87724
C 2.38496 -1.59638 2.14601
C 1.85749 -3.68288 0.87643
C 0.99459 -3.39419 3.18503
C 0.13877 3.46963 2.91055
C 0.15030 3.88168 0.45813
C 0.14738 -0.11982 5.52898
C -2.06065 0.62978 6.40214
H -0.95583 3.50036 2.93544
H 0.47986 2.83735 3.73593
H 0.50743 4.48851 3.08702
H 0.50332 3.55778 -0.52729
H -0.94488 3.90020 0.42976
H 0.49816 4.90851 0.63328
H 2.55563 2.26455 2.37773
H 2.60822 2.59975 0.64428
H 2.56779 3.94562 1.80693
H -0.79435 -2.74675 1.35097

H 0.17054 -1.84880 0.21887
H 1.10841 -4.45299 0.65871
H 2.12517 -3.20205 -0.07202
H 2.75294 -4.18587 1.26546
H 0.62772 -2.71235 3.95732
H 0.22940 -4.16390 3.02835
H 1.89077 -3.88859 3.58038
H 2.58627 -1.00527 1.24610
H 2.06848 -0.88830 2.91986
H 3.32221 -2.06101 2.47920
H -2.81882 0.40729 3.80472
H -1.48629 1.51138 3.94460
H 0.69829 -0.69643 4.77821
H 0.51311 0.91259 5.48656
H 0.40740 -0.52686 6.51429
H -1.72597 1.67366 6.40065
H -3.14840 0.62855 6.26626
H -1.84510 0.20916 7.39330
H -2.94963 -1.67195 5.24921
H -1.41853 -2.24526 4.57738
H -1.60872 -2.07964 6.33118
H -1.48055 1.47481 1.04676
H -2.38536 0.88284 -0.36287
H -4.35839 1.13628 2.40890
H -4.75409 1.72737 0.79021
H -5.75543 0.46933 1.53987
H -4.46469 0.23822 -1.23467
H -3.78455 -1.38512 -1.06307
H -5.42134 -1.03972 -0.46214
H -3.25674 -2.31041 1.21046
H -3.40681 -1.31680 2.67173
H -4.85588 -1.86438 1.83218
H 1.25169 0.00534 -5.48271
H 3.75509 0.84816 -4.62585
H 6.57447 0.26020 -0.21968
H 6.99166 2.68454 -0.12119
H 5.45004 4.25778 -1.22964
H 3.49639 -1.28230 -1.49542
H 6.27957 -1.86905 -0.36417
H 4.87446 -1.47136 0.64456
H 4.86262 -2.91382 -0.37521
H 4.68633 -1.15879 -3.68747
H 6.23664 -1.39621 -2.86480
H 5.02947 -2.69261 -2.88236
H 2.24466 3.25225 -2.83205
H 2.62492 4.79634 -0.85244
H 3.86973 5.63119 -1.79663
H 2.20296 5.61866 -2.36243
H 4.78950 4.55749 -3.93262
H 3.92875 3.20826 -4.68322
H 3.15330 4.79361 -4.56896
H -3.55285 1.26251 -4.26703
H -4.22230 -1.11200 -4.29950
H -2.57095 -2.87601 -3.81199
H -0.08341 2.42590 -3.44580
H -3.03804 3.19143 -3.21282
H -1.95683 2.82131 -1.85981
H -1.64668 4.22848 -2.89046
H -0.47720 2.30630 -5.90892
H -2.15079 2.82497 -5.67214
H -0.82256 3.92412 -5.27471
H 0.94854 -2.18715 -2.76806
H -0.28237 -3.68309 -5.14319
H 1.01803 -2.48841 -5.24574
H 1.29504 -4.02598 -4.41468
H -0.83263 -3.31586 -1.40256
H -1.27213 -4.29624 -2.81495
H 0.33486 -4.44240 -2.10808
129
2 - Cu 2 steps tautomerisation TS - Intermediate.
C 3.80795 -0.97227 -1.93818
C 3.27211 0.28247 -2.28480
C 3.96825 1.48942 -2.07597
C 5.21131 1.41029 -1.44056
C 5.74525 0.18815 -1.04811
C 5.05494 -0.98939 -1.30521
N 1.99861 0.30975 -2.96183
C 0.76222 0.29799 -2.37055
N -0.09112 0.21684 -3.43563
C 0.58800 0.17288 -4.64067

C	1.90683	0.22599	-4.34117
C	-1.52500	0.08619	-3.37522
C	-2.31696	1.24781	-3.30754
C	-3.70424	1.07876	-3.33161
C	-4.27542	-0.18562	-3.42435
C	-3.46752	-1.31324	-3.49552
C	-2.07343	-1.20575	-3.47593
C	-1.71160	2.64253	-3.27582
C	-2.44950	3.59247	-2.32612
C	-1.22019	-2.46107	-3.57978
C	-1.46528	-3.19365	-4.90718
Cu	0.25076	0.61868	-0.51150
Ta	-0.56901	-0.28802	2.28842
C	-0.57940	0.27400	4.39966
C	-1.70477	0.57709	5.41147
C	-2.51319	-0.69589	5.68912
C	3.45062	2.82929	-2.57818
C	3.79254	3.99822	-1.64696
C	3.12669	-2.28152	-2.30425
C	3.07111	-3.27131	-1.13790
C	3.99011	3.12247	-3.98938
C	3.81544	-2.91417	-3.52488
C	-0.20046	1.45735	1.24288
C	0.67211	2.71220	1.47217
C	0.67205	3.62232	0.22965
C	2.11616	2.30269	1.79681
C	0.11802	3.54944	2.63922
C	-1.43761	-3.39749	-2.38345
C	-1.65046	3.23316	-4.69420
C	-2.33989	-1.01330	1.93440
C	-3.75473	-0.89403	1.40117
C	-3.99474	0.50026	0.80570
C	0.98132	-1.86251	2.10562
C	1.29845	-3.01162	3.10155
C	0.00615	-3.63769	3.64775
C	-3.99432	-1.94951	0.30556
C	-4.77800	-1.13482	2.52899
C	2.15049	-2.48759	4.26744
C	2.10408	-4.11779	2.39663
C	-1.09615	1.07178	6.73647
C	-2.63689	1.66352	4.85891
H	-0.91879	3.84737	2.44658
H	0.13357	2.98684	3.57553
H	0.70979	4.46342	2.78168
H	1.08338	3.09928	-0.64197
H	-0.34915	3.93012	-0.01960
H	1.26669	4.53052	0.39622
H	2.15398	1.68993	2.70523
H	2.55200	1.71420	0.98082
H	2.75152	3.18225	1.96375
H	0.65562	-2.31833	1.14983
H	1.92278	-1.33538	1.86605
H	1.53710	-4.54723	1.56249
H	3.04570	-3.72451	1.99740
H	2.35022	-4.93334	3.08890
H	-0.58009	-2.91631	4.22765
H	-0.62650	-4.00434	2.83075
H	0.22770	-4.48830	4.30453
H	3.10054	-2.07938	3.90210
H	1.64276	-1.69476	4.82488
H	2.38346	-3.29316	4.97457
H	0.18972	1.06620	4.46678
H	-1.25688	1.77342	1.06880
H	-2.08853	2.59073	4.65911
H	-3.08921	1.33062	3.91966
H	-3.43963	1.89471	5.57072
H	-2.89647	-1.11614	4.75515
H	-1.88908	-1.45634	6.17563
H	-3.36187	-0.48924	6.35296
H	-0.41653	0.32289	7.16062
H	-0.52398	1.99532	6.58692
H	-1.87424	1.27882	7.48247
H	-0.04456	-0.63508	4.75143
H	-2.12223	-2.04107	2.31573
H	-4.63490	-2.12138	2.98473
H	-4.67978	-0.38347	3.31771
H	-5.80459	-1.08987	2.14141
H	-3.84588	1.27953	1.56137
H	-3.30449	0.69129	-0.02266
H	-5.01877	0.59195	0.42261

H -3.31222 -1.79383 -0.53422
H -3.82938 -2.96079 0.69568
H -5.02413 -1.89853 -0.07320
H 0.07315 0.09711 -5.58509
H 2.78022 0.19831 -4.97220
H 5.49259 -1.94041 -1.01722
H 6.71073 0.15379 -0.55091
H 5.77093 2.32040 -1.25105
H 2.09242 -2.05791 -2.58287
H 4.06822 -3.61242 -0.83992
H 2.58842 -2.82817 -0.26420
H 2.50058 -4.15987 -1.42757
H 3.81629 -2.24002 -4.38731
H 4.85759 -3.16557 -3.29899
H 3.30345 -3.83724 -3.81713
H 2.35845 2.76273 -2.64286
H 3.51781 3.78753 -0.61119
H 4.86061 4.23988 -1.67656
H 3.25289 4.89564 -1.96526
H 5.08429 3.17667 -3.97865
H 3.70103 2.35437 -4.71151
H 3.60829 4.08283 -4.35239
H -4.34825 1.95068 -3.27885
H -5.35650 -0.29136 -3.43877
H -3.92413 -2.29637 -3.56379
H -0.68501 2.55180 -2.90513
H -3.45516 3.83521 -2.68580
H -2.54005 3.16342 -1.32447
H -1.90125 4.53640 -2.24456
H -1.06450 2.60361 -5.37113
H -2.65627 3.33273 -5.11717
H -1.19147 4.22759 -4.67690
H -0.16840 -2.15918 -3.56503
H -2.49553 -3.55788 -4.97967
H -1.28291 -2.54237 -5.76820
H -0.80193 -4.06101 -4.99130
H -1.22120 -2.89145 -1.43853
H -2.46972 -3.76063 -2.33884
H -0.78231 -4.27159 -2.46452
129
2 - Cu 2 steps tautomerisation TS - Second H trans.
C 4.04392 -0.89702 -2.04371
C 3.43340 0.34012 -2.31660
C 4.02851 1.57255 -1.98084
C 5.24848 1.52935 -1.30020
C 5.85804 0.31903 -0.98558
C 5.26607 -0.87866 -1.36296
N 2.18303 0.33169 -3.03423
C 0.93396 0.36267 -2.47606
N 0.10533 0.23386 -3.55607
C 0.81400 0.11526 -4.73916
C 2.12592 0.17796 -4.40992
C -1.33416 0.17335 -3.52308
C -2.06666 1.35846 -3.72321
C -3.45926 1.25151 -3.78194
C -4.09308 0.02157 -3.64667
C -3.34360 -1.13089 -3.44286
C -1.94771 -1.08410 -3.37641
C -1.39663 2.71075 -3.90702
C -2.05220 3.80649 -3.05749
C -1.15680 -2.36751 -3.18410
C -1.22034 -3.24526 -4.44340
Cu 0.34463 0.73384 -0.65802
Ta -0.80008 -0.27227 2.05615
C -0.85736 0.17300 3.99997
C -1.39229 0.44499 5.39787
C -1.59414 -0.87009 6.17745
C 3.42280 2.90319 -2.40143
C 3.72982 4.04789 -1.43060
C 3.45701 -2.22494 -2.49554
C 3.22821 -3.18165 -1.32151
C 3.88847 3.28155 -3.81870
C 4.34037 -2.87296 -3.57312
C -0.41872 1.49737 0.99910
C 0.24623 2.82203 1.43624
C 0.38701 3.79244 0.24911
C 1.63982 2.54782 2.02047
C -0.60989 3.52486 2.50404
C -1.61783 -3.14566 -1.94477
C -1.37383 3.11543 -5.38970

C	-2.63488	-1.04724	1.87721
C	-4.11861	-0.74412	1.76086
C	-4.37748	0.76916	1.74780
C	0.77082	-1.82726	1.78385
C	1.09690	-2.98010	2.77204
C	-0.18812	-3.67627	3.24276
C	-4.61572	-1.33795	0.42823
C	-4.91273	-1.39969	2.90684
C	1.86269	-2.45272	3.99288
C	1.98519	-4.02858	2.07796
C	-0.37922	1.31786	6.16191
C	-2.73164	1.19410	5.33501
H	-1.60407	3.76451	2.10719
H	-0.74397	2.87042	3.36935
H	-0.14438	4.46360	2.83349
H	0.99015	3.35058	-0.55277
H	-0.59626	4.03347	-0.17029
H	0.86160	4.73580	0.55281
H	1.56793	1.91001	2.90892
H	2.27695	2.03428	1.28983
H	2.13855	3.47935	2.31866
H	0.44067	-2.28526	0.82932
H	1.71108	-1.30977	1.52535
H	1.48558	-4.44926	1.19727
H	2.93175	-3.58557	1.74858
H	2.22367	-4.85917	2.75491
H	-0.82748	-2.98507	3.80185
H	-0.76258	-4.05987	2.39018
H	0.04088	-4.52704	3.89686
H	2.78908	-1.95053	3.68837
H	1.26108	-1.73956	4.56304
H	2.13526	-3.27370	4.66767
H	0.24928	0.01559	4.01950
H	-1.43848	1.72044	0.60215
H	-2.62507	2.14127	4.79743
H	-3.49469	0.60037	4.82297
H	-3.10237	1.40902	6.34480
H	-2.32293	-1.51463	5.67299
H	-0.65508	-1.42807	6.25878
H	-1.96135	-0.67569	7.19374
H	0.58808	0.80973	6.25108
H	-0.21334	2.26919	5.64672
H	-0.73851	1.53583	7.17528
H	-1.96382	-0.70468	3.38050
H	-2.45413	-2.14271	1.91348
H	-4.75947	-2.48511	2.91552
H	-4.60078	-1.01207	3.88168
H	-5.98877	-1.21240	2.79959
H	-4.01933	1.24405	2.66589
H	-3.86074	1.23937	0.90484
H	-5.44958	0.98058	1.65174
H	-4.07911	-0.89646	-0.41655
H	-4.46266	-2.42305	0.39901
H	-5.68873	-1.14702	0.29677
H	0.32245	-0.00718	-5.69096
H	3.01576	0.11492	-5.01554
H	5.75786	-1.81838	-1.12814
H	6.80419	0.31264	-0.45143
H	5.73155	2.45723	-1.01285
H	2.47942	-2.03063	-2.94725
H	4.16871	-3.45550	-0.83176
H	2.57513	-2.73346	-0.56924
H	2.76076	-4.10793	-1.67252
H	4.47928	-2.21241	-4.43519
H	5.33332	-3.11574	-3.17953
H	3.88689	-3.80421	-3.92902
H	2.33437	2.77734	-2.42879
H	3.48570	3.78374	-0.39859
H	4.78401	4.34370	-1.47111
H	3.13971	4.92912	-1.70028
H	4.97778	3.39538	-3.84876
H	3.60886	2.52661	-4.55887
H	3.44101	4.23303	-4.12571
H	-4.05572	2.14539	-3.93726
H	-5.17673	-0.03828	-3.69646
H	-3.84896	-2.08597	-3.33398
H	-0.35964	2.61727	-3.56774
H	-3.06393	4.04310	-3.40397
H	-2.11335	3.51046	-2.00711
H	-1.46545	4.72883	-3.11822

H -0.85061 2.37737 -6.00564
H -2.39161 3.21545 -5.78296
H -0.86863 4.07893 -5.51691
H -0.10945 -2.09596 -3.02035
H -2.24924 -3.55416 -4.65797
H -0.84177 -2.71635 -5.32414
H -0.62081 -4.15199 -4.30895
H -1.59081 -2.51833 -1.04909
H -2.63938 -3.52348 -2.05986
H -0.96596 -4.01031 -1.78110
129
2 - Au
Ta 9.34095 4.14596 17.77171
Au 10.43545 4.77442 15.01505
N 11.81206 4.54107 12.28756
N 9.68536 4.56342 11.98242
C 10.60634 5.36940 17.02388
C 11.59309 6.51670 17.23888
C 11.12971 7.78319 16.49124
H 11.05749 7.59194 15.41498
H 10.14314 8.10306 16.83756
H 11.83475 8.61055 16.65136
C 13.00473 6.14976 16.74149
H 13.38335 5.26045 17.25232
H 13.00034 5.93325 15.66856
H 13.70733 6.97440 16.92376
C 11.68836 6.86218 18.73640
H 10.71227 7.15494 19.13331
H 12.04848 6.00681 19.31528
H 12.38503 7.69506 18.89781
C 10.36863 2.61976 18.93293
H 9.49209 2.16042 19.43851
H 10.56677 1.94699 18.06938
C 11.55715 2.52306 19.90862
C 11.68506 1.07751 20.42540
H 10.77625 0.76503 20.95368
H 11.84592 0.37815 19.59639
H 12.52836 0.97404 21.11995
C 11.31924 3.45027 21.10892
H 11.25540 4.49631 20.79364
H 10.38264 3.19820 21.62108
H 12.13242 3.36651 21.84049
C 12.86114 2.90776 19.20421
H 13.07111 2.22538 18.37219
H 12.79211 3.91630 18.79154
H 13.71093 2.86632 19.89669
C 8.21790 5.27550 19.26846
H 7.79359 4.43833 19.86245
H 9.06346 5.64365 19.88307
C 7.15078 6.39085 19.19645
C 6.74132 6.80456 20.62252
H 6.33066 5.95252 21.17705
H 7.60374 7.18307 21.18320
H 5.97862 7.59362 20.60566
C 7.70126 7.62274 18.46805
H 8.57692 8.02876 18.98603
H 8.00709 7.37003 17.44846
H 6.94534 8.41679 18.42002
C 5.89757 5.89925 18.45859
H 6.12893 5.60453 17.42906
H 5.45133 5.03633 18.96617
H 5.13581 6.68769 18.41826
C 7.99710 3.11365 16.34580
H 7.30609 3.97079 16.18592
H 8.40229 2.92007 15.34184
C 7.14683 1.88115 16.76908
C 7.99279 0.60176 16.69574
H 8.39408 0.45083 15.68735
H 8.83974 0.63993 17.38777
H 7.39277 -0.28054 16.95050
C 6.58076 2.02125 18.19082
H 7.37033 2.05730 18.95002
H 5.97554 2.92793 18.28887
H 5.94019 1.16549 18.43788
C 5.95294 1.73514 15.80752
H 5.29403 2.60913 15.86778
H 6.29035 1.64919 14.76998
H 5.35431 0.84584 16.04582
C 10.62816 4.56528 12.97154
C 10.26840 4.54214 10.72586

H 9.67776 4.53886 9.82404
C 11.60778 4.52110 10.91837
H 12.42764 4.48868 10.21926
C 13.12938 4.52132 12.86967
C 13.61707 3.31354 13.40250
C 14.91564 3.31871 13.92040
H 15.31985 2.40415 14.34444
C 15.69956 4.46562 13.89358
H 16.70680 4.44411 14.30034
C 15.19852 5.63863 13.34193
H 15.82106 6.52829 13.32014
C 13.90320 5.69733 12.81937
C 12.82069 2.01883 13.39284
H 11.81425 2.24164 13.02703
C 12.66318 1.43285 14.80149
H 13.62818 1.14313 15.23162
H 12.19281 2.15804 15.47191
H 12.03545 0.53589 14.76834
C 13.45079 1.00031 12.43032
H 13.53030 1.40148 11.41451
H 14.45762 0.71543 12.75465
H 12.84475 0.08881 12.38927
C 13.39964 6.99315 12.19966
H 12.32809 6.88103 12.00459
C 13.56362 8.19523 13.13895
H 13.08411 8.01708 14.10409
H 14.61791 8.42643 13.32390
H 13.10987 9.08503 12.68954
C 14.09561 7.26390 10.85622
H 15.17415 7.39717 10.99445
H 13.95476 6.44188 10.14729
H 13.70172 8.17693 10.39709
C 8.25805 4.52212 12.16416
C 7.57414 5.70504 12.49863
C 6.18418 5.62533 12.63178
H 5.62469 6.51943 12.89021
C 5.50580 4.43021 12.42470
H 4.42536 4.39389 12.53306
C 6.20614 3.28436 12.06667
H 5.66497 2.35877 11.89250
C 7.59675 3.30142 11.92607
C 8.26995 7.04937 12.63831
H 9.34924 6.87233 12.66188
C 7.90857 7.76362 13.94523
H 6.84534 8.02286 13.99145
H 8.15212 7.13845 14.80844
H 8.47627 8.69582 14.03171
C 7.96701 7.93437 11.41845
H 8.27006 7.45116 10.48366
H 6.89625 8.15516 11.34645
H 8.50051 8.88789 11.49608
C 8.32243 2.03920 11.47964
H 9.39909 2.23125 11.52070
C 7.96855 1.69438 10.02432
H 6.90196 1.46777 9.92086
H 8.19561 2.52061 9.34290
H 8.53074 0.81575 9.69037
C 8.04700 0.84507 12.40068
H 8.32455 1.07128 13.43312
H 6.99060 0.55685 12.39163
H 8.62644 -0.02487 12.07329
129
2 - Au with dispersion
Ta 9.30833 4.08401 17.59535
Au 10.44835 4.70685 14.97830
N 11.77495 4.55196 12.26006
N 9.64464 4.56273 12.01226
C 10.66302 5.27096 16.98040
C 11.72168 6.34775 17.15688
C 11.30484 7.64017 16.43264
H 11.12975 7.43997 15.37044
H 10.38212 8.04772 16.85031
H 12.08789 8.40455 16.52276
C 13.07697 5.90480 16.57674
H 13.42237 4.97351 17.03060
H 12.99914 5.73220 15.49962
H 13.84112 6.67477 16.74449
C 11.89360 6.66619 18.64916
H 10.93394 6.94363 19.09442
H 12.28534 5.80182 19.19064

H	12.59404	7.49883	18.79046
C	10.26835	2.48365	18.69042
H	9.40609	1.99830	19.19251
H	10.49711	1.82832	17.82466
C	11.45569	2.46374	19.66138
C	11.61978	1.05926	20.26121
H	10.72248	0.76320	20.81735
H	11.78495	0.31683	19.47193
H	12.47254	1.01572	20.94999
C	11.19398	3.45994	20.79625
H	11.10670	4.47828	20.40731
H	10.25889	3.21936	21.31606
H	12.00427	3.44481	21.53495
C	12.73437	2.84052	18.91434
H	12.97351	2.08751	18.15461
H	12.59501	3.79128	18.39798
H	13.58862	2.91949	19.59703
C	8.15524	5.21095	19.05424
H	7.57389	4.40283	19.54289
H	8.92263	5.49582	19.79750
C	7.21876	6.41055	18.82024
C	6.44880	6.73058	20.10975
H	5.83083	5.87910	20.41754
H	7.14136	6.95497	20.92859
H	5.78860	7.59691	19.97735
C	8.03939	7.63284	18.40801
H	8.75243	7.91018	19.19217
H	8.60867	7.40909	17.50372
H	7.39246	8.49742	18.21676
C	6.21100	6.10016	17.70713
H	6.71934	5.92928	16.75273
H	5.62200	5.20705	17.94147
H	5.51259	6.93453	17.56939
C	8.01106	3.16193	16.06305
H	7.33896	4.01780	15.85276
H	8.44836	2.93296	15.08275
C	7.14329	1.94981	16.49515
C	7.98485	0.66846	16.49239
H	8.45352	0.51180	15.51573
H	8.78216	0.71060	17.23877
H	7.36471	-0.20801	16.71516
C	6.53760	2.14428	17.89130
H	7.30461	2.18659	18.67253
H	5.95202	3.06719	17.94383
H	5.87374	1.30946	18.14552
C	5.98654	1.77648	15.50191
H	5.35327	2.66991	15.48344
H	6.36609	1.62781	14.48740
H	5.35895	0.91505	15.76468
C	10.61271	4.54409	12.96529
C	10.19070	4.59167	10.73780
H	9.57388	4.62037	9.85420
C	11.53848	4.57769	10.89478
H	12.34186	4.58488	10.17699
C	13.06784	4.57595	12.87797
C	13.53573	3.41558	13.51389
C	14.79135	3.48208	14.12170
H	15.17850	2.60550	14.63192
C	15.54790	4.64728	14.08384
H	16.52261	4.67547	14.56182
C	15.05438	5.78151	13.44997
H	15.64372	6.69295	13.44302
C	13.79438	5.77623	12.84809
C	12.74507	2.12375	13.54896
H	11.77953	2.30657	13.07198
C	12.46396	1.67705	14.98708
H	13.38752	1.41061	15.51181
H	11.96929	2.47385	15.55147
H	11.81203	0.79736	14.98889
C	13.45503	1.02862	12.74572
H	13.62101	1.33923	11.70918
H	14.42960	0.78435	13.18152
H	12.85423	0.11328	12.73762
C	13.24520	7.03645	12.20818
H	12.18197	6.87415	12.00339
C	13.34418	8.24127	13.14813
H	12.87954	8.02720	14.11245
H	14.38499	8.52748	13.33037
H	12.83953	9.10596	12.70515
C	13.94635	7.32270	10.87504

H 15.01630 7.49721 11.03079
H 13.84830 6.48555 10.17715
H 13.52443 8.21400 10.39942
C 8.24392 4.51731 12.31108
C 7.63211 5.65155 12.86093
C 6.26990 5.55729 13.16319
H 5.76246 6.41382 13.59504
C 5.55782 4.39397 12.90616
H 4.49942 4.34347 13.14391
C 6.19276 3.28903 12.34684
H 5.62231 2.38730 12.15556
C 7.55524 3.31955 12.05137
C 8.36532 6.96248 13.06581
H 9.43781 6.77250 12.96927
C 8.14113 7.53424 14.46601
H 7.09222 7.79189 14.64340
H 8.45876 6.81481 15.22604
H 8.73247 8.44491 14.60010
C 7.96577 7.96110 11.97261
H 8.17160 7.56130 10.97431
H 6.89675 8.19396 12.02506
H 8.52120 8.89763 12.08832
C 8.28500 2.09274 11.53202
H 9.07912 2.43153 10.85824
C 7.39146 1.14572 10.73181
H 6.64737 0.65641 11.36883
H 6.86182 1.66906 9.92975
H 7.99809 0.35419 10.28158
C 8.96180 1.34817 12.69030
H 9.58146 2.01637 13.29392
H 8.20756 0.91304 13.35176
H 9.59179 0.53645 12.31145
129
2 - Au 1 step tautomerisation TS
C 13.71868 3.59411 13.28156
C 13.13572 4.79130 12.82615
C 13.82135 6.02186 12.83196
C 15.13014 6.02746 13.32312
C 15.72692 4.86388 13.79370
C 15.02596 3.66430 13.77257
N 11.80929 4.75023 12.26626
C 10.63723 4.65692 12.96426
N 9.68106 4.65537 11.98978
C 10.24389 4.75083 10.72731
C 11.58464 4.80304 10.90127
C 8.26105 4.50718 12.17330
C 7.50094 5.62005 12.57455
C 6.11633 5.44799 12.67248
C 5.51673 4.23199 12.36770
C 6.29345 3.15492 11.95710
C 7.68272 3.26383 11.85185
C 8.11022 6.98783 12.83647
C 7.72779 7.53496 14.21686
C 8.49707 2.07152 11.36793
C 8.18200 1.75080 9.89860
Au 10.47907 4.72505 15.02170
Ta 9.31347 3.82416 17.74251
C 8.16345 5.00747 18.83136
C 7.55187 6.17144 19.58565
C 6.72570 7.06077 18.63537
C 13.20776 7.31443 12.31305
C 13.27445 8.44564 13.34785
C 13.01386 2.24867 13.21879
C 12.93595 1.57866 14.59675
C 13.87074 7.74801 10.99612
C 13.68733 1.32987 12.18766
C 10.68036 5.07020 17.08412
C 11.68930 6.17306 17.41653
C 11.17729 7.55020 16.95277
C 13.03162 5.88315 16.71833
C 11.97274 6.23093 18.92830
C 8.29749 0.83193 12.24862
C 7.72692 7.97225 11.72041
C 7.97118 2.87040 16.21054
C 6.94391 1.75206 16.57300
C 6.16973 2.06046 17.86383
C 10.06329 2.16248 18.99657
C 11.27394 2.00036 19.93482
C 11.16725 2.99816 21.09675
C 5.91459 1.62117 15.43646

C	7.65300	0.39947	16.73555
C	12.58028	2.22487	19.16251
C	11.29591	0.57499	20.51947
C	6.61271	5.58987	20.66229
C	8.60727	7.03567	20.28547
H	11.05617	6.35588	19.50639
H	12.46015	5.31243	19.26507
H	12.64044	7.07043	19.16202
H	10.98217	7.54576	15.87479
H	10.23909	7.81159	17.45427
H	11.90899	8.33840	17.17450
H	13.40748	4.89406	16.99732
H	12.93233	5.90545	15.62902
H	13.78190	6.62965	17.00964
H	9.16805	1.80770	19.53827
H	10.19265	1.44266	18.15732
H	10.38799	0.37549	21.10096
H	11.35306	-0.17561	19.72208
H	12.15815	0.42631	21.18243
H	11.17193	4.02915	20.73297
H	10.23247	2.84802	21.64951
H	11.99926	2.87591	21.80219
H	12.70326	1.46341	18.38226
H	12.58005	3.20091	18.66933
H	13.45071	2.16444	19.82778
H	7.33485	4.35001	18.45282
H	9.21983	5.61727	17.74115
H	9.22514	6.43132	20.95697
H	9.26512	7.52929	19.56390
H	8.12421	7.82075	20.87955
H	7.36462	7.50016	17.86190
H	5.94484	6.47839	18.13345
H	6.23941	7.87922	19.18186
H	5.82134	4.98251	20.20865
H	7.16835	4.95321	21.35784
H	6.13394	6.39415	21.23472
H	7.41776	3.71312	15.76276
H	8.59668	2.49384	15.38341
H	8.19344	0.12673	15.82110
H	8.37410	0.41629	17.55803
H	6.92976	-0.39844	16.94491
H	6.82752	2.10214	18.73935
H	5.64199	3.01888	17.78937
H	5.41747	1.28552	18.05809
H	5.35426	2.55416	15.30837
H	6.40576	1.39917	14.48437
H	5.19357	0.81858	15.64147
H	9.63890	4.76775	9.83520
H	12.39388	4.86907	10.19226
H	15.50289	2.75923	14.13716
H	16.74313	4.89175	14.17702
H	15.68667	6.95989	13.34179
H	11.98467	2.41784	12.88857
H	13.92996	1.33512	14.98731
H	12.43499	2.22885	15.32011
H	12.37172	0.64237	14.52824
H	13.70946	1.78828	11.19347
H	14.72049	1.10167	12.47148
H	13.14630	0.38054	12.11228
H	12.14865	7.12947	12.10728
H	12.80539	8.15309	14.29047
H	14.30754	8.73895	13.56228
H	12.75553	9.33227	12.96808
H	14.93434	7.96443	11.14418
H	13.79750	6.97242	10.22703
H	13.39616	8.65525	10.60719
H	5.49861	6.28661	12.98032
H	4.43850	4.12407	12.44601
H	5.81407	2.21038	11.71628
H	9.19904	6.88140	12.82638
H	6.65009	7.71137	14.30196
H	8.02688	6.84097	15.00743
H	8.23115	8.49121	14.39489
H	8.03815	7.60698	10.73617
H	6.64379	8.13326	11.68753
H	8.20329	8.94418	11.88832
H	9.55753	2.33537	11.42802
H	7.13488	1.45461	9.77414
H	8.35919	2.61207	9.24637
H	8.80651	0.92387	9.54404

H 8.54253 1.04521 13.29232
H 7.26519 0.46825 12.21233
H 8.94375 0.01753 11.90374
129
3 - Au
C 3.61982 -1.14025 -1.94735
C 3.17082 0.12336 -2.37341
C 3.92177 1.30089 -2.19348
C 5.15030 1.18259 -1.53696
C 5.61166 -0.04970 -1.08792
C 4.85605 -1.19682 -1.29581
N 1.92238 0.19751 -3.09110
C 0.67982 0.32391 -2.53795
N -0.15978 0.29337 -3.61367
C 0.53999 0.15041 -4.79907
C 1.85187 0.08455 -4.46945
C -1.59964 0.32321 -3.56656
C -2.25670 1.56323 -3.47714
C -3.65507 1.54825 -3.47243
C -4.36382 0.35598 -3.56218
C -3.68565 -0.85290 -3.66748
C -2.28848 -0.89966 -3.67442
C -1.51470 2.88961 -3.44150
C -1.95922 3.77051 -2.26775
C -1.57806 -2.23525 -3.83647
C -1.78377 -2.79334 -5.25362
Au 0.19192 0.77532 -0.58018
Ta -0.72684 -0.26851 2.21290
C -1.52411 0.09377 3.92095
C -2.16876 0.70088 5.14823
C -3.22192 -0.25736 5.73768
C 3.46676 2.64864 -2.73362
C 3.79143 3.81480 -1.79269
C 2.84826 -2.42108 -2.22432
C 2.71890 -3.31309 -0.98476
C 4.07725 2.91106 -4.12096
C 3.49161 -3.19334 -3.38758
C -0.22826 1.58230 1.34092
C 0.77635 2.68716 1.74644
C 0.77790 3.83699 0.72110
C 2.19906 2.12114 1.86573
C 0.37896 3.28565 3.10569
C -2.01055 -3.25774 -2.77908
C -1.66829 3.62883 -4.78007
C -2.28572 -1.28621 1.02312
C -3.67144 -1.82676 1.44373
C -4.58293 -0.65783 1.83646
C 0.97033 -1.63400 2.44242
C 1.53198 -2.41470 3.64967
C 0.47850 -3.38182 4.20691
C -4.32067 -2.57695 0.26613
C -3.54382 -2.80318 2.61985
C 1.97030 -1.43890 4.74966
C 2.75643 -3.23906 3.20960
C -1.11173 0.98154 6.23576
C -2.86217 2.02023 4.77094
H -0.62029 3.73202 3.05661
H 0.36488 2.51211 3.87781
H 1.08211 4.07299 3.40768
H 1.06744 3.48228 -0.27422
H -0.22075 4.28062 0.63623
H 1.47361 4.63286 1.01906
H 2.24832 1.34640 2.63876
H 2.52871 1.67219 0.92142
H 2.91207 2.90902 2.14044
H 0.77330 -2.35377 1.62158
H 1.77407 -0.98276 2.04152
H 2.48216 -3.97197 2.44144
H 3.53619 -2.59146 2.79196
H 3.19318 -3.78799 4.05373
H -0.39746 -2.84486 4.58439
H 0.13585 -4.07973 3.43350
H 0.88802 -3.97409 5.03433
H 2.76807 -0.77748 4.38983
H 1.13461 -0.80882 5.06813
H 2.35495 -1.97782 5.62450
H -1.33625 -1.02044 4.04487
H -1.24010 2.03539 1.24171
H -2.14442 2.73551 4.36264
H -3.63766 1.85152 4.01691

H -3.33400 2.47310 5.65189
H -4.01119 -0.47202 5.01105
H -2.76644 -1.20982 6.03375
H -3.68925 0.18047 6.62886
H -0.61958 0.05486 6.55049
H -0.34009 1.66403 5.86775
H -1.57449 1.43404 7.12274
H -2.43058 -0.63048 0.14450
H -1.69024 -2.13511 0.62191
H -2.88244 -3.64077 2.36458
H -3.13306 -2.30203 3.50036
H -4.52056 -3.22209 2.89265
H -4.13172 -0.08441 2.65080
H -4.73143 0.02144 0.98768
H -5.57001 -1.01285 2.15840
H -4.41577 -1.92552 -0.61038
H -3.72067 -3.44724 -0.02582
H -5.32386 -2.93848 0.52737
H 0.04172 0.10480 -5.75403
H 2.73317 -0.03863 -5.07789
H 5.23146 -2.15496 -0.94963
H 6.56847 -0.11609 -0.57741
H 5.75432 2.06929 -1.37380
H 1.83351 -2.14538 -2.52792
H 3.68628 -3.71685 -0.66781
H 2.28959 -2.76491 -0.14244
H 2.06927 -4.16676 -1.20500
H 3.53658 -2.59025 -4.30010
H 4.51480 -3.49534 -3.13834
H 2.91909 -4.10035 -3.60972
H 2.37708 2.61160 -2.84479
H 3.43810 3.62579 -0.77652
H 4.86747 4.01536 -1.74972
H 3.31027 4.72883 -2.15521
H 5.17067 2.94409 -4.06052
H 3.80686 2.13645 -4.84404
H 3.73224 3.87281 -4.51563
H -4.19552 2.48774 -3.40281
H -5.45016 0.36918 -3.55503
H -4.24863 -1.77838 -3.74549
H -0.45012 2.67825 -3.29889
H -3.00783 4.07310 -2.35881
H -1.83418 3.24674 -1.31588
H -1.35661 4.68416 -2.23444
H -1.30610 3.02518 -5.61874
H -2.71753 3.87476 -4.97695
H -1.10188 4.56621 -4.76740
H -0.50462 -2.06882 -3.70104
H -2.84240 -2.99692 -5.44771
H -1.43679 -2.09352 -6.02083
H -1.23482 -3.73274 -5.37911
H -1.85861 -2.87101 -1.76836
H -3.06793 -3.52346 -2.87892
H -1.42939 -4.17972 -2.88878
129
3 - Au with dispersion
C 3.48567 -1.20872 -1.76516
C 3.10392 0.06804 -2.19868
C 3.74958 1.24721 -1.79293
C 4.83304 1.10862 -0.92375
C 5.24294 -0.14584 -0.48116
C 4.57829 -1.29206 -0.89791
N 1.95278 0.15922 -3.05154
C 0.69580 0.31288 -2.56319
N -0.10379 0.21510 -3.65393
C 0.63582 0.00236 -4.80563
C 1.93838 -0.04182 -4.42269
C -1.53467 0.23806 -3.56185
C -2.18181 1.46980 -3.40504
C -3.57223 1.44478 -3.26258
C -4.26994 0.24345 -3.27397
C -3.59492 -0.96372 -3.43122
C -2.20790 -0.99397 -3.57588
C -1.43077 2.78608 -3.41897
C -1.79688 3.66576 -2.22158
C -1.44726 -2.30353 -3.67459
C -2.21959 -3.39333 -4.41869
Au 0.14870 0.87005 -0.68228
Ta -0.77606 -0.19379 1.92581
C -1.49232 0.03510 3.68089

C	-2.06346	0.54950	4.97392
C	-3.10385	-0.43880	5.52707
C	3.28687	2.60624	-2.28443
C	3.74438	3.75855	-1.39154
C	2.76941	-2.45934	-2.23505
C	2.48550	-3.43466	-1.09316
C	3.74554	2.85507	-3.72836
C	3.56676	-3.13813	-3.35586
C	-0.31333	1.70794	1.20227
C	0.73070	2.74520	1.63967
C	0.78365	3.91238	0.64164
C	2.11509	2.09461	1.74411
C	0.35130	3.30742	3.01502
C	-1.03907	-2.78358	-2.27623
C	-1.65894	3.51463	-4.74857
C	-2.39697	-1.03996	0.72718
C	-3.76247	-1.56740	1.19604
C	-4.57619	-0.41450	1.78833
C	0.89674	-1.59878	1.97231
C	1.58410	-2.26176	3.17727
C	0.60646	-3.18046	3.91694
C	-4.52878	-2.15449	0.00093
C	-3.57652	-2.66496	2.24771
C	2.09706	-1.17998	4.13307
C	2.77500	-3.10469	2.69424
C	-0.94544	0.72245	6.01691
C	-2.74065	1.90347	4.72416
H	-0.63635	3.77932	2.98071
H	0.31432	2.50276	3.75343
H	1.07552	4.06210	3.34691
H	1.04617	3.55825	-0.36087
H	-0.19438	4.40104	0.57261
H	1.51990	4.66725	0.94573
H	2.10702	1.29338	2.48983
H	2.42120	1.65349	0.78881
H	2.87367	2.82679	2.04787
H	0.55690	-2.38952	1.27462
H	1.65948	-1.03516	1.39979
H	2.44010	-3.91316	2.03445
H	3.48406	-2.48539	2.13272
H	3.31278	-3.55857	3.53612
H	-0.21867	-2.61079	4.35405
H	0.17788	-3.92606	3.23666
H	1.11050	-3.71514	4.73053
H	2.85405	-0.55849	3.64070
H	1.27580	-0.52776	4.44631
H	2.55640	-1.62227	5.02539
H	-1.32530	-1.08746	3.70147
H	-1.31103	2.18567	1.11135
H	-2.02497	2.62265	4.32094
H	-3.55592	1.79967	4.00173
H	-3.15322	2.30849	5.65610
H	-3.92027	-0.58712	4.81449
H	-2.64658	-1.41557	5.72387
H	-3.53089	-0.07061	6.46799
H	-0.45090	-0.23446	6.21443
H	-0.18738	1.42469	5.65803
H	-1.34712	1.10238	6.96516
H	-2.56073	-0.31332	-0.08994
H	-1.85131	-1.86941	0.23642
H	-2.97320	-3.48921	1.84727
H	-3.06876	-2.27076	3.13154
H	-4.54186	-3.07712	2.56504
H	-4.02926	0.03185	2.62303
H	-4.74114	0.36733	1.03665
H	-5.55621	-0.75627	2.14304
H	-4.66001	-1.39956	-0.78116
H	-3.98301	-2.99897	-0.43761
H	-5.52147	-2.51668	0.29704
H	0.16964	-0.10023	-5.77215
H	2.84302	-0.20117	-4.98604
H	4.90053	-2.26330	-0.53702
H	6.08305	-0.22695	0.20229
H	5.35285	1.99252	-0.57296
H	1.80098	-2.15932	-2.64653
H	3.40569	-3.85142	-0.67188
H	1.93877	-2.94421	-0.28567
H	1.88603	-4.27415	-1.45881
H	3.73306	-2.46093	-4.19913
H	4.54747	-3.46151	-2.99109

H 3.03469 -4.02029 -3.72646
H 2.18913 2.59334 -2.27311
H 3.49747 3.58191 -0.34295
H 4.82453 3.92285 -1.47211
H 3.25104 4.68399 -1.70201
H 4.83895 2.83466 -3.78899
H 3.35359 2.10647 -4.42005
H 3.40502 3.83739 -4.07166
H -4.11094 2.37872 -3.13831
H -5.34925 0.24431 -3.15368
H -4.15295 -1.89317 -3.42423
H -0.36210 2.56484 -3.34013
H -2.84105 3.99255 -2.26193
H -1.63966 3.12629 -1.28332
H -1.16976 4.56261 -2.20686
H -1.34898 2.89770 -5.59810
H -2.71762 3.76053 -4.88364
H -1.08900 4.44903 -4.77752
H -0.52666 -2.11696 -4.23888
H -3.09024 -3.73288 -3.84860
H -2.56758 -3.04634 -5.39653
H -1.57702 -4.26553 -4.57283
H -0.47085 -2.01939 -1.73805
H -1.92760 -3.01009 -1.68070
H -0.42825 -3.68960 -2.34409
129
2 - Au 2 steps tautomerisation TS - First H trans.
C 4.30919 -0.41619 -1.46842
C 3.51859 0.52945 -2.15166
C 3.89097 1.88115 -2.27908
C 5.08596 2.28113 -1.67227
C 5.87381 1.37655 -0.97309
C 5.48865 0.04391 -0.87642
N 2.32203 0.08440 -2.82478
C 1.06239 -0.00093 -2.29455
N 0.29727 -0.41738 -3.34767
C 1.05536 -0.57452 -4.49547
C 2.32892 -0.25827 -4.16692
C -1.12946 -0.62588 -3.36560
C -1.96187 0.46801 -3.66418
C -3.33186 0.21887 -3.78936
C -3.84760 -1.06134 -3.63191
C -3.00036 -2.12293 -3.33680
C -1.62252 -1.93311 -3.19673
C -1.43105 1.87425 -3.89028
C -2.08767 2.88908 -2.94597
C -0.71358 -3.12158 -2.92504
C -0.46778 -3.92532 -4.21251
Au 0.43907 0.60052 -0.42948
Ta -1.23174 0.16675 2.20105
C -1.95280 0.82774 4.19098
C -1.60831 0.30639 5.60434
C -2.17092 1.26735 6.66810
C 3.08088 2.88532 -3.08560
C 2.91086 4.22878 -2.36573
C 3.94240 -1.89254 -1.41483
C 4.45922 -2.60069 -0.15831
C 3.71199 3.10346 -4.47097
C 4.45381 -2.63023 -2.66492
C -0.07505 1.52354 1.39251
C 0.52523 2.92078 1.57933
C 0.05662 3.86902 0.45906
C 2.06187 2.81738 1.55517
C 0.11508 3.55112 2.92126
C -1.25366 -4.03692 -1.81960
C -1.59492 2.29384 -5.35892
C -2.79109 0.51750 0.93153
C -4.26385 0.16801 1.24263
C -4.40951 -0.99798 2.23473
C -0.64461 -1.96075 1.80137
C 0.60621 -2.69794 2.35563
C 0.31022 -3.30498 3.73468
C -5.00606 1.40401 1.78498
C -4.93484 -0.25965 -0.07488
C 1.80926 -1.75176 2.47358
C 0.98486 -3.85387 1.41173
C -2.24489 -1.07457 5.81812
C -0.08758 0.21677 5.79462
H -0.97192 3.66993 2.98724
H 0.44440 2.93587 3.76447

H 0.56515 4.54559 3.03368
H 0.33636 3.47970 -0.52489
H -1.03373 3.97893 0.47540
H 0.49698 4.86756 0.58041
H 2.41670 2.15029 2.34757
H 2.41749 2.41368 0.60129
H 2.51768 3.80446 1.70899
H -1.53145 -2.58927 1.99777
H -0.57034 -1.93973 0.70010
H 0.14863 -4.55338 1.29788
H 1.24155 -3.47512 0.41560
H 1.84665 -4.41883 1.79154
H 0.06428 -2.53626 4.47258
H -0.53583 -4.00095 3.68378
H 1.17717 -3.86021 4.11443
H 2.02136 -1.26552 1.51544
H 1.62216 -0.94974 3.19717
H 2.70700 -2.29227 2.80153
H -3.04878 0.91486 4.11991
H -1.60311 1.87561 4.12027
H 0.36913 -0.47034 5.07423
H 0.38264 1.19791 5.66097
H 0.16790 -0.14102 6.79993
H -1.73355 2.26724 6.56506
H -3.25800 1.36728 6.56878
H -1.95782 0.91028 7.68415
H -3.33701 -1.01355 5.74073
H -1.90009 -1.79524 5.06982
H -2.00377 -1.47531 6.81053
H -1.73697 1.62685 1.23541
H -2.74520 0.97509 -0.06151
H -4.90509 0.55131 -0.81107
H -4.42345 -1.12385 -0.51044
H -5.98660 -0.52757 0.08996
H -3.93016 -1.90031 1.84037
H -3.96480 -0.77581 3.20921
H -5.46844 -1.22713 2.40883
H -4.57117 1.74602 2.72973
H -4.94557 2.23377 1.07173
H -6.06817 1.18442 1.95912
H 0.61659 -0.88702 -5.42920
H 3.23228 -0.24192 -4.75458
H 6.11645 -0.65279 -0.33151
H 6.79574 1.70896 -0.50390
H 5.40036 3.31731 -1.74970
H 2.84821 -1.95893 -1.40230
H 5.54793 -2.72382 -0.17972
H 4.19116 -2.06080 0.75255
H 4.02431 -3.60246 -0.09486
H 4.03416 -2.22309 -3.58841
H 5.54544 -2.56226 -2.73095
H 4.18508 -3.69097 -2.61630
H 2.07941 2.46778 -3.23329
H 2.50712 4.09775 -1.35938
H 3.85904 4.77084 -2.28378
H 2.22293 4.86821 -2.92864
H 4.72090 3.52025 -4.37677
H 3.79037 2.17146 -5.03864
H 3.11189 3.80583 -5.05945
H -4.00198 1.04201 -4.02007
H -4.91518 -1.23289 -3.73654
H -3.41463 -3.11888 -3.21513
H -0.36063 1.87351 -3.66275
H -3.16307 2.98046 -3.13219
H -1.94474 2.59892 -1.90155
H -1.64402 3.88028 -3.08861
H -1.09065 1.59651 -6.03577
H -2.65135 2.32963 -5.64632
H -1.17168 3.29080 -5.52227
H 0.25083 -2.73240 -2.58120
H -1.40778 -4.33032 -4.60328
H -0.01788 -3.31199 -4.99929
H 0.20497 -4.76721 -4.01647
H -1.45543 -3.48003 -0.90117
H -2.17574 -4.54373 -2.12383
H -0.51875 -4.81476 -1.58946
129
2 - Au 2 steps tautomerisation TS - Intermediate.
C 4.02329 -0.28933 -1.51672
C 3.26741 0.62418 -2.27715

C	3.67918	1.95115	-2.50288
C	4.88407	2.36027	-1.92161
C	5.64125	1.48786	-1.15172
C	5.21416	0.17860	-0.95501
N	2.04999	0.17835	-2.90956
C	0.80744	0.15605	-2.33881
N	-0.01613	-0.19127	-3.36974
C	0.69428	-0.38136	-4.54411
C	1.99565	-0.14992	-4.25384
C	-1.45506	-0.27455	-3.35162
C	-2.19716	0.90870	-3.52511
C	-3.58672	0.78663	-3.61919
C	-4.20659	-0.45574	-3.56203
C	-3.44632	-1.60679	-3.39231
C	-2.05449	-1.54461	-3.27788
C	-1.55460	2.28051	-3.65197
C	-2.02893	3.23413	-2.54749
C	-1.25196	-2.82309	-3.10092
C	-1.26229	-3.66811	-4.38389
Au	0.37358	0.63424	-0.37366
Ta	-0.74574	-0.43500	2.35671
C	-0.60409	-0.33644	4.53312
C	-1.63925	-0.04687	5.64132
C	-0.93744	-0.02266	7.01182
C	2.89939	2.92489	-3.37484
C	2.58971	4.24278	-2.65322
C	3.60040	-1.74123	-1.35246
C	4.08328	-2.36794	-0.04159
C	3.64502	3.18878	-4.69285
C	4.08310	-2.58404	-2.54580
C	0.09961	1.34055	1.60823
C	1.29908	2.16774	2.14139
C	1.80798	3.18129	1.09892
C	2.46585	1.24306	2.52234
C	0.86216	2.97164	3.37857
C	-1.74891	-3.64216	-1.90257
C	-1.79712	2.87743	-5.04653
C	-2.63932	-0.60744	1.98133
C	-3.97255	-0.05812	1.51717
C	-3.85288	1.43872	1.19804
C	0.33650	-2.28520	1.82399
C	0.25271	-3.70937	2.43438
C	-1.19834	-4.09465	2.75753
C	-4.42594	-0.80412	0.24885
C	-5.04772	-0.25317	2.60406
C	1.09767	-3.79643	3.71393
C	0.81118	-4.73578	1.43131
C	-2.30365	1.31545	5.40147
C	-2.71238	-1.14159	5.66085
H	0.05944	3.67245	3.12113
H	0.49057	2.31859	4.17164
H	1.69944	3.55567	3.78161
H	2.22582	2.66783	0.22639
H	0.99221	3.82878	0.75688
H	2.59349	3.82131	1.52345
H	2.18094	0.54875	3.32197
H	2.78739	0.65204	1.65695
H	3.32847	1.82014	2.87870
H	0.03106	-2.34816	0.76099
H	1.39934	-1.98366	1.78913
H	0.22445	-4.73809	0.50582
H	1.84945	-4.50216	1.17060
H	0.79101	-5.75248	1.84461
H	-1.62347	-3.44416	3.52977
H	-1.83326	-4.01898	1.86732
H	-1.25807	-5.12723	3.12387
H	2.14851	-3.56115	3.50684
H	0.74747	-3.10168	4.48337
H	1.05904	-4.80676	4.13904
H	0.30018	0.27187	4.72153
H	-0.78731	2.00665	1.52819
H	-3.19764	-1.22032	4.68397
H	-2.27180	-2.11679	5.90457
H	-3.48077	-0.92739	6.41396
H	-0.44330	-0.97986	7.21721
H	-0.17277	0.76258	7.04893
H	-1.65072	0.16705	7.82408
H	-1.56257	2.12298	5.40314
H	-2.81085	1.32504	4.43164
H	-3.04110	1.53869	6.18296

H -0.24099 -1.37901 4.66710
H -2.67874 -1.70588 2.18584
H -5.16057 -1.31346 2.85828
H -4.78667 0.28560 3.51956
H -6.02277 0.11448 2.25818
H -3.54020 2.00466 2.08250
H -3.11251 1.60536 0.40894
H -4.81307 1.84604 0.85760
H -3.69009 -0.68946 -0.55133
H -4.54377 -1.87561 0.44928
H -5.39108 -0.42214 -0.11064
H 0.20610 -0.65515 -5.46551
H 2.87971 -0.17838 -4.87017
H 5.81859 -0.49196 -0.35378
H 6.57171 1.82616 -0.70414
H 5.22969 3.37824 -2.07609
H 2.50479 -1.76566 -1.33888
H 5.17042 -2.50427 -0.02693
H 3.80089 -1.76274 0.82426
H 3.63547 -3.35830 0.07925
H 3.68839 -2.21495 -3.49673
H 5.17699 -2.57358 -2.60868
H 3.76155 -3.62483 -2.43215
H 1.93900 2.46348 -3.62553
H 2.03201 4.06947 -1.72978
H 3.50218 4.79169 -2.39803
H 1.98944 4.89142 -3.30015
H 4.61105 3.67133 -4.50930
H 3.83881 2.26249 -5.24298
H 3.05872 3.85012 -5.33964
H -4.18973 1.68066 -3.74957
H -5.28742 -0.52721 -3.64409
H -3.94135 -2.57205 -3.34095
H -0.47375 2.16202 -3.52889
H -3.10777 3.41418 -2.60413
H -1.80311 2.82873 -1.55706
H -1.52618 4.20260 -2.64280
H -1.42796 2.21592 -5.83701
H -2.86336 3.04974 -5.22859
H -1.28517 3.84082 -5.14317
H -0.21378 -2.54424 -2.89337
H -2.27947 -3.98373 -4.64042
H -0.86204 -3.11417 -5.23927
H -0.65579 -4.57055 -4.25258
H -1.75191 -3.04290 -0.98805
H -2.76486 -4.01876 -2.06217
H -1.09988 -4.51001 -1.74633
129
2 - Au 2 steps tautomerisation TS - Second H trans.
C 4.20519 -0.03763 -1.67591
C 3.42025 0.82956 -2.45942
C 3.77418 2.16991 -2.70127
C 4.95639 2.63868 -2.11878
C 5.74600 1.81008 -1.33252
C 5.37281 0.48762 -1.11585
N 2.22880 0.31960 -3.09064
C 0.99396 0.23366 -2.51256
N 0.18580 -0.17780 -3.53286
C 0.89966 -0.34121 -4.70949
C 2.18748 -0.03153 -4.42976
C -1.24198 -0.36628 -3.47900
C -2.07580 0.76102 -3.59950
C -3.45595 0.53884 -3.63006
C -3.98195 -0.74521 -3.55717
C -3.13317 -1.83985 -3.44449
C -1.74527 -1.67819 -3.40032
C -1.54408 2.17880 -3.73452
C -2.07107 3.09277 -2.62030
C -0.84485 -2.89981 -3.30242
C -0.80709 -3.66576 -4.63434
Au 0.50558 0.77340 -0.57707
Ta -0.86651 -0.20957 2.07887
C -0.90331 -0.05380 4.06839
C -1.42694 0.14122 5.48329
C -2.00474 -1.17483 6.04214
C 2.95071 3.09870 -3.58166
C 2.55467 4.39043 -2.85456
C 3.83658 -1.50018 -1.48220
C 4.24290 -2.04809 -0.11116
C 3.69438 3.41424 -4.88888

C	4.44290	-2.36128	-2.60328
C	0.02859	1.55961	1.32296
C	1.10556	2.46292	1.97083
C	1.67359	3.47666	0.96047
C	2.26955	1.61838	2.51022
C	0.47925	3.25347	3.13119
C	-1.25970	-3.83168	-2.15717
C	-1.86081	2.75316	-5.12383
C	-2.82343	-0.42924	1.76116
C	-4.16502	0.27547	1.67225
C	-4.01079	1.78687	1.89245
C	0.26486	-2.05702	1.60319
C	0.26867	-3.39784	2.38039
C	-1.16394	-3.83002	2.72363
C	-4.71864	0.03829	0.25374
C	-5.17050	-0.30099	2.68716
C	1.08333	-3.27579	3.67503
C	0.91623	-4.49290	1.51265
C	-0.26713	0.59248	6.39036
C	-2.52060	1.21879	5.51767
H	-0.31602	3.91540	2.76629
H	0.03784	2.56924	3.86151
H	1.22832	3.87760	3.63570
H	2.19995	2.96155	0.14870
H	0.86970	4.07691	0.51784
H	2.38221	4.16374	1.44286
H	1.92923	0.93768	3.29923
H	2.71547	1.01866	1.70799
H	3.05642	2.25331	2.93709
H	-0.10584	-2.25745	0.57851
H	1.31138	-1.74118	1.44679
H	0.36037	-4.63558	0.57889
H	1.94669	-4.22588	1.25119
H	0.94373	-5.45667	2.03738
H	-1.63989	-3.10257	3.38979
H	-1.77803	-3.91631	1.81842
H	-1.17453	-4.80591	3.22532
H	2.11687	-2.97692	3.46218
H	0.64844	-2.53354	4.35038
H	1.11674	-4.23398	4.20797
H	0.11793	-0.50675	4.08108
H	-0.86136	2.18705	1.09417
H	-2.13934	2.17408	5.14367
H	-3.37873	0.93347	4.90178
H	-2.88421	1.36862	6.54174
H	-2.84480	-1.52321	5.43068
H	-1.24581	-1.96455	6.04907
H	-2.36668	-1.04316	7.07028
H	0.52763	-0.16216	6.41668
H	0.17049	1.52906	6.03095
H	-0.61503	0.74984	7.41874
H	-2.16761	-0.50732	3.30361
H	-2.93411	-1.52542	1.61524
H	-5.30704	-1.37745	2.53190
H	-4.82884	-0.15406	3.71656
H	-6.15133	0.18093	2.58660
H	-3.58321	2.00610	2.87516
H	-3.34824	2.21909	1.13547
H	-4.98170	2.29271	1.82397
H	-4.02875	0.42527	-0.50140
H	-4.86219	-1.03099	0.06070
H	-5.68934	0.53572	0.12953
H	0.42486	-0.65284	-5.62579
H	3.06885	-0.01912	-5.05059
H	6.00091	-0.14694	-0.49932
H	6.65853	2.19461	-0.88531
H	5.25822	3.66899	-2.28354
H	2.74583	-1.57620	-1.54784
H	5.33025	-2.13181	-0.00605
H	3.86698	-1.41832	0.69994
H	3.83015	-3.05249	0.02190
H	4.10446	-2.04089	-3.59338
H	5.53702	-2.30290	-2.58788
H	4.15905	-3.41141	-2.47536
H	2.02266	2.58221	-3.84669
H	1.99901	4.17599	-1.93845
H	3.43054	4.98963	-2.58437
H	1.92384	5.00770	-3.50327
H	4.62563	3.95647	-4.69225
H	3.95262	2.50396	-5.43941

H 3.07547 4.04016 -5.54057
H -4.12740 1.38799 -3.71956
H -5.05774 -0.89341 -3.58699
H -3.55385 -2.83932 -3.38826
H -0.45534 2.14541 -3.63127
H -3.16013 3.20076 -2.66595
H -1.80631 2.69915 -1.63449
H -1.63597 4.09336 -2.71592
H -1.45226 2.12488 -5.92210
H -2.94117 2.83433 -5.28536
H -1.43364 3.75623 -5.22897
H 0.17120 -2.55361 -3.08641
H -1.80153 -4.04162 -4.89909
H -0.46234 -3.03407 -5.45903
H -0.13202 -4.52528 -4.56349
H -1.31039 -3.29334 -1.20731
H -2.23739 -4.29058 -2.33884
H -0.53369 -4.64453 -2.05191
129
2 - Ag
Ta 9.33747 4.13332 17.84310
Ag 10.37916 4.71055 15.05759
N 11.80547 4.52961 12.26111
N 9.68784 4.56893 11.93749
C 10.58508 5.36169 17.12116
C 11.57069 6.51698 17.24279
C 11.07764 7.74885 16.45758
H 10.97692 7.51402 15.39144
H 10.09879 8.07595 16.81885
H 11.78039 8.58737 16.56094
C 12.96624 6.13272 16.71413
H 13.36655 5.26948 17.25247
H 12.92649 5.86630 15.65239
H 13.67211 6.96657 16.83070
C 11.71514 6.92672 18.72150
H 10.74993 7.22942 19.13727
H 12.09696 6.09590 19.32183
H 12.41203 7.76875 18.82661
C 10.39051 2.60295 18.98990
H 9.52842 2.12336 19.50173
H 10.60335 1.93162 18.12911
C 11.58460 2.54240 19.96207
C 11.74496 1.10827 20.50099
H 10.84493 0.78564 21.03826
H 11.91622 0.39929 19.68224
H 12.59316 1.03261 21.19338
C 11.33369 3.48423 21.14823
H 11.25203 4.52338 20.81443
H 10.40189 3.22546 21.66582
H 12.14928 3.42622 21.87979
C 12.87779 2.94432 19.24726
H 13.10078 2.25300 18.42582
H 12.78256 3.94421 18.81865
H 13.73071 2.93367 19.93718
C 8.20300 5.26617 19.33330
H 7.78587 4.43340 19.93920
H 9.05365 5.64364 19.93568
C 7.13207 6.37659 19.26027
C 6.74056 6.81318 20.68468
H 6.34141 5.96869 21.25885
H 7.60938 7.20379 21.22690
H 5.97442 7.59904 20.66604
C 7.66628 7.59845 18.50293
H 8.55540 8.00885 18.99393
H 7.94708 7.33230 17.47933
H 6.91069 8.39348 18.46285
C 5.87062 5.86679 18.54911
H 6.08912 5.55800 17.52084
H 5.43865 5.00821 19.07637
H 5.10255 6.64918 18.50819
C 8.01694 3.13377 16.35584
H 7.31618 3.99065 16.24023
H 8.38739 2.96454 15.33387
C 7.18078 1.88394 16.75779
C 8.04125 0.61636 16.65527
H 8.44390 0.49348 15.64338
H 8.88834 0.64960 17.34769
H 7.45235 -0.27896 16.88989
C 6.62345 1.99241 18.18560
H 7.41850 2.02010 18.93959

H 6.01151 2.89211 18.30549
H 5.99234 1.12664 18.42184
C 5.98293 1.74361 15.80052
H 5.31494 2.60903 15.88169
H 6.31513 1.68194 14.75929
H 5.39493 0.84340 16.02386
C 10.61818 4.55303 12.93636
C 10.27889 4.55903 10.68435
H 9.69650 4.57157 9.77711
C 11.61659 4.52557 10.88897
H 12.44268 4.49553 10.19691
C 13.11660 4.50113 12.85656
C 13.58905 3.29291 13.40270
C 14.88074 3.29193 13.93809
H 15.27285 2.37697 14.37245
C 15.67293 4.43305 13.91574
H 16.67453 4.40667 14.33584
C 15.18708 5.60672 13.35197
H 15.81567 6.49224 13.33487
C 13.89935 5.67185 12.81204
C 12.78496 2.00271 13.39058
H 11.78360 2.22947 13.01326
C 12.61151 1.42230 14.79995
H 13.57027 1.12220 15.23663
H 12.14772 2.15231 15.47040
H 11.97325 0.53298 14.76579
C 13.41827 0.97629 12.43861
H 13.50817 1.37223 11.42167
H 14.42092 0.68832 12.77294
H 12.80821 0.06751 12.39693
C 13.41260 6.97014 12.18398
H 12.34551 6.86124 11.96449
C 13.55824 8.16880 13.13076
H 13.05463 7.98969 14.08345
H 14.60860 8.39483 13.34239
H 13.11940 9.06189 12.67309
C 14.13854 7.24291 10.85696
H 15.21388 7.37496 11.01886
H 14.01263 6.42239 10.14341
H 13.75569 8.15727 10.39131
C 8.25893 4.53405 12.11078
C 7.57973 5.71696 12.45566
C 6.18885 5.64331 12.58439
H 5.63332 6.53764 12.85031
C 5.50505 4.45350 12.36563
H 4.42428 4.42152 12.47172
C 6.20083 3.30698 12.00082
H 5.65576 2.38507 11.81962
C 7.59173 3.31835 11.86284
C 8.28187 7.05576 12.61634
H 9.36045 6.87320 12.64046
C 7.91674 7.75449 13.93112
H 6.85611 8.02497 13.97064
H 8.14152 7.11651 14.79048
H 8.49376 8.67883 14.03706
C 7.98909 7.95961 11.40793
H 8.29425 7.48795 10.46801
H 6.91975 8.18644 11.33432
H 8.52680 8.90928 11.50158
C 8.31211 2.05478 11.41201
H 9.38963 2.24130 11.45629
C 7.96010 1.71874 9.95424
H 6.89260 1.49843 9.84676
H 8.19378 2.54707 9.27763
H 8.51841 0.83867 9.61763
C 8.02763 0.85824 12.32744
H 8.30479 1.07716 13.36167
H 6.96941 0.57706 12.31576
H 8.60173 -0.01403 11.99685
129
2 - Ag with dispersion
Ta 9.31208 4.08900 17.65947
Ag 10.37127 4.65118 15.01053
N 11.75576 4.56892 12.24576
N 9.63449 4.58836 11.97453
C 10.63865 5.28257 17.05478
C 11.69286 6.36952 17.12566
C 11.23225 7.62774 16.36931
H 11.02882 7.38785 15.31940
H 10.31560 8.03402 16.80136

H	12.00388	8.40823	16.40553
C	13.02193	5.91122	16.49995
H	13.40263	5.00904	16.98315
H	12.89073	5.68115	15.43828
H	13.78505	6.69590	16.58409
C	11.93646	6.75024	18.59468
H	10.99895	7.04906	19.07212
H	12.34807	5.90456	19.15124
H	12.64606	7.58403	18.67038
C	10.31791	2.48365	18.72374
H	9.47964	1.97297	19.24143
H	10.55847	1.82946	17.86107
C	11.51883	2.50965	19.67938
C	11.71993	1.12502	20.31280
H	10.83711	0.82667	20.89057
H	11.88685	0.36543	19.54030
H	12.58396	1.11510	20.98894
C	11.25567	3.53150	20.79101
H	11.15135	4.53736	20.37383
H	10.32920	3.29318	21.32710
H	12.07375	3.54735	21.52130
C	12.77942	2.89439	18.90620
H	13.02478	2.12827	18.16139
H	12.60953	3.82975	18.37080
H	13.64103	3.00821	19.57472
C	8.15788	5.20469	19.13296
H	7.58299	4.39412	19.62639
H	8.94005	5.48324	19.86338
C	7.22037	6.40754	18.92909
C	6.51579	6.75277	20.24946
H	5.91258	5.90837	20.60272
H	7.24897	6.98921	21.02861
H	5.85134	7.61861	20.13544
C	8.02646	7.61866	18.45860
H	8.78271	7.89804	19.20030
H	8.54678	7.37975	17.52887
H	7.37685	8.48666	18.29260
C	6.15647	6.08505	17.87334
H	6.61650	5.89209	16.89887
H	5.57480	5.20017	18.15435
H	5.45663	6.92113	17.75412
C	8.03076	3.22149	16.06720
H	7.33734	4.07750	15.93905
H	8.40780	3.04358	15.05013
C	7.19318	1.97841	16.46934
C	8.06282	0.71767	16.41116
H	8.52022	0.60614	15.42318
H	8.86994	0.75513	17.14746
H	7.46712	-0.18065	16.61264
C	6.60909	2.12000	17.88084
H	7.38855	2.15132	18.65065
H	6.00924	3.03098	17.97067
H	5.96445	1.26648	18.12184
C	6.02402	1.81643	15.48918
H	5.37144	2.69592	15.51516
H	6.38967	1.71547	14.46369
H	5.41876	0.93254	15.72870
C	10.58815	4.54492	12.93912
C	10.19178	4.64908	10.70582
H	9.58468	4.69883	9.81627
C	11.53784	4.62773	10.87784
H	12.34950	4.65102	10.16950
C	13.04200	4.55887	12.87733
C	13.46788	3.38868	13.52627
C	14.71479	3.42334	14.15462
H	15.06814	2.53919	14.67617
C	15.50559	4.56549	14.12205
H	16.47269	4.56864	14.61596
C	15.05575	5.70838	13.47182
H	15.67164	6.60217	13.46761
C	13.80565	5.73632	12.85039
C	12.64531	2.11614	13.55502
H	11.69721	2.31508	13.05041
C	12.31828	1.69208	14.99050
H	13.22120	1.40265	15.53818
H	11.84008	2.50717	15.54443
H	11.63796	0.83437	14.98759
C	13.34811	0.99374	12.78390
H	13.54838	1.28723	11.74852
H	14.30440	0.73003	13.24780

H 12.72442 0.09388 12.77120
C 13.30679 7.01153 12.19866
H 12.25005 6.87294 11.94890
C 13.39014 8.20548 13.15429
H 12.87119 7.99594 14.09159
H 14.42763 8.46049 13.39283
H 12.93248 9.08767 12.69493
C 14.06710 7.29428 10.89773
H 15.13258 7.44999 11.09751
H 13.98423 6.46280 10.19086
H 13.68002 8.19549 10.41136
C 8.23081 4.50975 12.25426
C 7.58806 5.61472 12.82786
C 6.22300 5.48618 13.10474
H 5.69257 6.32066 13.55203
C 5.53769 4.31691 12.80634
H 4.47722 4.23956 13.02668
C 6.20447 3.23802 12.23338
H 5.65754 2.32723 12.01645
C 7.56997 3.30431 11.95829
C 8.29364 6.92908 13.09707
H 9.36988 6.76834 12.98595
C 8.05909 7.42017 14.52661
H 7.00278 7.63095 14.72045
H 8.40325 6.67674 15.25247
H 8.61922 8.34253 14.70553
C 7.86842 7.97659 12.06096
H 8.07643 7.63512 11.04176
H 6.79548 8.18536 12.13085
H 8.40592 8.91635 12.22465
C 8.33137 2.09731 11.43942
H 9.17190 2.45725 10.83744
C 7.49273 1.18715 10.54243
H 6.70448 0.67684 11.10534
H 7.02140 1.74573 9.72793
H 8.12661 0.41085 10.10326
C 8.92129 1.30989 12.61657
H 9.50417 1.95574 13.27887
H 8.12078 0.86246 13.21272
H 9.57039 0.50419 12.25757
129
2 - Ag 1 step tautomerisation TS
C 13.64645 3.50812 13.27417
C 13.11395 4.72855 12.81771
C 13.84015 5.93551 12.85292
C 15.13423 5.89333 13.37948
C 15.67918 4.70684 13.85587
C 14.94111 3.53092 13.80209
N 11.79590 4.73771 12.23762
C 10.61777 4.65293 12.92349
N 9.67474 4.69079 11.93860
C 10.24895 4.80232 10.68258
C 11.58928 4.82292 10.87088
C 8.25220 4.55516 12.11582
C 7.50522 5.66180 12.55830
C 6.12013 5.49832 12.66499
C 5.50727 4.29601 12.33372
C 6.27066 3.22491 11.88473
C 7.65948 3.32614 11.76594
C 8.12893 7.01622 12.85560
C 7.72765 7.54994 14.23615
C 8.45685 2.13924 11.24212
C 8.11324 1.85174 9.77244
Ag 10.40575 4.67648 15.05436
Ta 9.33140 3.81262 17.79765
C 8.15480 4.95594 18.90790
C 7.51439 6.10422 19.66200
C 6.53740 6.87207 18.74908
C 13.28510 7.25169 12.32694
C 13.37371 8.37847 13.36496
C 12.90474 2.18469 13.17274
C 12.75161 1.50583 14.54009
C 13.99040 7.66251 11.02474
C 13.59189 1.25288 12.16244
C 10.64462 5.09726 17.17796
C 11.64104 6.23013 17.39869
C 11.10986 7.56553 16.84370
C 12.96927 5.89336 16.69365
C 11.95802 6.40920 18.89587
C 8.26423 0.88354 12.10137

C	7.78047	8.02334	11.74823
C	8.00705	2.90135	16.20161
C	7.04126	1.72102	16.53803
C	6.28327	1.93778	17.85697
C	10.15022	2.14313	19.01772
C	11.31456	2.08992	20.02620
C	11.07118	3.10250	21.15439
C	5.99282	1.58843	15.41916
C	7.82002	0.40036	16.62773
C	12.64125	2.40022	19.32140
C	11.41302	0.68316	20.64663
C	6.72429	5.50919	20.84558
C	8.55026	7.08665	20.21836
H	11.05778	6.62234	19.47333
H	12.41330	5.50380	19.30521
H	12.66173	7.23885	19.04429
H	10.90943	7.48700	15.76874
H	10.17141	7.84811	17.33251
H	11.83284	8.37628	17.00500
H	13.36743	4.93944	17.05246
H	12.84200	5.81207	15.60901
H	13.71661	6.67306	16.89022
H	9.26115	1.70731	19.51030
H	10.38827	1.43928	18.19026
H	10.49092	0.42445	21.18059
H	11.57461	-0.07657	19.87248
H	12.24400	0.61598	21.36108
H	11.01987	4.12226	20.76181
H	10.11984	2.89787	21.65917
H	11.86988	3.05755	21.90614
H	12.86639	1.63597	18.56703
H	12.59091	3.36426	18.80767
H	13.47513	2.42159	20.03430
H	7.34684	4.24919	18.57905
H	9.17302	5.59877	17.83401
H	9.26610	6.57277	20.86723
H	9.10549	7.57785	19.41295
H	8.05836	7.87105	20.80605
H	7.06852	7.31682	17.90057
H	5.76830	6.20234	18.34769
H	6.03129	7.67780	19.29678
H	5.95675	4.80975	20.49526
H	7.39189	4.96391	21.51994
H	6.22370	6.30072	21.41761
H	7.39767	3.74035	15.82528
H	8.59753	2.58764	15.32370
H	8.34949	0.19296	15.68989
H	8.56150	0.42226	17.43206
H	7.14428	-0.44201	16.82120
H	6.95723	1.97451	18.72057
H	5.70875	2.87160	17.83523
H	5.57421	1.11927	18.03458
H	5.38057	2.49479	15.34978
H	6.47192	1.44019	14.44664
H	5.32018	0.73919	15.59937
H	9.65423	4.85035	9.78450
H	12.40650	4.88583	10.17063
H	15.37934	2.60721	14.16845
H	16.68446	4.69807	14.26779
H	15.72054	6.80654	13.42209
H	11.89574	2.38673	12.80127
H	13.72159	1.23265	14.96934
H	12.24064	2.16167	15.25161
H	12.16549	0.58608	14.44046
H	13.66621	1.71648	11.17329
H	14.60600	0.99311	12.48490
H	13.02726	0.32009	12.05938
H	12.22406	7.10663	12.09954
H	12.88300	8.10050	14.30090
H	14.41252	8.63869	13.59381
H	12.88906	9.28183	12.97944
H	15.05830	7.83699	11.19530
H	13.90339	6.89228	10.25175
H	13.55934	8.58840	10.62918
H	5.51238	6.33216	13.00363
H	4.42928	4.19417	12.42226
H	5.78127	2.29076	11.62423
H	9.21643	6.89454	12.86308
H	6.65320	7.75285	14.29910
H	7.98781	6.83874	15.02571

H 8.25001 8.49029 14.44122
H 8.10718 7.66999 10.76471
H 6.69998 8.19684 11.69687
H 8.26461 8.98675 11.94123
H 9.52001 2.39456 11.28741
H 7.06236 1.56427 9.66039
H 8.28409 2.72605 9.13601
H 8.72627 1.02907 9.38915
H 8.53371 1.07263 13.14375
H 7.22781 0.53071 12.08076
H 8.89476 0.07014 11.72622
129
3 - Ag
C 3.71771 -0.84767 -2.18283
C 3.21380 0.36884 -2.67893
C 3.94432 1.57208 -2.62909
C 5.20918 1.53192 -2.03525
C 5.72342 0.34960 -1.51547
C 4.98531 -0.82512 -1.59264
N 1.92297 0.37024 -3.31895
C 0.71619 0.39463 -2.68127
N -0.18488 0.35463 -3.70379
C 0.44144 0.30727 -4.93798
C 1.77385 0.31085 -4.69450
C -1.61748 0.29611 -3.56416
C -2.33541 1.48734 -3.35431
C -3.72768 1.38907 -3.26395
C -4.37412 0.16545 -3.39104
C -3.63802 -0.99283 -3.61369
C -2.24359 -0.95746 -3.70305
C -1.66988 2.85174 -3.27440
C -2.03362 3.59634 -1.98350
C -1.47123 -2.24091 -3.96933
C -1.74518 -2.76203 -5.38877
Ag 0.35047 0.68449 -0.59706
Ta -0.56702 -0.34175 2.29278
C -1.53596 0.19004 3.86740
C -2.23742 1.04034 4.90311
C -3.47310 0.30849 5.46162
C 3.42941 2.87142 -3.23044
C 3.56617 4.06183 -2.27288
C 2.97101 -2.16592 -2.30834
C 2.78343 -2.85400 -0.95100
C 4.13766 3.17249 -4.56143
C 3.67628 -3.09516 -3.30861
C 0.16254 1.40522 1.45124
C 1.30269 2.39375 1.78521
C 1.12852 3.70366 0.99536
C 2.67982 1.79771 1.45539
C 1.28732 2.74420 3.28574
C -1.76791 -3.32305 -2.92345
C -2.00766 3.69337 -4.51491
C -2.04623 -1.35915 0.97401
C -3.50350 -1.77328 1.29307
C -4.36362 -0.51902 1.49130
C 1.00525 -1.76813 2.79858
C 1.28497 -2.65466 4.02913
C 0.11653 -3.62248 4.26228
C -4.08489 -2.58518 0.12131
C -3.56849 -2.64556 2.55281
C 1.48656 -1.78189 5.27431
C 2.56359 -3.48052 3.79451
C -1.28786 1.35462 6.07671
C -2.69347 2.36116 4.26172
H 0.32490 3.17441 3.57725
H 1.44743 1.85152 3.89811
H 2.07186 3.47478 3.52579
H 1.11760 3.51109 -0.08382
H 0.17978 4.18909 1.25216
H 1.93774 4.41361 1.21200
H 2.83475 0.84760 1.97784
H 2.78798 1.60433 0.38143
H 3.48385 2.48047 1.75848
H 1.02728 -2.40850 1.89280
H 1.86750 -1.07996 2.66073
H 2.45530 -4.13510 2.92129
H 3.42518 -2.82583 3.61756
H 2.79652 -4.11343 4.66038
H -0.80893 -3.08272 4.48775
H -0.06509 -4.24193 3.37556

H 0.32466 -4.29519 5.10337
H 2.35698 -1.12530 5.15433
H 0.61416 -1.14548 5.44922
H 1.65435 -2.39936 6.16542
H -1.50985 -0.90606 4.14021
H -0.80702 1.95601 1.41832
H -1.84169 2.90450 3.84231
H -3.40389 2.17601 3.44930
H -3.18012 3.00690 5.00341
H -4.18684 0.07265 4.66631
H -3.18542 -0.63243 5.94543
H -3.98781 0.92507 6.20964
H -0.96208 0.43335 6.57189
H -0.39579 1.88014 5.72489
H -1.78654 1.98201 6.82772
H -2.06169 -0.81051 0.01556
H -1.47241 -2.28422 0.74229
H -2.95448 -3.54742 2.43744
H -3.20896 -2.09700 3.42765
H -4.59783 -2.96705 2.75540
H -3.96376 0.08505 2.31115
H -4.36639 0.09936 0.58490
H -5.40417 -0.78191 1.72089
H -4.05917 -2.00489 -0.80795
H -3.51243 -3.50670 -0.04091
H -5.12790 -2.87144 0.31098
H -0.11477 0.27032 -5.86092
H 2.62014 0.27151 -5.36118
H 5.40171 -1.74579 -1.19449
H 6.70689 0.34299 -1.05380
H 5.79925 2.44173 -1.97847
H 1.97182 -1.95524 -2.70126
H 3.74039 -3.14620 -0.50593
H 2.27052 -2.19762 -0.24270
H 2.18520 -3.76363 -1.06889
H 3.77044 -2.62847 -4.29453
H 4.68383 -3.35553 -2.96658
H 3.11339 -4.02723 -3.42633
H 2.36208 2.74446 -3.44056
H 3.09789 3.85695 -1.30745
H 4.61464 4.32074 -2.09163
H 3.08554 4.94581 -2.70507
H 5.21319 3.31248 -4.40727
H 4.01143 2.36264 -5.28667
H 3.74050 4.09022 -5.00816
H -4.31318 2.28868 -3.09832
H -5.45678 0.11379 -3.31824
H -4.15343 -1.94348 -3.71502
H -0.58615 2.69952 -3.26390
H -3.10453 3.81932 -1.93053
H -1.76440 3.00977 -1.10010
H -1.49656 4.54939 -1.93469
H -1.70915 3.18715 -5.43873
H -3.08278 3.89364 -4.57820
H -1.49095 4.65829 -4.47443
H -0.40234 -2.01448 -3.90296
H -2.80091 -3.02446 -5.51663
H -1.49611 -2.01645 -6.15094
H -1.15203 -3.66087 -5.58834
H -1.57538 -2.96186 -1.90993
H -2.81090 -3.65308 -2.96577
H -1.13874 -4.20149 -3.10362
129
3 - Ag with dispersion
C 14.08235 4.27147 13.59347
C 13.29212 5.16178 12.85487
C 13.55290 6.53707 12.76443
C 14.65308 7.02458 13.47226
C 15.44110 6.17268 14.23988
C 15.16071 4.81212 14.29862
N 12.12312 4.65375 12.20087
C 10.92971 4.53804 12.83642
N 10.09271 4.08397 11.87242
C 10.74640 3.92369 10.65967
C 12.03873 4.28162 10.86958
C 8.68971 3.85088 12.05070
C 7.82440 4.95156 12.05740
C 6.45530 4.68481 12.14568
C 5.98487 3.38173 12.23035
C 6.87393 2.31150 12.26081

C	8.24976	2.52303	12.17539
C	8.31865	6.38272	11.99028
C	7.98959	7.12502	13.29051
C	9.24469	1.38425	12.29394
C	8.69223	0.03577	11.83477
Ag	10.59605	5.06990	14.84102
Ta	9.31933	4.15509	17.41445
C	8.70244	4.47050	19.19822
C	8.38367	5.06410	20.54400
C	7.09521	4.44421	21.10912
C	12.64626	7.46511	11.97860
C	11.68081	8.19802	12.91682
C	13.77737	2.78755	13.64652
C	13.20502	2.39916	15.01118
C	13.43196	8.45064	11.11048
C	15.00411	1.94288	13.29090
C	10.43158	5.81031	16.86549
C	11.76857	6.36497	17.37756
C	12.42892	7.28849	16.34443
C	12.73961	5.22395	17.69832
C	11.51963	7.16604	18.66176
C	9.75030	1.30406	13.74074
C	7.76001	7.11492	10.76650
C	7.50767	3.96771	16.18030
C	6.04770	4.08253	16.66229
C	5.82216	5.47093	17.26643
C	10.43940	2.28838	17.35028
C	10.21620	0.99060	18.14270
C	8.75462	0.54764	18.00960
C	5.08671	3.89848	15.48061
C	5.73587	3.00839	17.70666
C	10.55830	1.20451	19.61916
C	11.12071	-0.11540	17.57733
C	9.53793	4.79434	21.52585
C	8.18234	6.57942	20.40328
H	10.81905	7.98859	18.47927
H	11.08777	6.51729	19.42695
H	12.45258	7.59473	19.04912
H	12.69583	6.73377	15.43862
H	11.74946	8.09842	16.05775
H	13.34943	7.73719	16.74061
H	12.32659	4.56904	18.47373
H	12.93586	4.62093	16.80637
H	13.69814	5.61507	18.06028
H	10.37673	2.04480	16.27301
H	11.47983	2.62886	17.49853
H	10.88875	-0.30304	16.52216
H	12.17524	0.17613	17.64226
H	10.99620	-1.05910	18.12317
H	8.07586	1.27646	18.46374
H	8.47304	0.44689	16.95457
H	8.58397	-0.41901	18.49851
H	11.61010	1.49085	19.73517
H	9.95069	2.00627	20.04742
H	10.38991	0.28978	20.19992
H	8.44844	3.36698	19.13773
H	9.68722	6.62931	16.77351
H	9.06278	7.04969	19.96127
H	7.32711	6.79733	19.75679
H	7.99785	7.03670	21.38302
H	6.24903	4.63124	20.44110
H	7.20236	3.35931	21.22468
H	6.85617	4.86707	22.09263
H	9.69329	3.71827	21.65426
H	10.47191	5.22260	21.15040
H	9.32702	5.23008	22.51125
H	7.63623	4.65287	15.32299
H	7.65727	2.96029	15.73658
H	5.88127	2.00521	17.28835
H	6.38858	3.11525	18.57595
H	4.69701	3.08351	18.04973
H	6.49451	5.61686	18.11563
H	6.03601	6.25332	16.52739
H	4.78587	5.59697	17.60334
H	5.26014	4.66492	14.71856
H	5.23426	2.92181	15.00644
H	4.03935	3.96735	15.80160
H	10.23164	3.57536	9.77877
H	12.89293	4.30866	10.21259
H	15.78459	4.15937	14.90115

H 16.28048 6.57434 14.79965
H 14.88251 8.08473 13.44064
H 13.00587 2.57770 12.89826
H 13.92986 2.58187 15.81121
H 12.30762 2.98191 15.23702
H 12.93270 1.33986 15.03487
H 15.41548 2.22421 12.31658
H 15.79871 2.05370 14.03568
H 14.73362 0.88285 13.25711
H 12.04051 6.85067 11.30404
H 11.09503 7.49245 13.51396
H 12.22791 8.84185 13.61243
H 10.98902 8.82235 12.34151
H 13.99987 9.16258 11.71764
H 14.13654 7.93150 10.45367
H 12.74561 9.03175 10.48682
H 5.75195 5.51166 12.15231
H 4.91750 3.19738 12.29898
H 6.49131 1.30149 12.35540
H 9.40831 6.36503 11.89373
H 6.90903 7.17257 13.45975
H 8.44098 6.62517 14.15441
H 8.37272 8.14970 13.25288
H 8.01366 6.58999 9.84024
H 6.66968 7.20162 10.81390
H 8.17062 8.12821 10.71002
H 10.10648 1.61942 11.65792
H 7.91454 -0.33312 12.51146
H 8.26905 0.09168 10.82698
H 9.49223 -0.71047 11.82895
H 10.20505 2.24709 14.05490
H 8.92164 1.09397 14.42434
H 10.49667 0.51069 13.85067
129
2 - Ag 2 steps tautomerisation TS - First H trans.
C 4.31209 -0.50146 -1.53177
C 3.51271 0.48298 -2.14534
C 3.87953 1.84243 -2.18747
C 5.07386 2.20667 -1.55792
C 5.86978 1.26122 -0.92354
C 5.49341 -0.07669 -0.91625
N 2.31283 0.07355 -2.83520
C 1.05376 -0.01625 -2.30716
N 0.29398 -0.41118 -3.37078
C 1.05245 -0.55671 -4.51982
C 2.32666 -0.25150 -4.18177
C -1.13147 -0.62945 -3.39022
C -1.97181 0.45861 -3.68874
C -3.34047 0.20029 -3.81013
C -3.84752 -1.08272 -3.64740
C -2.99284 -2.13818 -3.35189
C -1.61574 -1.93961 -3.21682
C -1.44930 1.86702 -3.92267
C -2.13130 2.89062 -3.00591
C -0.69919 -3.12247 -2.94604
C -0.46352 -3.93339 -4.23081
Ag 0.37556 0.53688 -0.35498
Ta -1.27658 0.18632 2.24330
C -2.00087 0.89106 4.23442
C -1.62722 0.34902 5.63281
C -2.20736 1.26579 6.72564
C 3.06589 2.88734 -2.93720
C 2.97466 4.22653 -2.19574
C 3.96292 -1.98201 -1.58072
C 4.38502 -2.74557 -0.32087
C 3.63900 3.10879 -4.34748
C 4.58772 -2.64629 -2.82039
C -0.13175 1.55529 1.51466
C 0.49448 2.94204 1.59886
C 0.05972 3.81873 0.40899
C 2.02796 2.80385 1.60012
C 0.07534 3.66630 2.89153
C -1.22360 -4.03105 -1.82747
C -1.59194 2.26530 -5.39964
C -2.81336 0.56944 0.94731
C -4.28048 0.18090 1.23724
C -4.40686 -0.98456 2.23278
C -0.62147 -1.93506 1.85232
C 0.65855 -2.64537 2.37226
C 0.41854 -3.22738 3.77294

C	-5.06205	1.39709	1.76938
C	-4.92294	-0.26796	-0.08696
C	1.85110	-1.68082	2.43347
C	1.02024	-3.81515	1.43889
C	-2.21550	-1.05693	5.82312
C	-0.10194	0.30467	5.80413
H	-1.01141	3.79670	2.93302
H	0.38214	3.10001	3.77614
H	0.53573	4.66114	2.94736
H	0.35862	3.36591	-0.54307
H	-1.02935	3.93869	0.39374
H	0.50761	4.81933	0.47243
H	2.35858	2.18105	2.43752
H	2.38341	2.33097	0.67746
H	2.50769	3.78724	1.69342
H	-1.48887	-2.57854	2.08932
H	-0.59185	-1.94289	0.74736
H	0.18805	-4.52488	1.36556
H	1.24052	-3.45334	0.42768
H	1.90006	-4.36447	1.79993
H	0.17852	-2.44647	4.49992
H	-0.41378	-3.94142	3.76342
H	1.30824	-3.75599	4.13777
H	2.02434	-1.20614	1.46075
H	1.67589	-0.86978	3.14910
H	2.76829	-2.20313	2.73695
H	-3.10005	0.94881	4.17668
H	-1.67752	1.94594	4.18080
H	0.36867	-0.34882	5.06120
H	0.33306	1.30384	5.68673
H	0.17824	-0.06819	6.79747
H	-1.80235	2.28097	6.64156
H	-3.29801	1.33437	6.63941
H	-1.97245	0.89209	7.73112
H	-3.30972	-1.03133	5.75466
H	-1.85275	-1.75155	5.05820
H	-1.95351	-1.47084	6.80496
H	-1.77590	1.66634	1.31321
H	-2.77758	1.07876	-0.02146
H	-4.89988	0.53997	-0.82687
H	-4.38594	-1.12266	-0.51029
H	-5.97124	-0.55795	0.06298
H	-3.89425	-1.87473	1.85206
H	-3.98771	-0.74202	3.21452
H	-5.46076	-1.24566	2.39164
H	-4.64753	1.74856	2.71983
H	-5.01248	2.22875	1.05734
H	-6.12100	1.15169	1.92895
H	0.61534	-0.85458	-5.45922
H	3.23263	-0.23261	-4.76538
H	6.12858	-0.80640	-0.42530
H	6.79173	1.56735	-0.43688
H	5.38376	3.24680	-1.56619
H	2.87333	-2.06337	-1.66467
H	5.47380	-2.84567	-0.25102
H	4.02522	-2.25924	0.58827
H	3.97163	-3.75829	-0.34717
H	4.24326	-2.19161	-3.75313
H	5.67996	-2.56509	-2.79042
H	4.33006	-3.71038	-2.85240
H	2.04540	2.50339	-3.04329
H	2.63135	4.09731	-1.16704
H	3.93889	4.74543	-2.17106
H	2.26900	4.88731	-2.70960
H	4.66476	3.48988	-4.29146
H	3.65828	2.18619	-4.93454
H	3.03698	3.84229	-4.89456
H	-4.01667	1.01818	-4.04137
H	-4.91431	-1.26116	-3.74794
H	-3.40059	-3.13633	-3.22609
H	-0.38237	1.87830	-3.67847
H	-3.20181	2.97771	-3.21987
H	-2.01733	2.61516	-1.95391
H	-1.68671	3.88123	-3.14925
H	-1.06778	1.56515	-6.05814
H	-2.64380	2.28379	-5.70483
H	-1.17776	3.26498	-5.56935
H	0.26762	-2.72745	-2.61594
H	-1.40547	-4.34558	-4.60913
H	-0.02524	-3.32224	-5.02592

H 0.21544 -4.77072 -4.03668
H -1.41648 -3.46828 -0.91061
H -2.14806 -4.54224 -2.11658
H -0.48406 -4.80531 -1.60002
129
2 - Ag 2 steps tautomerisation TS - Intermediate.
C 3.80064 -1.12292 -2.03022
C 3.28783 0.15045 -2.33865
C 3.98310 1.34166 -2.05085
C 5.21287 1.22223 -1.39688
C 5.73213 -0.02216 -1.05613
C 5.03543 -1.18013 -1.37565
N 2.03487 0.22053 -3.05039
C 0.78772 0.25554 -2.49214
N -0.04320 0.22159 -3.57336
C 0.66071 0.16055 -4.76370
C 1.97369 0.15503 -4.43300
C -1.48246 0.16808 -3.53591
C -2.21059 1.37024 -3.48238
C -3.60547 1.27608 -3.50340
C -4.24328 0.04335 -3.57792
C -3.49619 -1.12682 -3.63978
C -2.09863 -1.09408 -3.62560
C -1.54095 2.73480 -3.45744
C -2.09636 3.63662 -2.34840
C -1.31231 -2.39288 -3.72553
C -1.60889 -3.12204 -5.04443
Ag 0.21311 0.60423 -0.45083
Ta -0.61738 -0.33498 2.41376
C -0.68557 0.11254 4.55253
C -1.83709 0.40286 5.53807
C -1.26189 0.84409 6.89651
C 3.46860 2.70847 -2.47834
C 3.83953 3.82820 -1.49929
C 3.10080 -2.41042 -2.43538
C 2.94466 -3.38660 -1.26497
C 3.97677 3.06510 -3.88626
C 3.83642 -3.07598 -3.60959
C -0.21861 1.48590 1.51855
C 0.72598 2.67199 1.80025
C 0.74980 3.66591 0.62376
C 2.15388 2.17271 2.06642
C 0.23524 3.45275 3.03437
C -1.56662 -3.30676 -2.51927
C -1.65389 3.41794 -4.82949
C -2.38008 -1.03135 1.96750
C -3.77743 -0.85809 1.40365
C -3.99202 0.58098 0.91347
C 0.93695 -1.89487 2.17823
C 1.23956 -3.09701 3.11231
C -0.06024 -3.76113 3.59081
C -3.98636 -1.81716 0.21678
C -4.83648 -1.18257 2.47575
C 2.06011 -2.63469 4.32577
C 2.06989 -4.15304 2.36061
C -2.73113 1.52309 4.99003
C -2.67715 -0.86232 5.75059
H -0.78751 3.81599 2.88343
H 0.23751 2.82713 3.93028
H 0.87630 4.32305 3.22672
H 1.11362 3.18692 -0.29297
H -0.25771 4.04615 0.42136
H 1.39750 4.52629 0.83993
H 2.17938 1.49916 2.93121
H 2.54446 1.61960 1.20397
H 2.83438 3.00795 2.27590
H 0.62738 -2.29635 1.19260
H 1.88123 -1.35498 1.98301
H 1.51955 -4.54312 1.49656
H 3.01074 -3.72531 1.99593
H 2.31812 -5.00265 3.01004
H -0.66530 -3.07628 4.19518
H -0.67092 -4.08542 2.73986
H 0.15159 -4.64563 4.20475
H 3.01401 -2.19843 4.00591
H 1.53165 -1.87953 4.91537
H 2.28493 -3.47791 4.99036
H 0.10202 0.87780 4.68291
H -1.25180 1.86943 1.36071
H -3.04524 -1.24443 4.79433

H -2.08123 -1.65128 6.22697
H -3.53864 -0.66030 6.39933
H -0.60737 0.07036 7.31546
H -0.67064 1.76203 6.79413
H -2.05894 1.03969 7.62539
H -2.15697 2.44171 4.82586
H -3.16522 1.22151 4.03175
H -3.54732 1.75546 5.68611
H -0.19233 -0.83003 4.87646
H -2.17754 -2.08734 2.27232
H -4.70934 -2.20257 2.85665
H -4.76118 -0.49621 3.32406
H -5.85025 -1.10254 2.06118
H -3.86772 1.29862 1.73173
H -3.27110 0.83200 0.12807
H -5.00143 0.70884 0.50279
H -3.27780 -1.59407 -0.58540
H -3.83593 -2.85865 0.52452
H -5.00386 -1.72892 -0.18776
H 0.16511 0.11857 -5.72039
H 2.86054 0.09850 -5.04333
H 5.45631 -2.14771 -1.11885
H 6.68885 -0.08784 -0.54534
H 5.77333 2.11776 -1.15002
H 2.09258 -2.15547 -2.77602
H 3.91231 -3.75125 -0.90433
H 2.42578 -2.92025 -0.42429
H 2.36656 -4.26144 -1.58056
H 3.91237 -2.40787 -4.47350
H 4.85382 -3.36395 -3.32328
H 3.30912 -3.98185 -3.92717
H 2.37437 2.65324 -2.51731
H 3.57850 3.57227 -0.46985
H 4.90955 4.06068 -1.53501
H 3.30453 4.74498 -1.76606
H 5.07145 3.10818 -3.89985
H 3.66085 2.33591 -4.63692
H 3.59693 4.04584 -4.19223
H -4.20000 2.18384 -3.46311
H -5.32848 -0.00530 -3.58882
H -4.00508 -2.08470 -3.69778
H -0.47722 2.58335 -3.24756
H -3.14315 3.90506 -2.52628
H -2.03202 3.14824 -1.37223
H -1.52431 4.56906 -2.30159
H -1.21110 2.80778 -5.62337
H -2.70189 3.59743 -5.09354
H -1.14018 4.38528 -4.81996
H -0.24597 -2.14609 -3.72420
H -2.65677 -3.43480 -5.10269
H -1.40403 -2.48693 -5.91245
H -0.99064 -4.02204 -5.12867
H -1.30370 -2.81004 -1.58124
H -2.61848 -3.60404 -2.45549
H -0.96814 -4.22033 -2.60462
129
2 - Ag 2 steps tautomerisation TS - Second H trans.
C 4.12786 -0.80670 -2.12875
C 3.48287 0.39343 -2.47551
C 4.03480 1.66138 -2.20427
C 5.25739 1.69429 -1.52809
C 5.90643 0.52308 -1.15043
C 5.34963 -0.71197 -1.45374
N 2.23479 0.30784 -3.19212
C 0.98934 0.31560 -2.63321
N 0.16090 0.13323 -3.70092
C 0.86710 0.00490 -4.88504
C 2.17842 0.11450 -4.56325
C -1.27716 0.05937 -3.64985
C -2.02039 1.23946 -3.83368
C -3.41381 1.12570 -3.85105
C -4.03700 -0.10681 -3.69483
C -3.27565 -1.25530 -3.51105
C -1.87899 -1.20122 -3.48277
C -1.36999 2.59876 -4.03205
C -1.86610 3.62254 -3.00244
C -1.07597 -2.47858 -3.29974
C -1.18240 -3.37901 -4.53986
Ag 0.35438 0.75536 -0.63741
Ta -0.85127 -0.22249 2.16542

C	-0.92765	0.13013	4.13031
C	-1.48814	0.35808	5.52646
C	-1.78132	-0.98334	6.22888
C	3.37527	2.94914	-2.67573
C	3.63257	4.13936	-1.74547
C	3.56986	-2.17596	-2.48309
C	3.33020	-3.03202	-1.23503
C	3.82651	3.29700	-4.10530
C	4.48191	-2.89827	-3.48631
C	-0.41186	1.59228	1.21292
C	0.34865	2.84947	1.68242
C	0.50019	3.87324	0.54254
C	1.74634	2.46870	2.19204
C	-0.42746	3.53651	2.81981
C	-1.48787	-3.23555	-2.03020
C	-1.58240	3.10672	-5.46628
C	-2.70434	-0.93236	1.92868
C	-4.17358	-0.57601	1.78341
C	-4.38296	0.94471	1.80330
C	0.68322	-1.80985	1.85227
C	0.98178	-2.99838	2.80558
C	-0.31961	-3.67539	3.25785
C	-4.65095	-1.11937	0.42208
C	-5.01977	-1.23329	2.89045
C	1.76145	-2.52530	4.04013
C	1.84397	-4.04518	2.07661
C	-0.45662	1.13524	6.36481
C	-2.78471	1.17972	5.46500
H	-1.41896	3.85448	2.47510
H	-0.57016	2.84205	3.65174
H	0.10394	4.42645	3.18243
H	1.05982	3.44553	-0.29762
H	-0.48159	4.18202	0.16503
H	1.02838	4.77515	0.88122
H	1.67611	1.76820	3.03222
H	2.33151	1.98450	1.40024
H	2.29980	3.35099	2.53846
H	0.35224	-2.23381	0.88246
H	1.63567	-1.30488	1.61450
H	1.33143	-4.42657	1.18546
H	2.79872	-3.61333	1.75602
H	2.06675	-4.90173	2.72614
H	-0.93957	-2.98243	3.83630
H	-0.90422	-4.01999	2.39559
H	-0.11220	-4.54958	3.88800
H	2.69989	-2.03807	3.74838
H	1.17875	-1.81336	4.63148
H	2.01415	-3.37167	4.69089
H	0.17660	-0.03735	4.16246
H	-1.41926	1.90031	0.85138
H	-2.60976	2.14827	4.98668
H	-3.55855	0.65722	4.89480
H	-3.17905	1.35680	6.47334
H	-2.52703	-1.56103	5.67097
H	-0.87489	-1.59354	6.30553
H	-2.16874	-0.82303	7.24371
H	0.47963	0.57224	6.45623
H	-0.22483	2.10130	5.90512
H	-0.83664	1.32126	7.37698
H	-2.04921	-0.67577	3.45096
H	-2.56150	-2.03400	1.92841
H	-4.89896	-2.32275	2.87808
H	-4.72487	-0.87719	3.88254
H	-6.08615	-1.01082	2.75688
H	-4.02873	1.38576	2.73976
H	-3.83483	1.41819	0.98223
H	-5.44548	1.19366	1.69175
H	-4.07316	-0.67806	-0.39538
H	-4.53507	-2.20826	0.37047
H	-5.71205	-0.88712	0.26372
H	0.37509	-0.15117	-5.83182
H	3.06777	0.06118	-5.17058
H	5.86870	-1.62095	-1.16344
H	6.85430	0.57663	-0.62201
H	5.71032	2.65152	-1.29243
H	2.59914	-2.03342	-2.96788
H	4.26431	-3.24108	-0.70299
H	2.65035	-2.53469	-0.53873
H	2.88897	-3.99495	-1.51337
H	4.62893	-2.30832	-4.39687

H 5.46996 -3.09580 -3.05684
H 4.04636 -3.86147 -3.77260
H 2.29290 2.77766 -2.69685
H 3.39983 3.90042 -0.70475
H 4.67315 4.47860 -1.79614
H 3.00590 4.98508 -2.04515
H 4.91013 3.45533 -4.13950
H 3.57999 2.50623 -4.81938
H 3.34050 4.21782 -4.44549
H -4.01785 2.01740 -3.99160
H -5.12125 -0.17269 -3.71299
H -3.77301 -2.21257 -3.38578
H -0.29233 2.48335 -3.87776
H -2.93558 3.82847 -3.11804
H -1.69706 3.26794 -1.98177
H -1.33366 4.57148 -3.12702
H -1.19128 2.40083 -6.20620
H -2.64628 3.25596 -5.68068
H -1.07530 4.06647 -5.61230
H -0.02410 -2.20089 -3.18036
H -2.21653 -3.69786 -4.70982
H -0.84114 -2.86394 -5.44377
H -0.57243 -4.27971 -4.41236
H -1.41595 -2.59526 -1.14660
H -2.51650 -3.60594 -2.09453
H -0.83587 -4.10275 -1.88159
3
CO2
O -3.85320 0.93035 -0.36091
C -3.61177 2.07084 -0.30256
O -3.37005 3.21138 -0.24420
132
2 - Cu + CO2 - C-C coupling adduct
C -1.67573 2.11860 -3.63216
C -1.50709 0.72032 -3.55237
C -2.58202 -0.17882 -3.68290
C -3.85638 0.36178 -3.88406
C -4.05443 1.73438 -3.94978
C -2.97465 2.60059 -3.82123
N -0.16501 0.19417 -3.46865
C 0.62239 0.07382 -2.35323
N 1.81892 -0.36002 -2.86351
C 1.76787 -0.51397 -4.23791
C 0.51918 -0.16238 -4.62011
C 3.05835 -0.50614 -2.13775
C 3.98301 0.55561 -2.19290
C 5.19901 0.38746 -1.52242
C 5.48462 -0.78510 -0.83631
C 4.56417 -1.82725 -0.82212
C 3.33464 -1.71941 -1.47844
C 3.74149 1.82650 -2.99653
C 4.56456 1.80117 -4.29547
C 2.37830 -2.90103 -1.52979
C 2.62272 -3.73789 -2.79778
Cu 0.26203 0.38616 -0.45509
C 0.32921 1.10234 1.38668
C 1.09911 2.41769 1.46008
C 0.85604 3.11199 2.81269
C -2.39894 -1.68849 -3.66151
C -3.47111 -2.39462 -2.82382
C -0.50462 3.08957 -3.59621
C 0.00674 3.36731 -5.02076
C -2.38646 -2.26122 -5.08859
C -0.83430 4.40963 -2.89055
Ta -0.33819 -0.45476 2.21963
C -1.69474 0.14882 3.81525
C -2.96881 0.98505 4.05293
C -4.15822 0.36339 3.30952
O -3.85747 0.93095 -0.36121
C -3.60341 2.06882 -0.30200
O -3.37414 3.21280 -0.24446
C -0.99442 -2.00730 0.75274
C -1.77593 -3.25751 1.25564
C -3.23810 -2.88947 1.53717
C 1.47360 -1.31714 3.17447
C 1.92893 -1.36372 4.65430
C 3.24172 -2.16491 4.75004
C 2.45735 -3.79730 -0.29047
C 4.04129 3.10621 -2.20582
C 0.67815 3.39865 0.35103

C	2.60816	2.13625	1.33493
C	-1.74685	-4.36067	0.18379
C	-1.15687	-3.83370	2.53765
C	0.88404	-2.05237	5.54425
C	2.19037	0.05219	5.18422
C	-3.30121	1.01446	5.55718
C	-2.76890	2.42557	3.57155
H	0.88339	2.98100	-0.64223
H	-0.39389	3.60951	0.41111
H	1.22121	4.34995	0.43722
H	2.94593	1.49196	2.15228
H	2.83434	1.61899	0.39688
H	3.18973	3.06834	1.37200
H	-0.19412	3.39006	2.92325
H	1.12550	2.45317	3.64336
H	1.46266	4.02412	2.89261
H	1.34888	-2.36890	2.84281
H	2.31265	-0.92683	2.58046
H	-0.05991	-1.49766	5.56333
H	0.67369	-3.06873	5.19058
H	1.24135	-2.12882	6.57865
H	2.93141	0.57241	4.56716
H	1.27511	0.65307	5.18275
H	2.56998	0.02346	6.21329
H	3.10259	-3.19042	4.38752
H	4.02819	-1.69997	4.14433
H	3.60331	-2.22158	5.78500
H	-1.86296	-0.85178	4.27407
H	-0.87557	0.59063	4.42757
H	-3.46700	0.00202	5.94429
H	-2.48163	1.46185	6.13145
H	-4.20769	1.60099	5.75416
H	-1.99022	2.92663	4.15621
H	-2.46020	2.44753	2.52292
H	-3.69344	3.00551	3.68335
H	-3.97087	0.30675	2.23322
H	-4.36224	-0.65160	3.66999
H	-5.06826	0.95562	3.46774
H	-1.51953	-1.60985	-0.13075
H	-0.02120	-2.35650	0.35501
H	-2.17425	-4.00339	-0.75806
H	-0.71966	-4.68635	-0.01673
H	-2.32009	-5.24199	0.50061
H	-0.11076	-4.12057	2.38216
H	-1.18767	-3.11653	3.36694
H	-1.70209	-4.72719	2.86631
H	-3.31193	-2.13519	2.32557
H	-3.72368	-2.48058	0.64419
H	-3.81128	-3.76841	1.85812
H	0.05827	-0.12210	-5.59365
H	2.61945	-0.84705	-4.80871
H	4.80754	-2.74218	-0.29283
H	6.43234	-0.89303	-0.31605
H	5.93117	1.18917	-1.54000
H	1.35889	-2.50181	-1.58108
H	3.40160	-4.35116	-0.24570
H	2.35416	-3.22160	0.63362
H	1.65481	-4.54013	-0.32090
H	2.48857	-3.15006	-3.71033
H	3.64133	-4.14164	-2.80391
H	1.92507	-4.58137	-2.83873
H	2.68256	1.85917	-3.27222
H	3.47184	3.14770	-1.27507
H	5.10407	3.19179	-1.95612
H	3.77988	3.98353	-2.80703
H	5.63744	1.77968	-4.07516
H	4.33682	0.92422	-4.90899
H	4.36266	2.69496	-4.89540
H	-3.14000	3.67130	-3.87772
H	-5.05364	2.13235	-4.10490
H	-4.70616	-0.30518	-3.98828
H	0.30414	2.61328	-3.03184
H	-1.52020	5.02759	-3.48051
H	-1.28182	4.24364	-1.90819
H	0.08175	4.99226	-2.75236
H	0.33269	2.45385	-5.52632
H	-0.77986	3.82684	-5.62966
H	0.85663	4.05776	-4.99300
H	-1.42821	-1.90256	-3.20096
H	-3.33929	-2.06728	-5.59359

H -1.59164 -1.82621 -5.70108
H -2.23411 -3.34549 -5.06338
H -3.52529 -1.98257 -1.81324
H -4.46440 -2.31265 -3.27760
H -3.24224 -3.46212 -2.74944
132
2 - Cu + CO2 - C-C coupling TS
C -1.85387 1.93279 -3.58923
C -1.57647 0.55003 -3.60969
C -2.58347 -0.42133 -3.76473
C -3.90418 0.02788 -3.86743
C -4.20931 1.38126 -3.81896
C -3.19337 2.32015 -3.68439
N -0.19956 0.11632 -3.56635
C 0.58921 -0.01253 -2.45477
N 1.79568 -0.40638 -2.96715
C 1.75283 -0.52638 -4.34540
C 0.49663 -0.19377 -4.72305
C 3.01857 -0.58833 -2.22268
C 3.96102 0.45837 -2.23046
C 5.16300 0.24904 -1.54617
C 5.41475 -0.94636 -0.88645
C 4.47185 -1.96822 -0.90853
C 3.25603 -1.82046 -1.58225
C 3.74454 1.76139 -2.98739
C 4.55133 1.76574 -4.29653
C 2.27107 -2.97706 -1.66467
C 2.51023 -3.79910 -2.94326
Cu 0.21058 0.32902 -0.57350
C 0.13704 1.12466 1.23248
C 0.96582 2.40197 1.36330
C 0.56058 3.16900 2.63576
C -2.28526 -1.90888 -3.87526
C -3.26206 -2.76594 -3.06268
C -0.75509 2.98460 -3.54173
C -0.25567 3.30427 -4.96175
C -2.29444 -2.36224 -5.34509
C -1.18032 4.27570 -2.83482
Ta -0.65265 -0.37634 2.10442
C -1.85979 0.22895 3.81166
C -3.10324 0.98053 4.32843
C -4.38663 0.39580 3.72247
O -2.86429 0.44355 0.73077
C -2.44313 1.54516 0.58750
O -2.39701 2.69223 0.33351
C -1.12314 -2.07148 0.72465
C -2.03402 -3.22556 1.23953
C -3.49044 -2.74956 1.33167
C 1.10507 -1.30099 3.09410
C 1.62377 -1.34045 4.55608
C 2.93345 -2.15249 4.59070
C 2.31072 -3.89438 -0.43877
C 4.08923 3.00126 -2.15239
C 0.80426 3.35719 0.16699
C 2.45350 2.01710 1.47595
C -1.96358 -4.41820 0.26945
C -1.59260 -3.73126 2.62142
C 0.61716 -2.02693 5.49010
C 1.92454 0.06802 5.08503
C -3.18492 0.83046 5.86117
C -3.01256 2.47664 4.00354
H 1.09830 2.86745 -0.76926
H -0.23111 3.68604 0.06629
H 1.43708 4.24537 0.29644
H 2.62399 1.36880 2.33953
H 2.78783 1.47296 0.58599
H 3.08013 2.91229 1.59156
H -0.48978 3.46796 2.58853
H 0.69878 2.54792 3.52615
H 1.17222 4.07317 2.75525
H 0.94078 -2.35410 2.79431
H 1.93667 -0.95573 2.46069
H -0.32164 -1.46872 5.55351
H 0.38635 -3.04080 5.14265
H 1.02229 -2.10767 6.50632
H 2.66141 0.57858 4.45560
H 1.02337 0.68872 5.11478
H 2.33067 0.02358 6.10334
H 2.77011 -3.17459 4.22895
H 3.69741 -1.69052 3.95457

H 3.33797 -2.21806 5.60896
H -1.92618 -0.81180 4.20701
H -0.97225 0.65154 4.33294
H -3.26682 -0.22393 6.15051
H -2.29179 1.24161 6.34593
H -4.05871 1.35735 6.26499
H -2.11766 2.92121 4.45227
H -2.96738 2.65827 2.92733
H -3.88546 3.01015 4.39910
H -4.39576 0.49204 2.63409
H -4.48707 -0.66788 3.96909
H -5.27011 0.91064 4.11968
H -1.50666 -1.75294 -0.25693
H -0.12348 -2.49532 0.51346
H -2.26066 -4.12358 -0.74122
H -0.94449 -4.81854 0.21579
H -2.62521 -5.23385 0.58986
H -0.55850 -4.09339 2.60387
H -1.65971 -2.95220 3.38978
H -2.22973 -4.56129 2.95139
H -3.59718 -1.92484 2.04300
H -3.85237 -2.38863 0.36304
H -4.15014 -3.56375 1.65703
H 0.03698 -0.14453 -5.69667
H 2.61194 -0.82979 -4.92139
H 4.68569 -2.89889 -0.39407
H 6.35199 -1.08638 -0.35497
H 5.90964 1.03717 -1.52990
H 1.26267 -2.55171 -1.71974
H 3.23713 -4.47766 -0.39288
H 2.21487 -3.32996 0.49308
H 1.48515 -4.61046 -0.48874
H 2.40332 -3.19312 -3.84757
H 3.51825 -4.22866 -2.94323
H 1.79222 -4.62389 -3.00651
H 2.68258 1.83018 -3.24580
H 3.55559 3.00711 -1.19958
H 5.16191 3.06450 -1.94101
H 3.81534 3.90774 -2.70234
H 5.62552 1.70604 -4.08974
H 4.29278 0.92147 -4.94256
H 4.36783 2.68833 -4.85753
H -3.44463 3.37487 -3.65519
H -5.24308 1.70784 -3.89070
H -4.70482 -0.69553 -3.98392
H 0.08202 2.56459 -2.97343
H -1.89339 4.85258 -3.43458
H -1.63260 4.07239 -1.86155
H -0.30559 4.91405 -2.67753
H 0.14008 2.41998 -5.46919
H -1.07021 3.70770 -5.57366
H 0.54110 4.05510 -4.92512
H -1.28194 -2.08336 -3.47133
H -3.28190 -2.20359 -5.79236
H -1.56548 -1.81797 -5.95220
H -2.06013 -3.42975 -5.41755
H -3.31883 -2.43208 -2.02391
H -4.27334 -2.74230 -3.48222
H -2.93731 -3.81121 -3.07054
132
2 - Cu + CO2 - C-C coupling product
C 3.52036 -1.66300 -1.69720
C 3.29177 -0.44213 -2.36122
C 4.24030 0.59849 -2.38791
C 5.44192 0.39103 -1.70300
C 5.68725 -0.79532 -1.02327
C 4.73676 -1.80994 -1.02417
N 2.06655 -0.27434 -3.10009
C 0.84807 0.04235 -2.56745
N 0.02805 0.10153 -3.65938
C 0.71694 -0.17117 -4.82875
C 2.00152 -0.41479 -4.47617
C -1.39320 0.34797 -3.63090
C -1.85763 1.66909 -3.46907
C -3.24172 1.85665 -3.42813
C -4.12126 0.78928 -3.57438
C -3.63344 -0.49407 -3.78130
C -2.25809 -0.74667 -3.81378
C -0.91175 2.86064 -3.43157
C -1.45550 4.05717 -2.64620

C	-1.76364	-2.15969	-4.08955
C	-2.06402	-2.56694	-5.54084
Cu	0.44477	0.52472	-0.73826
Ta	-0.82527	-0.16470	2.26850
C	1.24466	-0.49660	3.06042
C	1.71413	-1.43516	4.21724
C	1.40424	-0.82082	5.59048
C	4.02355	1.89337	-3.15814
C	4.35278	3.14024	-2.32724
C	2.53585	-2.82066	-1.76029
C	2.37599	-3.54726	-0.42072
C	4.84068	1.89173	-4.46058
C	2.94458	-3.80481	-2.86893
C	0.13194	1.42792	0.99952
C	-1.22906	1.94228	0.84464
O	-1.72540	3.03798	0.64233
C	1.23839	2.50076	1.23838
C	2.65810	1.91359	1.17611
C	1.03238	3.21059	2.59091
C	1.17417	3.58279	0.13707
C	-2.34624	-3.18418	-3.11031
C	-0.54769	3.28502	-4.86592
C	-1.68078	0.29453	4.20629
C	-2.95725	1.10466	4.54931
C	-2.77050	2.57588	4.15332
O	-2.05894	0.85190	1.16307
C	-1.11633	-2.13383	1.38107
C	-2.41272	-2.97770	1.50435
C	-2.76834	-3.24161	2.97499
C	-4.18901	0.54011	3.82941
C	-3.19121	1.02745	6.06897
C	-3.58516	-2.26070	0.82025
C	-2.18869	-4.34118	0.82535
C	3.24426	-1.59156	4.10972
C	1.09189	-2.83597	4.15439
H	1.33480	3.13489	-0.85221
H	0.20486	4.08136	0.12847
H	1.96037	4.33216	0.29902
H	2.87112	1.20864	1.97960
H	2.81792	1.38405	0.22859
H	3.39961	2.72044	1.23984
H	0.05338	3.69883	2.61978
H	1.09016	2.50816	3.42929
H	1.79749	3.98120	2.75064
H	1.76482	-0.82069	2.13977
H	1.68426	0.48330	3.27542
H	0.00322	-2.80076	4.27014
H	1.31593	-3.33260	3.20304
H	1.48638	-3.47223	4.95638
H	1.81940	0.19071	5.67245
H	0.32953	-0.75903	5.78062
H	1.84608	-1.42634	6.39135
H	3.52676	-2.04999	3.15481
H	3.74305	-0.61772	4.17102
H	3.63916	-2.22304	4.91644
H	-1.75529	-0.70949	4.67244
H	-0.82842	0.77375	4.71970
H	-3.34238	-0.00850	6.39558
H	-2.33490	1.43194	6.62120
H	-4.07903	1.60273	6.35921
H	-1.89560	3.00859	4.65296
H	-2.64462	2.69483	3.07373
H	-3.64646	3.16490	4.45069
H	-4.07560	0.61690	2.74407
H	-4.36010	-0.51058	4.09389
H	-5.08912	1.09904	4.11237
H	-0.88529	-1.98811	0.31063
H	-0.27139	-2.72006	1.77859
H	-1.92335	-4.22262	-0.23012
H	-1.37720	-4.89346	1.31356
H	-3.09296	-4.96050	0.87567
H	-1.95787	-3.76620	3.49328
H	-2.97416	-2.31329	3.51713
H	-3.66628	-3.86672	3.04806
H	-3.80897	-1.30219	1.29756
H	-3.36421	-2.05098	-0.23132
H	-4.49179	-2.87669	0.85878
H	0.23106	-0.17301	-5.79111
H	2.86520	-0.67369	-5.06692
H	4.94566	-2.73655	-0.49891

H 6.62561 -0.93268 -0.49311
H 6.19394 1.17426 -1.70051
H 1.55441 -2.41242 -2.02073
H 3.28562 -4.08379 -0.13055
H 2.12092 -2.84989 0.38197
H 1.57413 -4.28873 -0.49295
H 2.99445 -3.31418 -3.84617
H 3.92958 -4.23785 -2.66235
H 2.22342 -4.62630 -2.93986
H 2.96337 1.95401 -3.42577
H 3.80378 3.15084 -1.38312
H 5.42209 3.20745 -2.10024
H 4.08405 4.04183 -2.88754
H 5.91379 1.84086 -4.24592
H 4.59253 1.04017 -5.10147
H 4.65514 2.80828 -5.03056
H -3.63697 2.85499 -3.27741
H -5.19297 0.96284 -3.53449
H -4.32911 -1.31756 -3.91576
H 0.00930 2.54002 -2.93167
H -2.30616 4.52564 -3.15472
H -1.75741 3.77789 -1.63307
H -0.67580 4.82129 -2.56538
H -0.08512 2.47225 -5.43455
H -1.44241 3.60819 -5.40982
H 0.15570 4.12453 -4.84672
H -0.67680 -2.17559 -3.96023
H -3.14315 -2.59355 -5.72615
H -1.62592 -1.86715 -6.25973
H -1.66352 -3.56451 -5.75103
H -2.11649 -2.91331 -2.07721
H -3.43435 -3.26431 -3.20080
H -1.92690 -4.17705 -3.30576
132
2 - Cu + CO2 - C-O activation TS
C 3.47003 -1.57968 -1.63863
C 3.23722 -0.37306 -2.32651
C 4.17648 0.67533 -2.36849
C 5.37220 0.49440 -1.66607
C 5.61976 -0.67510 -0.95818
C 4.68048 -1.70030 -0.94978
N 2.01378 -0.22592 -3.07360
C 0.80335 0.14546 -2.56017
N -0.01198 0.18443 -3.65513
C 0.67098 -0.15652 -4.80950
C 1.94774 -0.42048 -4.44257
C -1.41899 0.50149 -3.64853
C -1.81278 1.85292 -3.58185
C -3.18441 2.11725 -3.58165
C -4.11805 1.08969 -3.66489
C -3.69797 -0.22955 -3.76628
C -2.33797 -0.55653 -3.76285
C -0.80320 2.99192 -3.59253
C -1.27940 4.24123 -2.84488
C -1.91335 -2.00848 -3.92495
C -2.24295 -2.51694 -5.33727
Cu 0.38395 0.66389 -0.75211
Ta -0.95638 -0.17674 2.19228
C 1.21035 -0.63804 2.89470
C 1.74054 -1.46514 4.10433
C 1.37788 -0.78062 5.43119
C 3.95884 1.94471 -3.18052
C 4.26854 3.22273 -2.39058
C 2.49567 -2.74656 -1.69705
C 2.38320 -3.51151 -0.37456
C 4.79076 1.90536 -4.47319
C 2.88218 -3.70035 -2.84044
C 0.11243 1.54867 1.01836
C -1.09993 2.11141 0.69335
O -1.89442 2.94704 0.45260
C 1.22253 2.61376 1.33889
C 2.62106 2.01967 1.11684
C 1.08550 3.10732 2.79032
C 1.10619 3.84136 0.41291
C -2.53463 -2.91839 -2.86019
C -0.42292 3.35034 -5.03994
C -1.83124 0.34439 4.09177
C -3.10991 1.14270 4.42414
C -2.93884 2.60336 3.98538
O -2.12010 0.41200 0.93679

C	-1.15139	-2.28228	1.57004
C	-2.43415	-3.14650	1.69840
C	-2.74502	-3.43730	3.17463
C	-4.32969	0.54424	3.71249
C	-3.34589	1.10514	5.94478
C	-3.65222	-2.46800	1.05786
C	-2.19075	-4.49542	0.99484
C	3.27897	-1.53950	4.02184
C	1.20493	-2.90197	4.14068
H	1.16933	3.54372	-0.64062
H	0.16494	4.37935	0.55338
H	1.92536	4.54159	0.61613
H	2.80612	1.14289	1.73780
H	2.74799	1.71229	0.07230
H	3.38927	2.76930	1.34505
H	0.10627	3.57003	2.95400
H	1.19874	2.29076	3.50860
H	1.85214	3.85922	3.01542
H	1.69359	-1.03864	1.98245
H	1.68161	0.34696	3.01025
H	0.11727	-2.92078	4.26084
H	1.45180	-3.44533	3.22078
H	1.64175	-3.46007	4.97889
H	1.72300	0.26068	5.44441
H	0.29740	-0.77826	5.60365
H	1.84598	-1.29546	6.27963
H	3.59638	-2.03534	3.09679
H	3.72022	-0.53580	4.02776
H	3.70521	-2.09875	4.86606
H	-1.89766	-0.66722	4.54850
H	-0.97000	0.81096	4.60638
H	-3.48428	0.07634	6.29787
H	-2.49512	1.53362	6.48763
H	-4.24128	1.67627	6.21982
H	-2.07047	3.06208	4.47351
H	-2.80773	2.67912	2.90221
H	-3.82194	3.19466	4.25577
H	-4.19933	0.58032	2.62675
H	-4.48924	-0.49975	4.00835
H	-5.23892	1.10177	3.96819
H	-0.90544	-2.18281	0.49551
H	-0.31669	-2.83953	2.01156
H	-1.98057	-4.35217	-0.07080
H	-1.33612	-5.02078	1.43708
H	-3.06733	-5.15076	1.07789
H	-1.90855	-3.94679	3.66618
H	-2.95533	-2.51747	3.73014
H	-3.62696	-4.08317	3.26533
H	-3.91366	-1.53864	1.56913
H	-3.46179	-2.20944	0.01224
H	-4.52354	-3.13432	1.09123
H	0.18603	-0.18590	-5.77194
H	2.80615	-0.72516	-5.01897
H	4.89208	-2.61253	-0.40151
H	6.55252	-0.79180	-0.41346
H	6.11815	1.28347	-1.67309
H	1.50263	-2.34271	-1.91956
H	3.30227	-4.05731	-0.13530
H	2.15508	-2.84229	0.45925
H	1.57920	-4.25073	-0.44198
H	2.89733	-3.19043	-3.80882
H	3.87766	-4.12538	-2.67074
H	2.16868	-4.52872	-2.90695
H	2.90170	1.98822	-3.46324
H	3.69686	3.27162	-1.46096
H	5.33137	3.29858	-2.13808
H	4.01628	4.10189	-2.99276
H	5.86166	1.87010	-4.24515
H	4.55566	1.02993	-5.08611
H	4.60464	2.80005	-5.07674
H	-3.52831	3.14349	-3.51228
H	-5.17924	1.32180	-3.65494
H	-4.43584	-1.02289	-3.84337
H	0.10198	2.63870	-3.08522
H	-2.09357	4.74809	-3.37495
H	-1.62061	4.00337	-1.83439
H	-0.45619	4.95888	-2.76857
H	-0.00469	2.49520	-5.57955
H	-1.30218	3.69884	-5.59312
H	0.32241	4.15311	-5.05199

H -0.82744 -2.06499 -3.79908
H -3.32334 -2.50771 -5.51668
H -1.77654 -1.89995 -6.11230
H -1.89186 -3.54636 -5.46652
H -2.28172 -2.57483 -1.85462
H -3.62618 -2.95193 -2.93763
H -2.16576 -3.94314 -2.97647
132
2 - Cu + CO2 - C-O activation product
C 2.73285 -2.44019 -1.88367
C 2.84628 -1.06840 -2.17030
C 3.94220 -0.28834 -1.75003
C 4.92937 -0.92652 -0.99447
C 4.83520 -2.27897 -0.67972
C 3.75112 -3.02538 -1.12270
N 1.82905 -0.45970 -2.98777
C 0.73435 0.21940 -2.53434
N 0.06007 0.53623 -3.67964
C 0.70852 0.05913 -4.80533
C 1.82711 -0.56766 -4.36967
C -1.17303 1.27890 -3.74843
C -1.10689 2.65740 -4.02541
C -2.31578 3.34931 -4.14148
C -3.53328 2.69618 -3.98939
C -3.56659 1.33305 -3.72211
C -2.39001 0.58833 -3.59687
C 0.20954 3.38843 -4.24147
C 0.32406 4.65516 -3.38475
C -2.45662 -0.91367 -3.36871
C -2.77631 -1.63566 -4.68809
Cu 0.14065 0.66553 -0.76106
Ta -0.46923 -0.74624 1.99642
C 1.72531 -0.37966 2.17063
C 2.64466 -0.67630 3.39326
C 1.93204 -0.38149 4.72278
C 4.09300 1.17196 -2.14994
C 4.79173 2.02493 -1.08602
C 1.58715 -3.30005 -2.39378
C 0.79096 -3.93241 -1.24613
C 4.83703 1.29003 -3.49141
C 2.09984 -4.36860 -3.37189
C -0.47544 1.69304 0.88707
C -1.70788 1.66968 0.41616
O -2.81804 1.58272 0.01762
C 0.14043 3.04520 1.34763
C 1.53070 3.23190 0.72311
C 0.27410 3.08617 2.87796
C -0.74019 4.23114 0.91593
C -3.45269 -1.30619 -2.27167
C 0.41111 3.71988 -5.72864
C -1.82227 -0.02441 3.56518
C -3.30826 0.39504 3.68750
C -3.47613 1.90148 3.44759
O -1.00227 -1.14297 0.37406
C -0.28201 -2.80188 2.76968
C -1.33230 -3.94315 2.84447
C -2.24493 -3.75115 4.06348
C -4.18402 -0.37020 2.68390
C -3.80334 0.09116 5.11511
C -2.18827 -4.01305 1.57361
C -0.59405 -5.28479 3.01348
C 3.88509 0.23407 3.30340
C 3.13774 -2.13037 3.38513
H -0.87790 4.24478 -0.17047
H -1.73123 4.18162 1.37994
H -0.28200 5.18256 1.21167
H 2.20529 2.41511 0.99529
H 1.46503 3.26102 -0.36930
H 1.98211 4.17133 1.06624
H -0.70292 2.99444 3.35932
H 0.91200 2.27814 3.24613
H 0.72212 4.03631 3.19488
H 2.19109 -0.81791 1.27112
H 1.77562 0.70257 1.98987
H 2.31635 -2.84562 3.46471
H 3.68245 -2.34705 2.45906
H 3.82039 -2.31019 4.22493
H 1.57853 0.65540 4.76383
H 1.06761 -1.03680 4.87552
H 2.60924 -0.53006 5.57295

H 4.41657 0.07320 2.35857
H 3.60402 1.29259 3.35546
H 4.58721 0.03401 4.12317
H -1.68136 -0.92651 4.19462
H -1.18914 0.73679 4.06291
H -3.75156 -0.98145 5.33527
H -3.19359 0.61473 5.86104
H -4.84478 0.40965 5.24925
H -2.89416 2.48266 4.17297
H -3.16417 2.18645 2.44141
H -4.52772 2.19172 3.56136
H -3.90181 -0.13032 1.65488
H -4.09279 -1.45336 2.81960
H -5.24211 -0.11098 2.81524
H 0.50751 -3.12949 2.06485
H 0.21957 -2.75073 3.74909
H 0.05504 -5.48682 2.15349
H 0.03381 -5.27780 3.91230
H -1.30056 -6.11988 3.10374
H -1.66114 -3.69541 4.99048
H -2.83784 -2.83613 3.98458
H -2.94358 -4.59108 4.16016
H -2.76249 -3.09448 1.42334
H -1.56461 -4.15208 0.68515
H -2.89186 -4.85342 1.62844
H 0.31609 0.20874 -5.79828
H 2.60772 -1.08595 -4.90312
H 3.69136 -4.08240 -0.87977
H 5.61609 -2.75280 -0.09128
H 5.78750 -0.35913 -0.64924
H 0.89568 -2.65621 -2.94549
H 1.41888 -4.58780 -0.63261
H 0.35349 -3.16407 -0.60343
H -0.02534 -4.54191 -1.64902
H 2.64555 -3.92318 -4.21040
H 2.77473 -5.07446 -2.87562
H 1.26164 -4.94315 -3.77989
H 3.08617 1.58182 -2.28607
H 4.33244 1.90191 -0.10193
H 5.85603 1.78016 -0.99903
H 4.72896 3.08297 -1.35941
H 5.84587 0.86998 -3.41174
H 4.31663 0.76288 -4.29604
H 4.93157 2.34094 -3.78579
H -2.30188 4.41410 -4.35571
H -4.46196 3.25301 -4.07906
H -4.52356 0.83463 -3.60466
H 1.02101 2.71949 -3.93699
H -0.41784 5.40905 -3.66846
H 0.18562 4.43053 -2.32402
H 1.31319 5.10835 -3.51143
H 0.38608 2.81988 -6.35101
H -0.37370 4.39334 -6.09004
H 1.37615 4.21355 -5.88650
H -1.46999 -1.24691 -3.03232
H -3.75896 -1.33550 -5.06901
H -2.03674 -1.41279 -5.46442
H -2.79201 -2.72038 -4.53687
H -3.22568 -0.79702 -1.33306
H -4.48615 -1.07788 -2.55495
H -3.39520 -2.38447 -2.09219
132
2 - Cu + CO2 4-Cu + TaO complex
C -2.23988 2.42234 -4.05931
C -0.83712 2.42940 -4.16742
C -0.10286 3.59426 -4.45836
C -0.82092 4.77908 -4.64521
C -2.20698 4.80342 -4.54118
C -2.90497 3.63759 -4.24977
N -0.12418 1.18970 -4.00656
C 0.26167 0.66304 -2.80847
N 0.88441 -0.49967 -3.15235
C 0.88369 -0.69233 -4.52327
C 0.24600 0.37525 -5.06411
C 1.46096 -1.43090 -2.21595
C 0.65443 -2.47073 -1.72016
C 1.23987 -3.36683 -0.81970
C 2.57328 -3.23920 -0.44835
C 3.34850 -2.20491 -0.96088
C 2.81079 -1.27286 -1.85307

C	-0.80116	-2.64811	-2.11893
C	-1.02780	-3.99750	-2.81634
C	3.67971	-0.14384	-2.38338
C	4.87095	-0.67986	-3.19010
Cu	-0.04486	1.36684	-1.06375
O	-0.98132	-4.51423	2.21864
Ta	-0.72630	-3.80568	3.77236
C	-0.59090	-5.41708	5.21463
C	-0.34584	-6.90296	4.86502
C	-0.20967	-7.71932	6.16168
C	1.41219	3.59910	-4.58713
C	1.84288	3.85050	-6.03989
C	-3.03807	1.16462	-3.75716
C	-3.80933	1.29264	-2.43620
C	2.06344	4.61157	-3.63554
C	-3.97514	0.80635	-4.91978
C	-0.39764	2.07788	0.68310
C	-0.40834	3.54939	1.09226
C	-1.24048	4.36195	0.08689
C	-0.59583	1.05279	1.45534
O	-0.77844	0.06303	2.10053
C	1.06527	-2.60332	3.54423
C	1.87784	-2.09701	4.76077
C	2.79475	-3.20799	5.29095
C	-2.39004	-2.50486	4.23918
C	-3.87117	-2.74212	3.87182
C	-4.73277	-1.63391	4.50169
C	0.93548	-1.63232	5.88343
C	2.74854	-0.90525	4.32559
C	4.14591	0.77828	-1.24778
C	-1.73152	-2.48517	-0.90932
C	1.03282	4.09075	1.09783
C	-1.01247	3.72894	2.49443
C	-4.05035	-2.71044	2.34863
C	-4.33423	-4.10237	4.41434
C	-1.52145	-7.45491	4.04715
C	0.94885	-7.03813	4.04885
H	-0.83617	4.25929	-0.92617
H	-2.27738	4.01140	0.06874
H	-1.24171	5.42800	0.34855
H	1.64992	3.54284	1.81723
H	1.49225	3.97575	0.11007
H	1.05429	5.15555	1.36487
H	-2.04375	3.36150	2.52427
H	-0.43480	3.17741	3.24466
H	-1.01985	4.78589	2.78733
H	1.73820	-3.05851	2.80352
H	0.62307	-1.73215	3.02039
H	2.22362	-4.08325	5.61971
H	3.49266	-3.54079	4.51424
H	3.38631	-2.85733	6.14499
H	0.25155	-0.85191	5.53130
H	0.33176	-2.46241	6.27939
H	1.49877	-1.22453	6.73121
H	3.43220	-1.19770	3.52085
H	2.12883	-0.08331	3.95238
H	3.35211	-0.52730	5.16061
H	-2.30789	-2.38949	5.33923
H	-2.05792	-1.53630	3.82043
H	-4.64223	-1.63518	5.59458
H	-4.42525	-0.64628	4.14070
H	-5.79289	-1.76823	4.25360
H	-3.72873	-1.74687	1.93878
H	-3.45949	-3.49459	1.86581
H	-5.10357	-2.85745	2.08039
H	-3.77765	-4.92514	3.95036
H	-4.19525	-4.16547	5.50077
H	-5.39837	-4.26636	4.20677
H	0.18432	-5.08160	5.93160
H	-1.54267	-5.32615	5.77642
H	0.63254	-7.36398	6.76725
H	-1.11695	-7.64228	6.77201
H	-0.04113	-8.78122	5.94490
H	-2.45748	-7.39410	4.61541
H	-1.64785	-6.89548	3.11474
H	-1.35626	-8.50873	3.79347
H	0.86460	-6.51115	3.09169
H	1.80660	-6.62720	4.59486
H	1.16699	-8.09072	3.83243
H	0.02068	0.62737	-6.08808

H 1.32948 -1.56227 -4.97866
H 0.63781 -4.16287 -0.39166
H 3.00992 -3.95029 0.24767
H 4.38811 -2.11346 -0.65854
H -1.05474 -1.86263 -2.83851
H -1.54167 -3.24882 -0.14874
H -1.59964 -1.50806 -0.43558
H -2.77725 -2.57592 -1.22357
H -0.38299 -4.11201 -3.69414
H -0.82497 -4.83499 -2.14081
H -2.06887 -4.08407 -3.14526
H 3.07033 0.46139 -3.06223
H 3.29381 1.18335 -0.69397
H 4.78542 0.24414 -0.53682
H 4.72525 1.61643 -1.65042
H 5.54436 -1.27445 -2.56356
H 4.54196 -1.31505 -4.01886
H 5.45370 0.14866 -3.60696
H -0.28492 5.69615 -4.87264
H -2.74538 5.73589 -4.68690
H -3.98786 3.66777 -4.16914
H 1.77798 2.60785 -4.30122
H 1.78393 5.64083 -3.88448
H 1.77062 4.42569 -2.59838
H 3.15457 4.54317 -3.69961
H 1.41509 3.10786 -6.72097
H 1.52143 4.83948 -6.38445
H 2.93345 3.80448 -6.13049
H -2.33180 0.33721 -3.63882
H -4.73216 1.58169 -5.08033
H -3.42362 0.68123 -5.85725
H -4.50162 -0.13030 -4.70812
H -3.13173 1.50029 -1.60243
H -4.55146 2.09729 -2.48028
H -4.34272 0.36142 -2.21815
132
2 - Au + CO2 - C-C coupling adduct
C -2.13120 1.07041 -2.92912
C -1.43791 -0.11353 -3.23866
C -2.08646 -1.34825 -3.43523
C -3.47533 -1.37676 -3.28154
C -4.18483 -0.22931 -2.94661
C -3.51849 0.97867 -2.77725
N -0.01422 -0.06015 -3.43864
C 0.93906 -0.02477 -2.46068
N 2.11626 -0.04897 -3.15796
C 1.89556 -0.10303 -4.52412
C 0.55428 -0.10290 -4.70145
C 3.44224 -0.04114 -2.59497
C 4.20342 1.14151 -2.68467
C 5.50928 1.10646 -2.18667
C 6.03466 -0.05083 -1.62449
C 5.26354 -1.20467 -1.55902
C 3.95379 -1.23296 -2.04766
C 3.67876 2.41577 -3.33174
C 4.30722 2.62183 -4.71972
C 3.17202 -2.53652 -2.01794
C 3.76545 -3.54424 -3.01485
Au 0.77181 0.18483 -0.41776
C 0.99659 0.70068 1.59155
C 2.19130 1.60428 1.89411
C 2.23714 1.93638 3.39707
C -1.34712 -2.61460 -3.84630
C -1.57669 -3.77281 -2.86800
C -1.44810 2.42508 -2.83147
C -1.81615 3.29748 -4.04224
C -1.72632 -3.02884 -5.27672
C -1.76051 3.14317 -1.51400
Ta -0.35285 -0.37499 2.39535
C -1.46149 0.95432 3.72842
C -2.33531 2.20558 3.48336
C -3.48769 1.87728 2.52353
O -7.34241 1.10354 1.18013
C -7.08913 1.39286 0.07861
O -6.84164 1.68255 -1.02655
C -1.70261 -1.41101 0.97661
C -2.66982 -2.53841 1.43144
C -3.34702 -2.19849 2.76632
C 0.87845 -1.76427 3.59798
C 0.78996 -2.18455 5.08681

C	1.68986	-3.41333	5.31778
C	3.09263	-3.13030	-0.60588
C	3.90557	3.65899	-2.46163
C	2.10334	2.93036	1.11618
C	3.50704	0.89355	1.52430
C	-3.77725	-2.72332	0.37908
C	-1.90944	-3.86493	1.57329
C	-0.63976	-2.55113	5.50541
C	1.29216	-1.04286	5.98245
C	-2.93631	2.68391	4.81824
C	-1.49920	3.34207	2.88425
H	2.06007	2.73859	0.03898
H	1.20123	3.48544	1.39008
H	2.97441	3.56644	1.32498
H	3.59663	-0.05513	2.06385
H	3.54729	0.67311	0.45310
H	4.37417	1.51724	1.78077
H	1.33465	2.47105	3.70589
H	2.31993	1.02593	3.99863
H	3.10248	2.57211	3.62614
H	0.67200	-2.66176	2.97162
H	1.93044	-1.52577	3.38969
H	-1.31292	-1.68938	5.43174
H	-1.04414	-3.35609	4.88103
H	-0.66623	-2.89653	6.54634
H	2.32733	-0.77814	5.73862
H	0.67918	-0.14320	5.86461
H	1.26252	-1.33246	7.04016
H	1.35345	-4.26546	4.71543
H	2.72719	-3.19636	5.03814
H	1.68246	-3.72314	6.37094
H	-2.08509	0.21613	4.27706
H	-0.65978	1.22646	4.44304
H	-3.56132	1.90508	5.27110
H	-2.14659	2.93718	5.53500
H	-3.56058	3.57575	4.67854
H	-0.69501	3.64084	3.56615
H	-1.03935	3.02848	1.94280
H	-2.12189	4.22626	2.69810
H	-3.11110	1.57504	1.53997
H	-4.11110	1.06523	2.91458
H	-4.13452	2.75213	2.38181
H	-2.31262	-0.53064	0.68196
H	-1.22714	-1.72209	0.03424
H	-4.36578	-1.80561	0.26838
H	-3.35362	-2.96230	-0.60089
H	-4.46345	-3.53314	0.66051
H	-1.42580	-4.14402	0.62993
H	-1.12854	-3.80250	2.33822
H	-2.58773	-4.68001	1.85445
H	-2.62161	-2.09798	3.57988
H	-3.90695	-1.25974	2.69701
H	-4.05233	-2.98594	3.06016
H	-0.04719	-0.13449	-5.59556
H	2.70737	-0.14332	-5.23185
H	5.68645	-2.10660	-1.12657
H	7.05053	-0.05427	-1.23920
H	6.12205	2.00150	-2.23884
H	2.14593	-2.32389	-2.33125
H	4.07970	-3.41819	-0.22789
H	2.65253	-2.41412	0.09376
H	2.46967	-4.03115	-0.61210
H	3.78619	-3.13990	-4.03230
H	4.79202	-3.81405	-2.74361
H	3.17147	-4.46449	-3.02711
H	2.59717	2.30695	-3.46461
H	3.49617	3.52797	-1.45764
H	4.96975	3.89858	-2.36395
H	3.41962	4.52739	-2.91902
H	5.39258	2.74745	-4.63984
H	4.12303	1.77409	-5.38676
H	3.89970	3.52008	-5.19582
H	-4.08856	1.87038	-2.53478
H	-5.26336	-0.27093	-2.82560
H	-4.00778	-2.31272	-3.42542
H	-0.36663	2.26204	-2.85606
H	-2.82650	3.37580	-1.41754
H	-1.45934	2.53258	-0.65838
H	-1.21253	4.08997	-1.46372
H	-1.55032	2.81017	-4.98618

H -2.89108 3.50742 -4.06779
H -1.28966 4.25694 -3.99561
H -0.27395 -2.40059 -3.83973
H -2.79049 -3.27819 -5.34742
H -1.52814 -2.22912 -5.99760
H -1.15560 -3.91152 -5.58456
H -1.28077 -3.49698 -1.85249
H -2.62704 -4.08138 -2.84129
H -0.98696 -4.64470 -3.17118
132
2 - Au + CO2 - C-C coupling TS
C -1.79291 1.90564 -3.69332
C -1.50593 0.52634 -3.75310
C -2.50452 -0.45103 -3.91217
C -3.83060 -0.01241 -3.99022
C -4.14587 1.33704 -3.91052
C -3.13639 2.28248 -3.76542
N -0.12697 0.10048 -3.72957
C 0.67021 -0.02870 -2.62776
N 1.87055 -0.43446 -3.13673
C 1.81808 -0.56290 -4.51375
C 0.56133 -0.22419 -4.88709
C 3.08639 -0.62801 -2.38488
C 4.03159 0.41419 -2.37410
C 5.22560 0.19284 -1.67978
C 5.46354 -1.00936 -1.02676
C 4.51309 -2.02426 -1.06199
C 3.30456 -1.86320 -1.74505
C 3.82282 1.72788 -3.11311
C 4.71186 1.79199 -4.36519
C 2.30307 -3.00461 -1.83045
C 2.57732 -3.87151 -3.07139
Au 0.27849 0.40858 -0.65194
C 0.10262 1.20160 1.28835
C 0.89478 2.49412 1.50911
C 0.47970 3.15688 2.83416
C -2.19660 -1.93480 -4.03968
C -3.07338 -2.79090 -3.11854
C -0.69820 2.95994 -3.62086
C -0.19710 3.31248 -5.03221
C -2.34199 -2.39944 -5.49786
C -1.12665 4.23181 -2.88236
Ta -0.71530 -0.30752 2.16938
C -1.82953 0.30048 3.93480
C -3.11834 0.95969 4.47024
C -4.36596 0.25732 3.91830
O -2.90701 0.49089 0.90379
C -2.50946 1.59499 0.71043
O -2.48449 2.73163 0.41697
C -1.23808 -2.03851 0.86185
C -2.15629 -3.18354 1.37723
C -3.61835 -2.71728 1.39859
C 1.02976 -1.28518 3.12989
C 1.60984 -1.33380 4.57007
C 2.90456 -2.16986 4.54492
C 2.27407 -3.87723 -0.57179
C 4.06304 2.95143 -2.21933
C 0.69358 3.53152 0.38791
C 2.39464 2.14638 1.58060
C -2.04260 -4.39863 0.43897
C -1.76351 -3.65156 2.78683
C 0.63411 -2.00638 5.54646
C 1.95728 0.06556 5.09308
C -3.14180 0.84243 6.00782
C -3.16303 2.44992 4.10917
H 1.00566 3.12803 -0.58201
H -0.35429 3.82623 0.30768
H 1.29066 4.43044 0.59134
H 2.59224 1.43465 2.38659
H 2.73339 1.68589 0.64660
H 2.99481 3.04828 1.76231
H -0.57654 3.43804 2.80927
H 0.63598 2.48142 3.68051
H 1.07170 4.06343 3.01517
H 0.81124 -2.33442 2.85443
H 1.84970 -0.98479 2.45880
H -0.28936 -1.43057 5.65774
H 0.36758 -3.01397 5.20674
H 1.08513 -2.09895 6.54211
H 2.67150 0.57055 4.43399

H 1.06714 0.69758 5.17088
H 2.40984 0.00713 6.09095
H 2.70710 -3.18605 4.18390
H 3.65031 -1.71779 3.88068
H 3.34906 -2.24977 5.54529
H -1.79328 -0.72913 4.36032
H -0.96558 0.80942 4.41257
H -3.12963 -0.20746 6.32331
H -2.27142 1.33648 6.45492
H -4.04346 1.30703 6.42648
H -2.29673 2.97988 4.51946
H -3.16838 2.60942 3.02828
H -4.06574 2.91808 4.52025
H -4.42287 0.34104 2.83013
H -4.36319 -0.80781 4.17826
H -5.27660 0.69769 4.34267
H -1.62275 -1.70715 -0.11370
H -0.24253 -2.46521 0.63770
H -2.31214 -4.13131 -0.58750
H -1.01802 -4.78837 0.42586
H -2.70579 -5.21335 0.75868
H -0.72927 -4.01231 2.81460
H -1.85774 -2.85143 3.52997
H -2.41035 -4.47437 3.11625
H -3.75595 -1.86663 2.07179
H -3.94595 -2.40044 0.40220
H -4.28346 -3.52396 1.73169
H 0.09459 -0.18272 -5.85783
H 2.67305 -0.87431 -5.09186
H 4.71387 -2.95892 -0.54905
H 6.39532 -1.15943 -0.48846
H 5.97672 0.97669 -1.65051
H 1.30680 -2.56267 -1.93898
H 3.18711 -4.47311 -0.46359
H 2.14848 -3.27505 0.33222
H 1.43799 -4.58058 -0.63049
H 2.52206 -3.29136 -3.99747
H 3.57497 -4.32129 -3.01671
H 1.84503 -4.68324 -3.14031
H 2.77951 1.77059 -3.44210
H 3.43698 2.92320 -1.32437
H 5.10752 3.02312 -1.89815
H 3.82937 3.86846 -2.77061
H 5.77268 1.76612 -4.09328
H 4.52430 0.95229 -5.04180
H 4.53025 2.71940 -4.91878
H -3.39738 3.33370 -3.70776
H -5.18294 1.65657 -3.96444
H -4.62591 -0.74155 -4.11125
H 0.13742 2.52857 -3.05835
H -1.85469 4.81362 -3.45888
H -1.56048 4.00424 -1.90595
H -0.25621 4.87606 -2.72484
H 0.19537 2.43910 -5.56125
H -1.00966 3.73342 -5.63498
H 0.60235 4.05937 -4.97754
H -1.15618 -2.09321 -3.73695
H -3.37099 -2.26369 -5.84817
H -1.68778 -1.84118 -6.17459
H -2.09342 -3.46221 -5.58918
H -3.01315 -2.44788 -2.08286
H -4.12567 -2.77078 -3.42104
H -2.74667 -3.83530 -3.15376
132
2 - Au + CO2 - C-C coupling product
C 3.52516 -1.78656 -1.76828
C 3.25707 -0.55756 -2.39747
C 4.16582 0.51821 -2.38688
C 5.36870 0.33519 -1.69844
C 5.65383 -0.86185 -1.05179
C 4.74223 -1.90988 -1.09067
N 2.02911 -0.41163 -3.13641
C 0.80721 -0.11061 -2.60752
N -0.01866 -0.06158 -3.69402
C 0.67345 -0.32820 -4.86322
C 1.96171 -0.55449 -4.51225
C -1.44120 0.17728 -3.66505
C -1.91276 1.49800 -3.52841
C -3.29809 1.67937 -3.49830
C -4.17160 0.60450 -3.62265

C	-3.67603	-0.68121	-3.79475
C	-2.29928	-0.92637	-3.81989
C	-0.97772	2.69728	-3.50143
C	-1.48024	3.84766	-2.62372
C	-1.79632	-2.34542	-4.04018
C	-2.14950	-2.84120	-5.45066
Au	0.37771	0.46246	-0.68672
Ta	-0.93478	-0.22198	2.42187
C	1.14383	-0.58095	3.15449
C	1.64170	-1.57112	4.25521
C	1.34715	-1.02893	5.66180
C	3.90442	1.82393	-3.12336
C	4.17593	3.05958	-2.25577
C	2.57780	-2.97293	-1.83934
C	2.20097	-3.49090	-0.44615
C	4.72976	1.88807	-4.41882
C	3.17082	-4.09321	-2.70749
C	0.01837	1.42487	1.16475
C	-1.35910	1.94799	1.06540
O	-1.84642	3.05099	0.90421
C	1.10793	2.50427	1.46645
C	2.54173	1.95069	1.40397
C	0.86816	3.14186	2.84868
C	1.04150	3.63798	0.41677
C	-2.32175	-3.31132	-2.97276
C	-0.71407	3.18757	-4.93608
C	-1.76137	0.17001	4.38158
C	-3.01687	0.98800	4.78163
C	-2.81857	2.46906	4.43090
O	-2.17598	0.86215	1.38543
C	-1.28593	-2.15482	1.49497
C	-2.58891	-2.98724	1.62292
C	-2.95204	-3.24152	3.09323
C	-4.27595	0.46752	4.07585
C	-3.21302	0.86291	6.30359
C	-3.75051	-2.26191	0.92903
C	-2.37474	-4.35591	0.95120
C	3.17134	-1.70287	4.11387
C	1.03483	-2.97456	4.13221
H	1.21340	3.23874	-0.59026
H	0.06819	4.12881	0.42384
H	1.81939	4.38447	0.62493
H	2.75356	1.20455	2.16985
H	2.73571	1.48266	0.43175
H	3.25876	2.77126	1.53487
H	-0.11954	3.61088	2.88999
H	0.93295	2.40218	3.65429
H	1.61588	3.91827	3.05354
H	1.64378	-0.85404	2.20649
H	1.58080	0.39095	3.40782
H	-0.05076	-2.96023	4.27842
H	1.24026	-3.41487	3.14959
H	1.45801	-3.64753	4.88822
H	1.75015	-0.01686	5.78712
H	0.27489	-0.99207	5.87208
H	1.81025	-1.66656	6.42479
H	3.44122	-2.10964	3.13249
H	3.66041	-0.72751	4.21527
H	3.58714	-2.36904	4.88119
H	-1.84481	-0.85006	4.80881
H	-0.89164	0.61538	4.89701
H	-3.36732	-0.18154	6.60022
H	-2.33857	1.24043	6.84640
H	-4.08673	1.43760	6.63466
H	-1.92118	2.87144	4.91549
H	-2.72760	2.62371	3.35245
H	-3.67483	3.05985	4.77778
H	-4.18451	0.56324	2.98992
H	-4.46866	-0.58326	4.32340
H	-5.15553	1.04261	4.38921
H	-1.07100	-1.98349	0.42565
H	-0.43849	-2.75647	1.86463
H	-2.10195	-4.24501	-0.10288
H	-1.57257	-4.91493	1.44702
H	-3.28635	-4.96453	0.99929
H	-2.14148	-3.75662	3.62138
H	-3.16810	-2.31051	3.62575
H	-3.84586	-3.87261	3.16551
H	-3.95595	-1.29134	1.39038
H	-3.52645	-2.07600	-0.12660

H -4.66753 -2.86142 0.97954
H 0.18504 -0.33854 -5.82429
H 2.82762 -0.80577 -5.10309
H 4.97991 -2.84496 -0.59176
H 6.59359 -0.97987 -0.51945
H 6.09175 1.14467 -1.66769
H 1.65256 -2.63915 -2.31847
H 3.06999 -3.89040 0.08747
H 1.76466 -2.69363 0.16179
H 1.46601 -4.29834 -0.52891
H 3.39901 -3.74043 -3.71850
H 4.09841 -4.48395 -2.27504
H 2.46512 -4.92676 -2.79039
H 2.84477 1.85037 -3.39834
H 3.61422 3.02518 -1.31949
H 5.23868 3.16044 -2.01115
H 3.88133 3.96527 -2.79616
H 5.80263 1.87220 -4.19767
H 4.51734 1.04424 -5.08265
H 4.51335 2.81123 -4.96694
H -3.69886 2.67949 -3.37385
H -5.24440 0.77320 -3.59141
H -4.36667 -1.51242 -3.90643
H -0.02312 2.36732 -3.07825
H -2.36995 4.32715 -3.04727
H -1.71298 3.51803 -1.60767
H -0.70662 4.61923 -2.55680
H -0.28592 2.40224 -5.56745
H -1.64432 3.52460 -5.40700
H -0.01602 4.03173 -4.92846
H -0.70497 -2.34092 -3.95684
H -3.23432 -2.89262 -5.59183
H -1.74905 -2.17938 -6.22540
H -1.74340 -3.84456 -5.61826
H -2.04498 -2.97043 -1.97218
H -3.41234 -3.40259 -3.00635
H -1.90212 -4.31182 -3.12380
132
2 - Au + CO2 - C-O activation TS
C 3.86919 -1.29364 -1.91449
C 3.44726 -0.10015 -2.52839
C 4.23058 1.06979 -2.54455
C 5.46705 1.02193 -1.89415
C 5.90261 -0.13680 -1.26142
C 5.11324 -1.28069 -1.27629
N 2.18797 -0.09472 -3.22827
C 0.95864 0.10666 -2.67064
N 0.09768 0.01683 -3.72492
C 0.77556 -0.23497 -4.90525
C 2.09083 -0.31040 -4.59246
C -1.34068 0.09383 -3.65591
C -1.95603 1.35879 -3.59612
C -3.35209 1.38544 -3.54611
C -4.09819 0.21209 -3.57186
C -3.46200 -1.01931 -3.65984
C -2.06714 -1.10928 -3.70462
C -1.15831 2.65225 -3.66460
C -1.75216 3.78024 -2.81509
C -1.40495 -2.47276 -3.83842
C -1.72289 -3.10449 -5.20279
Au 0.55122 0.68543 -0.76462
Ta -1.07920 -0.07978 2.26988
C 0.98139 -1.07452 2.65350
C 1.43843 -1.87139 3.91349
C 1.74304 -0.91019 5.07300
C 3.80260 2.33268 -3.27709
C 3.97668 3.59940 -2.43045
C 3.06099 -2.57970 -1.98032
C 2.92077 -3.26009 -0.61409
C 4.56079 2.46938 -4.60762
C 3.67134 -3.54043 -3.01373
C 0.26189 1.57320 1.14931
C -0.88227 2.32089 0.95200
O -1.57221 3.26532 0.86030
C 1.46635 2.46569 1.64700
C 2.82009 1.82120 1.31272
C 1.36442 2.66094 3.16778
C 1.45713 3.85425 0.97709
C -1.79066 -3.41896 -2.69573
C -1.00481 3.09969 -5.12835

C	-1.82894	0.41804	4.22718
C	-2.88839	1.44471	4.69126
C	-2.36702	2.87149	4.47208
O	-2.15029	0.76346	1.09237
C	-1.69431	-2.09554	1.62094
C	-3.14917	-2.62360	1.54799
C	-3.80043	-2.59370	2.93856
C	-4.20681	1.27253	3.92543
C	-3.15290	1.24498	6.19479
C	-4.00165	-1.80927	0.56751
C	-3.11621	-4.09129	1.07961
C	2.74029	-2.63135	3.59002
C	0.40624	-2.90198	4.39551
H	1.46015	3.76017	-0.11458
H	0.58352	4.44769	1.25936
H	2.35064	4.41675	1.27301
H	2.92877	0.82522	1.74519
H	2.95646	1.72590	0.23048
H	3.63140	2.44787	1.70359
H	0.42517	3.15258	3.44070
H	1.41650	1.70277	3.69249
H	2.18648	3.28924	3.53281
H	1.04179	-1.75993	1.78667
H	1.77822	-0.35067	2.45839
H	-0.54967	-2.43331	4.65543
H	0.21092	-3.66146	3.63021
H	0.76923	-3.42483	5.28964
H	2.50710	-0.17850	4.78559
H	0.85169	-0.35907	5.39016
H	2.11905	-1.45542	5.94794
H	2.57859	-3.35891	2.78628
H	3.52384	-1.93893	3.26082
H	3.11986	-3.17710	4.46465
H	-2.15294	-0.60208	4.53026
H	-0.89884	0.58201	4.80322
H	-3.53163	0.23652	6.39851
H	-2.23542	1.38230	6.77931
H	-3.89607	1.96274	6.56349
H	-1.42047	3.03218	5.00163
H	-2.21188	3.08103	3.40976
H	-3.08680	3.60661	4.85154
H	-4.05014	1.36299	2.84633
H	-4.65862	0.29480	4.12769
H	-4.93125	2.03568	4.23461
H	-1.25151	-2.12372	0.60743
H	-1.10337	-2.80869	2.21067
H	-2.64802	-4.18273	0.09383
H	-2.54726	-4.71632	1.77821
H	-4.13034	-4.50549	1.00908
H	-3.18885	-3.13051	3.67413
H	-3.93671	-1.56817	3.29264
H	-4.78944	-3.06782	2.91715
H	-4.03525	-0.75377	0.84793
H	-3.58775	-1.85840	-0.44552
H	-5.02660	-2.20015	0.53232
H	0.25871	-0.34540	-5.84482
H	2.95895	-0.50066	-5.20240
H	5.46966	-2.18263	-0.78794
H	6.86595	-0.15002	-0.75912
H	6.09783	1.90575	-1.88400
H	2.05052	-2.32743	-2.31627
H	3.88225	-3.62407	-0.23671
H	2.50147	-2.57743	0.12965
H	2.25602	-4.12639	-0.69522
H	3.72655	-3.08460	-4.00770
H	4.68701	-3.83274	-2.72532
H	3.06941	-4.45209	-3.09211
H	2.73597	2.24318	-3.50791
H	3.45990	3.51553	-1.47151
H	5.03127	3.81455	-2.22829
H	3.56720	4.46372	-2.96369
H	5.63802	2.56876	-4.43467
H	4.40898	1.60047	-5.25535
H	4.22436	3.35827	-5.15188
H	-3.86408	2.33993	-3.48477
H	-5.18248	0.25998	-3.52607
H	-4.05507	-1.92883	-3.69031
H	-0.15788	2.44910	-3.26757
H	-2.70490	4.14057	-3.21827
H	-1.91411	3.46741	-1.78073

H -1.06737 4.63461 -2.80765
H -0.51357 2.33612 -5.74004
H -1.98410 3.30555 -5.57455
H -0.40754 4.01600 -5.18891
H -0.32024 -2.33472 -3.78668
H -2.79559 -3.29805 -5.30949
H -1.42254 -2.45461 -6.03121
H -1.19955 -4.06018 -5.31403
H -1.53561 -2.98861 -1.72404
H -2.86340 -3.63746 -2.69378
H -1.26085 -4.37223 -2.79809
132
2 - Au + CO2 - C-O activation product (4-Au + TaO complex)
C -1.61655 -0.43621 -1.47420
C -1.00165 0.68710 -2.05516
C -1.41135 2.00547 -1.78609
C -2.47600 2.17652 -0.89715
C -3.09743 1.08521 -0.30106
C -2.67222 -0.20767 -0.58502
N 0.09280 0.48020 -2.97016
C 1.40556 0.43072 -2.60884
N 2.06760 0.22669 -3.78306
C 1.18548 0.15030 -4.84971
C -0.05881 0.31056 -4.33619
C 3.49579 0.10803 -3.91138
C 4.08394 -1.16194 -3.76911
C 5.47200 -1.24692 -3.91381
C 6.23758 -0.11997 -4.19022
C 5.62697 1.12083 -4.33189
C 4.24291 1.26508 -4.19731
C 3.27378 -2.41749 -3.49110
C 3.33067 -3.38395 -4.68369
C 3.60538 2.63444 -4.36862
C 3.79923 3.16268 -5.79783
Au 2.15605 0.58724 -0.73634
C 2.88584 0.72752 1.17924
C 4.35666 0.88554 1.57540
C 4.90807 2.19778 0.99193
C -0.74117 3.22125 -2.40475
C -1.72425 4.03314 -3.26022
C -1.17646 -1.86103 -1.76850
C -0.67388 -2.56153 -0.49807
C -0.08226 4.09750 -1.32965
C -2.30252 -2.66525 -2.43481
C 4.12938 3.63582 -3.33061
C 3.71861 -3.10636 -2.19408
Ta -3.80724 -2.64383 3.62138
C -4.15142 -4.72870 4.10495
C -4.21149 -5.88774 3.08551
C -4.38943 -7.21840 3.83692
C -1.72221 -2.17317 3.95602
C -1.18814 -1.72152 5.33751
C -1.87380 -2.50615 6.46785
C -5.23240 -1.41082 4.68854
C -6.43226 -0.66904 4.05959
C -7.22976 0.04471 5.16443
O -4.05483 -2.43649 1.92503
C -1.43388 -0.21722 5.52480
C 0.32761 -1.97676 5.40088
C 1.89942 0.67113 2.03567
O 0.96609 0.61308 2.76848
C 5.17151 -0.29195 1.01426
C 4.51523 0.91646 3.10391
C -5.93341 0.37240 3.04839
C -7.35024 -1.67320 3.34663
C -5.39602 -5.68858 2.13034
C -2.90625 -5.93796 2.27827
H 4.81881 2.19952 -0.09936
H 4.35004 3.05764 1.37660
H 5.96682 2.32852 1.25066
H 4.81562 -1.24142 1.42752
H 5.07507 -0.34187 -0.07543
H 6.23563 -0.18575 1.26218
H 3.96234 1.75509 3.54151
H 4.14305 -0.00886 3.55736
H 5.56946 1.02683 3.38386
H -1.31631 -3.18401 3.72877
H -1.31384 -1.52645 3.16850
H -2.95781 -2.31982 6.50106
H -1.71617 -3.58612 6.35835

H -1.47872 -2.21478 7.44796
H -0.92270 0.35627 4.74574
H -2.50106 0.03022 5.48381
H -1.05535 0.11969 6.49703
H 0.55371 -3.04387 5.28845
H 0.84084 -1.43072 4.60369
H 0.74175 -1.64578 6.36150
H -5.60148 -2.07760 5.49374
H -4.58724 -0.67867 5.21393
H -7.61433 -0.67102 5.90045
H -6.60377 0.76977 5.69717
H -8.08685 0.58599 4.74589
H -5.27915 1.10847 3.53101
H -5.37292 -0.10756 2.23975
H -6.77494 0.91637 2.60387
H -6.82591 -2.16979 2.52299
H -7.70946 -2.44300 4.04071
H -8.22966 -1.16969 2.92848
H -3.38042 -4.95373 4.86743
H -5.10250 -4.69397 4.67295
H -3.55179 -7.40286 4.51982
H -5.31124 -7.21605 4.43007
H -4.44343 -8.06225 3.13855
H -6.34496 -5.66917 2.67997
H -5.30042 -4.74833 1.57849
H -5.45063 -6.50770 1.40394
H -2.77233 -5.02236 1.69206
H -2.03676 -6.05674 2.93638
H -2.91071 -6.78331 1.58023
H -1.02873 0.31871 -4.80722
H 1.52443 -0.00966 -5.86071
H 5.95872 -2.21225 -3.80736
H 7.31526 -0.20932 -4.29659
H 6.23427 1.99529 -4.54836
H 2.22897 -2.12178 -3.35522
H 4.75484 -3.45620 -2.25640
H 3.63962 -2.42607 -1.34153
H 3.08755 -3.97903 -1.99482
H 2.97906 -2.90825 -5.60501
H 4.35189 -3.73808 -4.86192
H 2.70306 -4.26132 -4.49447
H 2.52898 2.52984 -4.20074
H 3.94454 3.28010 -2.31325
H 5.20596 3.80457 -3.44137
H 3.62901 4.60275 -3.45067
H 4.85894 3.32003 -6.02624
H 3.39980 2.46611 -6.54205
H 3.28759 4.12297 -5.92270
H -2.81501 3.18152 -0.66130
H -3.91724 1.24161 0.39419
H -3.15717 -1.04748 -0.09461
H 0.05520 2.86850 -3.06824
H -0.82589 4.50322 -0.63515
H 0.64479 3.52392 -0.74695
H 0.43684 4.94404 -1.79271
H -2.17849 3.41843 -4.04416
H -2.53533 4.44888 -2.65297
H -1.20959 4.87180 -3.74157
H -0.33946 -1.82077 -2.47339
H -3.16093 -2.77714 -1.76442
H -2.65514 -2.18192 -3.35206
H -1.95078 -3.66978 -2.69425
H 0.15991 -2.01327 -0.04912
H -1.47083 -2.64246 0.24812
H -0.33084 -3.57492 -0.73532
132
2 - Ag + CO2 - C-C coupling adduct
C -1.69723 2.06257 -3.73569
C -1.48929 0.66883 -3.69462
C -2.54087 -0.25859 -3.80872
C -3.83498 0.24832 -3.96441
C -4.07171 1.61615 -4.00141
C -3.01348 2.51082 -3.88386
N -0.13412 0.17582 -3.64849
C 0.66468 0.05494 -2.54709
N 1.85701 -0.36686 -3.06591
C 1.79632 -0.51178 -4.44158
C 0.54048 -0.16728 -4.81021
C 3.09314 -0.51334 -2.33602
C 4.01361 0.55091 -2.38166

C	5.22365	0.38622	-1.69948
C	5.50424	-0.78503	-1.00909
C	4.58295	-1.82693	-0.99682
C	3.35896	-1.72180	-1.66336
C	3.76827	1.82793	-3.17338
C	4.67071	1.87225	-4.41681
C	2.39190	-2.89522	-1.70246
C	2.63141	-3.75123	-2.95827
Ag	0.29236	0.37019	-0.45974
C	0.36137	1.07647	1.59175
C	1.15148	2.37674	1.68283
C	1.06968	2.94745	3.11136
C	-2.31516	-1.76211	-3.81111
C	-3.26450	-2.49165	-2.85333
C	-0.55111	3.06295	-3.70070
C	-0.11859	3.42977	-5.13064
C	-2.44590	-2.33182	-5.23290
C	-0.87987	4.32950	-2.90226
Ta	-0.33142	-0.47797	2.41040
C	-1.74017	0.16596	3.94848
C	-2.98502	1.07247	4.05240
C	-4.12659	0.49596	3.20490
O	-4.13357	1.03472	-0.45381
C	-3.78363	2.14581	-0.37637
O	-3.45451	3.26396	-0.30074
C	-1.01400	-2.05111	0.96518
C	-1.78999	-3.29725	1.48508
C	-3.25018	-2.92842	1.77651
C	1.45970	-1.33099	3.41038
C	1.82882	-1.46727	4.90934
C	3.12959	-2.28409	5.03298
C	2.45476	-3.77307	-0.44911
C	3.95326	3.09465	-2.32780
C	0.61888	3.44982	0.71438
C	2.63727	2.11182	1.36949
C	-1.77139	-4.40541	0.41802
C	-1.15980	-3.86337	2.76518
C	0.73237	-2.19124	5.70346
C	2.06959	-0.08483	5.53041
C	-3.45786	1.14702	5.51659
C	-2.66879	2.49216	3.56934
H	0.72794	3.12543	-0.32765
H	-0.44351	3.64146	0.89430
H	1.16561	4.39531	0.83417
H	3.05915	1.39717	2.08331
H	2.75854	1.68268	0.36894
H	3.22420	3.03927	1.42577
H	0.04101	3.20782	3.36884
H	1.43247	2.21831	3.84116
H	1.68424	3.85315	3.20185
H	1.38549	-2.35907	2.99610
H	2.32074	-0.87859	2.89839
H	-0.21343	-1.63900	5.68090
H	0.55037	-3.19433	5.30120
H	1.02198	-2.30401	6.75560
H	2.85034	0.45968	4.98731
H	1.16091	0.52582	5.51135
H	2.38911	-0.17453	6.57623
H	3.00347	-3.28824	4.61088
H	3.95013	-1.79607	4.49436
H	3.43531	-2.39716	6.08125
H	-2.00355	-0.81546	4.40147
H	-0.95745	0.57572	4.62557
H	-3.70847	0.15135	5.90171
H	-2.67646	1.56763	6.16027
H	-4.34979	1.77894	5.61595
H	-1.93125	2.96961	4.22362
H	-2.25506	2.47839	2.55637
H	-3.57058	3.11726	3.57865
H	-3.83375	0.40082	2.15486
H	-4.42234	-0.49717	3.56196
H	-5.01383	1.13957	3.25619
H	-1.56504	-1.65185	0.09933
H	-0.05644	-2.40415	0.53499
H	-2.21261	-4.05395	-0.52018
H	-0.74557	-4.72857	0.20588
H	-2.33769	-5.28708	0.74626
H	-0.11258	-4.14429	2.60528
H	-1.19085	-3.14028	3.58897
H	-1.69698	-4.75817	3.10361

H -3.31779 -2.17248 2.56403
H -3.74193 -2.52194 0.88537
H -3.82096 -3.80643 2.10422
H 0.06753 -0.12917 -5.77831
H 2.64625 -0.83292 -5.02198
H 4.82026 -2.73810 -0.45826
H 6.44765 -0.89122 -0.48073
H 5.95427 1.18975 -1.71066
H 1.37698 -2.48611 -1.76193
H 3.39237 -4.33673 -0.38986
H 2.35246 -3.18105 0.46477
H 1.64310 -4.50621 -0.47226
H 2.50911 -3.17271 -3.87861
H 3.64492 -4.16758 -2.95495
H 1.92368 -4.58663 -2.99199
H 2.72956 1.82167 -3.51855
H 3.30199 3.09034 -1.45066
H 4.98516 3.20484 -1.97854
H 3.71642 3.98084 -2.92639
H 5.72844 1.89654 -4.13333
H 4.52180 0.99854 -5.05920
H 4.46260 2.76868 -5.01057
H -3.20982 3.57753 -3.91690
H -5.08523 1.98833 -4.12426
H -4.66843 -0.44132 -4.05603
H 0.29713 2.58041 -3.20397
H -1.62638 4.95072 -3.40905
H -1.25444 4.09317 -1.90359
H 0.02179 4.94009 -2.79156
H 0.19761 2.55071 -5.70021
H -0.94323 3.90325 -5.67504
H 0.71837 4.13596 -5.10790
H -1.29387 -1.95146 -3.46437
H -3.45550 -2.17015 -5.62637
H -1.74121 -1.86450 -5.92758
H -2.25412 -3.41009 -5.23303
H -3.20110 -2.08342 -1.84151
H -4.30727 -2.42320 -3.18053
H -3.00805 -3.55500 -2.81163
132
2 - Ag + CO2 - C-C coupling TS
C -1.80522 1.89631 -3.72495
C -1.50590 0.51992 -3.78644
C -2.49752 -0.46691 -3.93273
C -3.82828 -0.04060 -3.99568
C -4.15508 1.30630 -3.91469
C -3.15297 2.26120 -3.78284
N -0.12294 0.10787 -3.77058
C 0.66649 -0.03271 -2.66599
N 1.87167 -0.41600 -3.17871
C 1.83070 -0.51829 -4.55917
C 0.57235 -0.18506 -4.93281
C 3.08311 -0.61725 -2.42188
C 4.02590 0.42717 -2.38866
C 5.21495 0.19945 -1.68781
C 5.45069 -1.01038 -1.04830
C 4.50289 -2.02675 -1.10391
C 3.29967 -1.86013 -1.79518
C 3.81955 1.75147 -3.10931
C 4.71235 1.83405 -4.35763
C 2.30382 -3.00483 -1.90429
C 2.58881 -3.84953 -3.15805
Ag 0.23697 0.32687 -0.60591
C 0.08639 1.17302 1.39304
C 0.90988 2.45208 1.52270
C 0.53505 3.18785 2.82308
C -2.17533 -1.94722 -4.06383
C -3.04343 -2.81519 -3.14569
C -0.72108 2.96237 -3.66830
C -0.27731 3.35154 -5.08918
C -2.31466 -2.40819 -5.52378
C -1.13918 4.21170 -2.88604
Ta -0.71062 -0.34359 2.23573
C -1.89930 0.24857 3.95926
C -3.14051 0.99866 4.48426
C -4.42670 0.41286 3.88533
O -2.91103 0.46631 0.88174
C -2.50166 1.57161 0.73209
O -2.46293 2.71518 0.46358
C -1.19904 -2.06044 0.87282

C	-2.12175	-3.20055	1.39809
C	-3.57480	-2.71159	1.47433
C	1.03846	-1.30026	3.20791
C	1.59411	-1.32753	4.65649
C	2.89453	-2.15474	4.66865
C	2.27189	-3.89875	-0.66059
C	4.05755	2.96157	-2.19681
C	0.70955	3.43678	0.35499
C	2.40426	2.07841	1.58294
C	-2.05814	-4.40149	0.43731
C	-1.69229	-3.69938	2.78604
C	0.60139	-1.99213	5.62102
C	1.92194	0.08240	5.16401
C	-3.21291	0.84713	6.01731
C	-3.05468	2.49522	4.16024
H	0.98688	2.97542	-0.60089
H	-0.33095	3.75797	0.28460
H	1.33737	4.32685	0.49501
H	2.60397	1.40141	2.41777
H	2.71858	1.56921	0.66488
H	3.02540	2.97545	1.71113
H	-0.51715	3.48368	2.80743
H	0.69770	2.54841	3.69579
H	1.14581	4.09175	2.94737
H	0.84023	-2.35390	2.93325
H	1.86102	-0.98749	2.54531
H	-0.33094	-1.42450	5.69581
H	0.35429	-3.00851	5.29258
H	1.02700	-2.06224	6.62966
H	2.64601	0.58090	4.51059
H	1.02683	0.71067	5.21220
H	2.35459	0.04355	6.17165
H	2.71096	-3.17720	4.31794
H	3.64994	-1.70679	4.01256
H	3.32036	-2.21774	5.67838
H	-1.96207	-0.79254	4.35322
H	-1.00836	0.67108	4.47482
H	-3.29181	-0.20762	6.30609
H	-2.31738	1.25884	6.49711
H	-4.08494	1.37259	6.42687
H	-2.15812	2.94123	4.60405
H	-3.01698	2.67836	3.08386
H	-3.92621	3.02663	4.56172
H	-4.44304	0.51136	2.79719
H	-4.52377	-0.65144	4.13030
H	-5.30853	0.92561	4.28900
H	-1.58879	-1.75049	-0.10805
H	-0.20684	-2.49906	0.65696
H	-2.36344	-4.11509	-0.57388
H	-1.03941	-4.80244	0.37889
H	-2.71820	-5.21412	0.76871
H	-0.66335	-4.07629	2.77494
H	-1.75035	-2.91249	3.54695
H	-2.34192	-4.51746	3.12157
H	-3.68054	-1.87738	2.17437
H	-3.92501	-2.36121	0.49720
H	-4.24360	-3.51634	1.80481
H	0.11003	-0.12980	-5.90511
H	2.69172	-0.81012	-5.13872
H	4.70165	-2.96730	-0.60114
H	6.37850	-1.16517	-0.50454
H	5.96381	0.98464	-1.64235
H	1.30604	-2.56595	-2.01247
H	3.18568	-4.49468	-0.55954
H	2.14237	-3.31332	0.25392
H	1.43732	-4.60249	-0.73389
H	2.53588	-3.25401	-4.07437
H	3.58825	-4.29548	-3.10506
H	1.86076	-4.66340	-3.24430
H	2.77720	1.79923	-3.44071
H	3.43322	2.91729	-1.30130
H	5.10233	3.03171	-1.87632
H	3.82011	3.88636	-2.73324
H	5.77229	1.80331	-4.08279
H	4.52636	1.00515	-5.04778
H	4.53313	2.76998	-4.89748
H	-3.42288	3.31027	-3.72478
H	-5.19561	1.61605	-3.95731
H	-4.61840	-0.77694	-4.10607
H	0.14172	2.52985	-3.14952

H -1.89390 4.79621 -3.42396
H -1.53790 3.95705 -1.90135
H -0.27224 4.86407 -2.74317
H 0.10657 2.49449 -5.65040
H -1.11714 3.77301 -5.65280
H 0.51371 4.10818 -5.04820
H -1.13324 -2.09557 -3.76159
H -3.34425 -2.27968 -5.87514
H -1.66359 -1.84209 -6.19699
H -2.05708 -3.46854 -5.61821
H -2.99203 -2.47162 -2.10962
H -4.09484 -2.80996 -3.45182
H -2.70221 -3.85495 -3.17960
132
2 - Ag + CO2 - C-C coupling product
C 3.59209 -1.75673 -1.92303
C 3.33881 -0.51879 -2.54213
C 4.25922 0.54694 -2.51729
C 5.45938 0.34335 -1.82967
C 5.73047 -0.86315 -1.19493
C 4.80652 -1.89984 -1.24447
N 2.11160 -0.35012 -3.27767
C 0.89409 -0.06325 -2.73473
N 0.06666 0.00969 -3.81621
C 0.75032 -0.22844 -4.99655
C 2.04105 -0.46171 -4.65663
C -1.35606 0.24268 -3.76325
C -1.82946 1.55918 -3.59386
C -3.21454 1.73428 -3.52981
C -4.08613 0.65762 -3.65268
C -3.58959 -0.62339 -3.85516
C -2.21286 -0.86254 -3.91412
C -0.89704 2.76076 -3.56435
C -1.39040 3.89997 -2.66681
C -1.70854 -2.27706 -4.15936
C -2.10774 -2.76973 -5.55847
Ag 0.44246 0.45770 -0.72827
Ta -0.88515 -0.16437 2.40141
C 1.18514 -0.55063 3.16902
C 1.64729 -1.53927 4.28668
C 1.35375 -0.97285 5.68393
C 4.01216 1.86685 -3.23292
C 4.26992 3.08283 -2.33362
C 2.63284 -2.93320 -2.00545
C 2.25563 -3.46577 -0.61755
C 4.85939 1.95605 -4.51242
C 3.21271 -4.04819 -2.88916
C 0.08491 1.44525 1.17681
C -1.26851 1.98035 1.01670
O -1.74744 3.08132 0.80493
C 1.20652 2.49885 1.41932
C 2.62214 1.90127 1.34790
C 1.01147 3.18721 2.78512
C 1.15297 3.60128 0.33667
C -2.18825 -3.24973 -3.07612
C -0.65346 3.26948 -4.99625
C -1.72194 0.25221 4.35817
C -2.97028 1.09312 4.73089
C -2.74778 2.56424 4.35338
O -2.11396 0.90338 1.33843
C -1.22308 -2.10259 1.45436
C -2.54448 -2.91034 1.55734
C -2.94057 -3.15129 3.02149
C -4.22858 0.57469 4.02203
C -3.18463 1.00062 6.25269
C -3.67883 -2.16751 0.83750
C -2.34312 -4.28462 0.89339
C 3.17408 -1.71461 4.16357
C 1.00274 -2.92678 4.17435
H 1.29456 3.16915 -0.66268
H 0.19362 4.11891 0.34481
H 1.95613 4.33074 0.50553
H 2.82455 1.17156 2.13184
H 2.78458 1.39865 0.38566
H 3.36832 2.70106 1.43851
H 0.03721 3.68393 2.82612
H 1.06572 2.46870 3.61005
H 1.78399 3.94784 2.95600
H 1.69631 -0.84624 2.23410
H 1.63690 0.41571 3.41944

H -0.08436 -2.87829 4.30081
H 1.21164 -3.38821 3.20215
H 1.39289 -3.60021 4.94766
H 1.78370 0.02893 5.80187
H 0.28093 -0.90325 5.88214
H 1.79084 -1.61440 6.45900
H 3.44338 -2.14186 3.19055
H 3.68781 -0.75117 4.25714
H 3.56445 -2.38126 4.94382
H -1.82622 -0.76167 4.79547
H -0.85338 0.69085 4.88053
H -3.35460 -0.03599 6.56770
H -2.31147 1.37812 6.79765
H -4.05485 1.59198 6.56331
H -1.84958 2.96288 4.83974
H -2.64256 2.69594 3.27313
H -3.59880 3.17455 4.67896
H -4.12459 0.64834 2.93545
H -4.43579 -0.46902 4.28780
H -5.10474 1.16572 4.31489
H -0.98798 -1.94849 0.38698
H -0.39634 -2.72058 1.84226
H -2.05083 -4.18037 -0.15653
H -1.55899 -4.85615 1.40363
H -3.26571 -4.87761 0.92672
H -2.14933 -3.67829 3.56687
H -3.14959 -2.21402 3.54649
H -3.84728 -3.76524 3.08018
H -3.87374 -1.18934 1.28702
H -3.43114 -1.99427 -0.21524
H -4.60788 -2.74935 0.87436
H 0.25711 -0.21768 -5.95534
H 2.90462 -0.69761 -5.25739
H 5.03259 -2.84204 -0.75369
H 6.66824 -0.99730 -0.66295
H 6.19106 1.14468 -1.78972
H 1.70937 -2.58512 -2.47780
H 3.12171 -3.88300 -0.09294
H 1.83191 -2.67377 0.00644
H 1.51082 -4.26321 -0.70789
H 3.44156 -3.68472 -3.89617
H 4.13755 -4.45309 -2.46402
H 2.49877 -4.87378 -2.98058
H 2.95770 1.90078 -3.52627
H 3.69026 3.02945 -1.40907
H 5.32784 3.17452 -2.06570
H 3.98831 4.00120 -2.85932
H 5.92844 1.93577 -4.27402
H 4.65804 1.12500 -5.19565
H 4.65225 2.88964 -5.04622
H -3.61654 2.73008 -3.37798
H -5.15856 0.82126 -3.59467
H -4.27939 -1.45578 -3.96298
H 0.06510 2.42695 -3.16087
H -2.28478 4.38299 -3.07622
H -1.61285 3.56089 -1.65124
H -0.61676 4.67163 -2.60070
H -0.23144 2.49357 -5.64309
H -1.59096 3.60956 -5.45021
H 0.04203 4.11571 -4.98711
H -0.61493 -2.26519 -4.11620
H -3.19631 -2.82711 -5.66364
H -1.73659 -2.10269 -6.34333
H -1.70193 -3.77015 -5.74326
H -1.87330 -2.91329 -2.08502
H -3.27907 -3.34340 -3.06669
H -1.77237 -4.24835 -3.24850
132
2 - Ag + CO2 - C-O activation TS
C 3.54147 -1.57082 -1.83262
C 3.28487 -0.35907 -2.50080
C 4.19286 0.71725 -2.50630
C 5.38189 0.55699 -1.78856
C 5.65383 -0.61979 -1.10059
C 4.74526 -1.67109 -1.12800
N 2.06435 -0.22979 -3.25575
C 0.84415 0.09254 -2.74058
N 0.02618 0.11479 -3.83042
C 0.71862 -0.18739 -4.99030
C 2.00486 -0.41097 -4.62714

C	-1.39272	0.37254	-3.80732
C	-1.84238	1.70497	-3.72835
C	-3.22427	1.91072	-3.70178
C	-4.11410	0.84411	-3.76674
C	-3.63939	-0.45642	-3.87646
C	-2.26718	-0.72494	-3.90132
C	-0.88717	2.88840	-3.75396
C	-1.33849	4.05552	-2.86922
C	-1.78333	-2.15851	-4.06142
C	-2.14317	-2.70413	-5.45205
Ag	0.38733	0.65948	-0.75523
Ta	-1.00074	-0.07115	2.35065
C	1.15710	-0.65961	3.02929
C	1.65207	-1.57102	4.19239
C	1.36508	-0.92056	5.55442
C	3.94815	1.99836	-3.29087
C	4.16290	3.26113	-2.44655
C	2.60393	-2.76563	-1.90881
C	2.30143	-3.36824	-0.53197
C	4.83021	2.03714	-4.54911
C	3.17225	-3.82901	-2.86241
C	0.11598	1.62374	1.20370
C	-1.05937	2.27541	0.91393
O	-1.80308	3.16001	0.69393
C	1.29646	2.61446	1.51517
C	2.65698	1.94758	1.26050
C	1.21099	3.08511	2.97845
C	1.23653	3.86646	0.61610
C	-2.31925	-3.07635	-2.95721
C	-0.67097	3.35983	-5.20230
C	-1.80890	0.37329	4.30522
C	-3.04649	1.21854	4.67922
C	-2.83533	2.67313	4.23766
O	-2.20605	0.64868	1.21060
C	-1.26966	-2.12056	1.59618
C	-2.59459	-2.92568	1.63800
C	-3.04705	-3.14001	3.09070
C	-4.31092	0.66878	4.00678
C	-3.23511	1.18555	6.20658
C	-3.71361	-2.22143	0.86003
C	-2.34994	-4.31189	1.01181
C	3.17934	-1.75166	4.07465
C	1.01496	-2.96666	4.18106
H	1.25050	3.58920	-0.44484
H	0.33778	4.46281	0.79398
H	2.10620	4.50538	0.81035
H	2.78797	1.03310	1.83929
H	2.76931	1.68553	0.20136
H	3.46747	2.63939	1.52192
H	0.26357	3.60172	3.16628
H	1.28549	2.24752	3.67701
H	2.02392	3.78583	3.20597
H	1.60301	-1.05615	2.09548
H	1.69269	0.28771	3.17765
H	-0.07019	-2.91309	4.31668
H	1.21124	-3.48862	3.23686
H	1.42059	-3.58786	4.99016
H	1.78671	0.09088	5.60475
H	0.29134	-0.84657	5.74915
H	1.80941	-1.50550	6.36982
H	3.44385	-2.22817	3.12308
H	3.69115	-0.78277	4.11354
H	3.58016	-2.37522	4.88579
H	-1.91753	-0.64806	4.72805
H	-0.92376	0.78616	4.82381
H	-3.39081	0.16049	6.56337
H	-2.35558	1.58910	6.72224
H	-4.10474	1.78154	6.51048
H	-1.92850	3.09393	4.68899
H	-2.74834	2.74668	3.14999
H	-3.68081	3.29923	4.54757
H	-4.20324	0.67529	2.91798
H	-4.51770	-0.35842	4.33049
H	-5.18458	1.27772	4.26938
H	-0.97022	-1.99329	0.53792
H	-0.47968	-2.73069	2.05154
H	-2.01674	-4.22295	-0.02818
H	-1.57866	-4.86223	1.56342
H	-3.26502	-4.91802	1.01870
H	-2.26905	-3.63864	3.68044

H -3.28724 -2.19076 3.57977
H -3.94694 -3.76605 3.13069
H -3.93941 -1.23728 1.27707
H -3.42907 -2.06440 -0.18549
H -4.62955 -2.82571 0.87326
H 0.23338 -0.22216 -5.95251
H 2.87252 -0.68160 -5.20698
H 4.97509 -2.58986 -0.59709
H 6.58194 -0.72063 -0.54495
H 6.10461 1.36726 -1.76831
H 1.65201 -2.42254 -2.32567
H 3.19338 -3.80691 -0.07247
H 1.90232 -2.61707 0.15492
H 1.55906 -4.16693 -0.62778
H 3.34232 -3.42342 -3.86511
H 4.12821 -4.21707 -2.49411
H 2.47988 -4.67301 -2.95088
H 2.90254 2.00264 -3.61635
H 3.55094 3.24900 -1.54135
H 5.20885 3.37659 -2.14380
H 3.89422 4.14923 -3.02820
H 5.89223 2.04415 -4.28100
H 4.65880 1.16985 -5.19431
H 4.62547 2.93989 -5.13433
H -3.60953 2.92211 -3.62722
H -5.18392 1.02997 -3.73596
H -4.34385 -1.28097 -3.93699
H 0.07932 2.54729 -3.36793
H -2.23176 4.54856 -3.26783
H -1.55514 3.73404 -1.84720
H -0.54925 4.81333 -2.82907
H -0.27845 2.55969 -5.83798
H -1.61340 3.70379 -5.64264
H 0.03879 4.19373 -5.23238
H -0.69176 -2.16402 -3.97910
H -3.22861 -2.74581 -5.59153
H -1.73274 -2.07965 -6.25241
H -1.75153 -3.71904 -5.57919
H -2.03676 -2.70704 -1.96843
H -3.41085 -3.15468 -2.98515
H -1.91380 -4.08704 -3.07456
132
2 - Ag + CO2 - C-O activation product (4-Ag + TaO complex)
C -2.47765 0.60703 -3.50396
C -1.43052 1.39013 -4.02227
C -1.63215 2.67755 -4.55203
C -2.93776 3.17673 -4.54895
C -3.99332 2.42676 -4.04349
C -3.76304 1.15676 -3.52860
N -0.09676 0.84507 -4.02566
C 0.81146 1.01257 -3.02514
N 1.90765 0.33439 -3.46410
C 1.68710 -0.24165 -4.70484
C 0.41894 0.08195 -5.05985
C 3.14789 0.21972 -2.74199
C 3.29578 -0.82584 -1.81286
C 4.52311 -0.92691 -1.15027
C 5.55465 -0.03022 -1.40196
C 5.37853 0.99344 -2.32586
C 4.17244 1.14410 -3.01631
C 2.19618 -1.83409 -1.52076
C 2.60256 -3.24370 -1.97598
C 4.01658 2.26845 -4.02795
C 4.91882 2.04065 -5.25026
Ag 0.52538 2.00478 -1.20751
C 0.19559 2.94339 0.63410
C 1.19829 3.81342 1.38355
C 1.58565 5.02450 0.51652
C -0.50159 3.52801 -5.10810
C -0.71939 3.85184 -6.59314
C -2.26411 -0.78602 -2.93434
C -2.73305 -0.87895 -1.47578
C -0.30992 4.80681 -4.28032
C -2.94649 -1.85084 -3.80609
C 4.27768 3.64248 -3.39650
C 1.79678 -1.82267 -0.03855
Ta -1.99641 -4.32088 4.17415
C -3.04548 -5.97861 5.09244
C -3.93227 -6.99682 4.34048
C -4.51779 -8.00413 5.34477

C	0.15136	-4.24702	4.52428
C	0.80925	-4.69051	5.85217
C	0.94059	-6.21984	5.89037
C	-2.89049	-2.45788	4.80443
C	-3.10223	-1.22297	3.90066
C	-3.62896	-0.05223	4.74792
O	-2.16395	-4.45446	2.46494
C	-0.02367	-4.21450	7.05358
C	2.21660	-4.07663	5.95476
C	-1.00730	2.63104	1.01552
O	-2.11839	2.29773	1.29629
C	2.46727	2.99849	1.69085
C	0.60489	4.32450	2.70705
C	-1.76891	-0.81229	3.25831
C	-4.12415	-1.54415	2.80170
C	-5.08260	-6.26344	3.63500
C	-3.09517	-7.75370	3.29962
H	2.02154	4.69334	-0.43285
H	0.70470	5.63185	0.28516
H	2.32035	5.65949	1.02872
H	2.22911	2.13726	2.32350
H	2.91610	2.61899	0.76603
H	3.21514	3.61243	2.20992
H	-0.29430	4.92365	2.52690
H	0.32867	3.48970	3.36034
H	1.32626	4.95090	3.24586
H	0.69446	-4.67907	3.67230
H	0.28093	-3.14939	4.40980
H	-0.03501	-6.71463	5.83166
H	1.54564	-6.58117	5.05122
H	1.42345	-6.54867	6.81790
H	-0.14193	-3.12451	7.04823
H	-1.02600	-4.66627	7.06183
H	0.45230	-4.48945	8.00205
H	2.83827	-4.38285	5.10618
H	2.16958	-2.98180	5.95678
H	2.72272	-4.39372	6.87491
H	-3.86035	-2.77182	5.23934
H	-2.27206	-2.16749	5.67786
H	-4.58576	-0.30487	5.22035
H	-2.92045	0.21033	5.54261
H	-3.78039	0.83889	4.12854
H	-1.01174	-0.60150	4.02453
H	-1.38579	-1.60626	2.60609
H	-1.88806	0.09185	2.65185
H	-3.78641	-2.38016	2.18105
H	-5.09600	-1.81058	3.23596
H	-4.27459	-0.67406	2.15357
H	-2.23785	-6.52245	5.62282
H	-3.63876	-5.50913	5.90240
H	-3.72197	-8.54745	5.86767
H	-5.13123	-7.49915	6.10009
H	-5.15128	-8.74350	4.84012
H	-5.69263	-5.70152	4.35291
H	-4.70140	-5.56322	2.88395
H	-5.74335	-6.97431	3.12514
H	-2.68195	-7.06701	2.55379
H	-2.26329	-8.28758	3.77553
H	-3.70720	-8.49658	2.77502
H	-0.15767	-0.15522	-5.93969
H	2.44323	-0.82112	-5.21017
H	4.66975	-1.72242	-0.42536
H	6.49976	-0.12876	-0.87504
H	6.18985	1.69076	-2.51455
H	1.31071	-1.54519	-2.09541
H	2.62578	-2.13979	0.60371
H	1.48484	-0.82379	0.28034
H	0.96305	-2.51153	0.13284
H	2.84804	-3.26804	-3.04281
H	3.47831	-3.60347	-1.42497
H	1.78540	-3.95078	-1.79870
H	2.97970	2.26655	-4.37891
H	3.62392	3.81346	-2.53658
H	5.31388	3.74132	-3.05620
H	4.09484	4.43661	-4.12816
H	5.97746	2.04190	-4.96867
H	4.70658	1.08196	-5.73447
H	4.77005	2.83421	-5.99040
H	-3.12754	4.17050	-4.94489
H	-4.99988	2.83574	-4.04750

H	-4.59365	0.58128	-3.13056
H	0.42598	2.95155	-5.03233
H	-1.19678	5.44823	-4.32347
H	-0.11788	4.57066	-3.22934
H	0.53751	5.38531	-4.66404
H	-0.82616	2.94154	-7.19199
H	-1.62023	4.45611	-6.74423
H	0.12938	4.42063	-6.98777
H	-1.18945	-0.99481	-2.94322
H	-4.03168	-1.70477	-3.83554
H	-2.58000	-1.82420	-4.83774
H	-2.75723	-2.85147	-3.40343
H	-2.25141	-0.12251	-0.85028
H	-3.81600	-0.73960	-1.39147
H	-2.49644	-1.86597	-1.06510