A reinterpretation of the Imidazolate Au(I) Cyclic Trinuclear Compounds reactivity with iodine and methyl iodide with the perspective of the Inverted Ligand Field Theory.

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Supporting Info

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1 Preparations

1.1 Reaction of [µ-Au-C2,N3-1-methylimidazolate]3 with Hydrochloric Acid. Preparation of compound [(ImMe-NHC-2yl)2-Au]Cl. Compound 6.

The [Au(µ-C2,N3-1-Methyl-imidazole)]3 (40 mg; 0.048 mmol) was dissolved in 4 ml of CH2Cl2, under nitrogen atmosphere, and 1 mL of a 1M watery solution of HCl (0.5 mmol) was added under vigorous magnetic stirring at room temperature for 1.5 Hour. The suspension was extracted with water (3 times), dried under Na2SO4. The solution turned pale pink and after filtration, was dried under a vacuum. The white solid was washed with cyclohexane and evaporated to dryness to obtain a microcrystalline. Yield 56%

1H NMR (δ, room temperature, CDCl3): 11.12 (s, broad, 2H), 7.09 (t, 3JH-H = 1.6Hz, 2H), 7.00 (t, 3JH-H = 1.6Hz, 2H), 3.85 (s, 6H, NCH3), 1.44 (s, trace of cyclohexane).

13C NMR (δ, room temperature, CDCl3): 167 (C2), 121(C4), 118 (C5), 38.4 (N-CH3).

MIR (cm⁻¹): 3293 (m, br), 3174 (m), 3145 (w), 3130 (w), 3012 (w), 2957 (m, sh), 2922 (m), 2853 (m), 1665 (w), 1575 (m), 1559 (m, sh), 1489 (w), 1452 (s), 1443 (m, sh), 1394 (m), 1348 (m), 1332 (m), 1312 (m, sh), 1281 (m), 1235 (m), 1127 (m, sh), 1098 (s), 1072 (s), 1009 (m), 969 (m,sh), 946 (m, sh), 922 (m), 893 (m, sh), 875 (m, sh), 832 (m), 726 (s).

FIR (cm⁻¹): 699 (w), 682 (w), 662 (m), 637 (m), 613 (m), 415 (w), 329 (s), 322 (s), 303 (w), 265 (s), 256 (m, sh), 239 (m) 230 (m), 221 (m), 215 (m), 206 (m), 200 (m, sh), 185 (s), 177 (s), 166 (m), 147 (m, sh), 139 (s), 123 (s), 112 (s), 103 (s).
Elemental analysis for CsH12AuClN4 calc %: C 24.23, H 3.05, N 14.13. Found: C 24.68, H 3.43, N 13.52.

The reaction of [µ-Au-C2,N3-1-benzylimidazolate], with Hydrochloric Acid. Preparation of compound [ImBz-NHC-2yl]2-Au]Cl. Compound 7.

The [Au(µ-C2,N2-1-Benzyl-imidazole)]3 (40 mg; 0.038 mmol) was dissolved in 3.5 ml of CH2Cl2, under nitrogen atmosphere, and 1 mL of a 1M watery solution of HCl (0.5 mmol) was added under vigorous magnetic stirring at room temperature for 1.5 Hour. The suspension was extracted with water (3 times), dried under Na2SO4, and after filtration, evaporated to dryness. A microcrystalline solid was obtained. Yield 81%

1H NMR (δ, room temperature, DMSO): 12.43 (s, broad, 2H), 7.65-7.42 (m, 14H), 5.41 (s, 4H).
$^{13}$C NMR ($\delta$, room temperature, DMSO): 180 (C2), 137 (Ph), 128 (Ph), 127.92 (Ph), 127.50 (Ph), 121.50 (C4), 119.52 (C5), 53.4 (CH2-Ph).

Elemental analysis for C$_{20}$H$_{22}$AuClN$_4$ calcd %: C 43.61, H 4.03, N 10.17. Found: C 44.02, H 3.83, N 9.72.

2 IR spectra

Crystals of compounds 1 and 2 are simultaneously formed as needles and platelets, respectively. Manual separation of the crystals was performed, and the IR spectra were recorded.

Figure S1. Overlapped IR spectra in the range 4000-400 cm$^{-1}$ of compound 1 (red lines, needles) and compound 2 (blue line, platelets)
Figure S2. Overlapped IR spectra in the range 700-200 cm\(^{-1}\) of compound 1 (red line, needles) and 2 (blue line, platelets)

3 NMR spectra

Crystals of compounds 1 and 2 are simultaneously formed as needles and platelets, respectively. Manual separation of the crystals was performed and the \(^1\)H and \(^{13}\)C NMR spectra were recorded in DMSO-d\(^6\). Both compounds are sparingly soluble in DMSO-d\(^6\). Compound 1 is less soluble than compound 2. The NMR spectra consist of several peaks but none of the presents can be attributed to the starting \(\text{CTC}^\text{Me}\). The solution of compound 1 in DMSO-d\(^6\) displays signals for the imidazole protons at 7.74 and 7.40 ppm, and 125.27 and 122.99 ppm, respectively, attributed to compound 1 but, predominantly, the signals due to compound 2 were observed (see figure S2-S5). It is likely that the fully iodized compound 1, upon the difficult dissolution, loses iodine to give compound 2. Moreover the overnight acquisition for the \(^{13}\)C NMR results in the rising of traces of additional compounds, likely due to the nine membered cycle rupture and the formation of carbene species (in example the signal at 13 ppm in \(^1\)H NMR figure S4, acquired after 12 hours from the preparation of the solution, and signals at 113 and 118 ppm in figures S5 and S6). The \(^1\)H NMR spectrum of compound 2 consists of six sharp doublets of the same intensity for the imidazole protons and three singlets of the same intensity for the N-methyl groups, none of them corresponds to the starting \(\text{CTC}^\text{Me}\) or to the free 1-methylimidazole; saturated solutions of compounds 1 and 2 exhibit nearly small singlets for the C2 atoms, 166.13 and 166.09 ppm, respectively (see inset image in figure S7).
**Figure S3.** $^1$HNMR spectrum of compound 1 in DMSO-d$_6$. The dissolution in DMSO-d$_6$ was obtained by heating and sonication. Stars indicate peaks due to compound 1, while red circles depict the formation of compound 2 in solution, due to the loss of an iodine molecule. Green triangles label peaks that are not assigned which rise upon a time. At 3.60 ppm and 1.76 ppm the signals of tetrahydrofuran.
Figure S4. $^{13}$C NMR spectra in DMSO-d$_6$ of compound 1 upon heating and sonication. The acquisition of the $^{13}$C NMR spectrum needed an accumulation time of several hours. Most of the peaks are due to compound 2.

Figure S5. $^1$H NMR spectrum of the sparingly soluble compound 2 in DMSO-d$_6$. The dissolution in DMSO-d$_6$ was obtained by heating and sonication. Small traces of compound 1 are present.
Figure S6. $^{13}$C NMR spectrum in DMSO-$d^6$ of compound 2 upon heating and sonication. The acquisition of the $^{13}$C NMR spectrum needed an accumulation time of several hours.
Figure S7. Overlapped $^{13}$C NMR spectra in DMSO-d$_6$ of compounds 1 and 2. In the inset image signals for the C2 of the imidazoles: in orange the signal due to the dissolution of compound 1 (166.13 ppm and 166.09 ppm) and the signal of the compound 2 (166.09 ppm). Compound 2 is present in the solution of compound 1 upon the dissociation of iodine from compound 1.
**Figure S8.** $^1$HNMR spectrum in CDCl$_3$ of compound 3 (orange line) overlapped with the spectrum of CTC$_{Me}$ (blue line). The signal at 2.19 ppm is the free MeI and the one at 1.78 ppm due to the CH$_3$-Au-I frame. Beyond the CTC$_{Me}$ and compound 3, also other species are generated in the solution. Inset images are enlargements of the chemical ranges indicated by the arrows. The attribution of the Me-Au-I at 1.78 ppm was made according to data reported in the literature.$^1$
*Figure S9.* $^{13}$C NMR spectrum in CDCl$_3$ of compound 3, revealing the presence of CTC$^\text{Me}$ and free MeI (29 ppm) in addition the compound 3, with methyl bound to Au at 20 ppm. Upon long accumulation, additional species are formed too.

*Figure S10.* Overlapped IR spectra in the range 4000 - 600 cm$^{-1}$ of the CTC$^\text{Me}$ (red line) and compound 3 (blue line). Although a good overlap of the bands is mostly observed, additional absorptions are observed at 1154 cm$^{-1}$ (CH$_3$ deformation) and 721 cm$^{-1}$ (CH$_3$ rocking) in the spectrum.
of compound 3, likely due to the deformation and rocking modes of the Methyl of the Me-Au-I moiety. The attribution was made according to data reported in the literature.\textsuperscript{2}

Figure S11. \textsuperscript{1}H NMR spectrum of compounds 4 and 5 recorded in DMSO-d\textsuperscript{6}.
**Figure S12.** $^{13}$C NMR spectrum recorded in acetone-d$_6$ for compounds 4 and 5. The peaks at 28 and 206 ppm are due to DMSO, the peak at 77 is due to CHCl$_3$, the peak at 54 ppm is due to CH$_2$Cl$_2$.

**Figure S13.** Overlapped FIR spectra of the solid consisting of compounds 4 and 5 (red line) and that of the starting CTC$_{Bz}$ (blue line).
4 Computational studies

4.1 Reactivity of the CTCMe with molecular I₂

As pointed out in the manuscript, the reactivity between CTCMe and I₂ evolves through the formation of an initial adduct, CTCMe₂2I₂, held together with the trinuclear moiety and two I₂ molecules with a free energy gain of -11.8 kcal mol⁻¹. Then, a triiodide moiety is released with the achievement of cationic species CTCMeI⁺ with a free energy cost +14.5 kcal mol⁻¹ and, then, the triiodide species reacts with CTCMeI⁺ to provide the first intermediate CTCMeI₂ together with a new I₂ molecule with a ΔG = -24.1 kcal mol⁻¹. CTCMeI₂ features a gold center in square planar coordination due to the formation of two new Au-I bonding. In the case of the methyl substituent at the imidazole ring, the process occurs stepwise for the two remaining metal centers. Briefly, a second adduct, CTCMeI₂⁻2I₂ is formed with a free energy gain of -9.2 kcal mol⁻¹, again a triiodide is released (ΔG = +12.2 kcal mol⁻¹) together with the formation of the cationic intermediate CTCMeI₃⁺. The complete iodination of the second gold, compound 2 is observed with a free energy gain of -19.3 kcal mol⁻¹. The third iodination follows similarly with a gain of -7.1 kcal mol⁻¹ followed by +10.4 kcal mol⁻¹ cost for the separation of the I₃⁻ and a further gain of -17.4 kcal mol⁻¹ occurs for the achievement of the fully iodinated species, 1. Scheme S1 summarizes the overall free energy pathway associated with the reactivity of CTCMe with di-iodine up to the final species 1.

![Scheme S1. Free Energy pathway for the reaction between the CTCMe and di-iodine molecules up to the final complete iodinated species 1.](image)
4.2 Computational studies on the reaction of HCl with CTC$^\text{Me}$ or CTC$^\text{Bz}$

The reactivity between the original CTCs with methyl iodide highlighted the not innocent behavior of the imidazole ligand and their ability to catch a methyl cation. Thus, we wonder if such a discrepancy is also operative for the reaction with the hydrochloric acid or not. Once again, the investigation of direct involvement in the reaction is excluded in both cases while the analysis revealed again that the incoming substrate reacts with the aromatic system of the imidazolyl ring. The computational analysis perfectly mirrors the experimental results since in both cases the formation of carbene and bis-carbene moieties is observed. Figure S16 shows the Transition State for the reaction of starting compound with benzyl, Figure S16a, and with methyl substituents, Figure S16b.
Figure S16. Optimized structure of Transition State for the interaction between HCl and: a) CTC\textsuperscript{Bz} and b) CTC\textsuperscript{Me}. The aryl rings are hidden for clarity in Figure S16a.

In both cases, the free energy barriers associated with the formation of the carbene and the cleavage of the Au1-N bonding are very small, being not higher than 7 kcal mol\textsuperscript{-1}. The structures feature an already stretched Au1-N bonding and the transferred proton in between the chlorine and the nitrogen center. In both cases, the H-Cl distance of the incoming hydrochloric acid is elongated by \textit{ca.} 0.24 Å, suggesting an already advanced stage of the process. After such a Transition State the process evolves toward the formation of the N-H linkage of compound CTC\textsubscript{HCl} with a free energy gain of -22.9 and -18.5 kcal mol\textsuperscript{-1} for CTC\textsuperscript{Bz} and CTC\textsuperscript{Me}, respectively. The somewhat higher energy gain in the case of the benzyl could be reasonably explained given a based on somewhat more pronounced stability of a benzyl carbene compared to the methyl one. The reaction proceeds in the same way with the final formation of three (NH-carbene)AuCl moieties with a total free energy gain of -26.3 and -23.2 kcal mol\textsuperscript{-1}.

### 4.3 Cartesian coordinates and free energies of all the structures optimized in the computational analysis (B97D-DFT level of theory).

**Compound CTC\textsuperscript{Me} in dichloromethane solution**

**Cartesian Coordinates**

|           | Au   | C    | H    | Cl   |
|-----------|------|------|------|------|
| Au -0.406798 | 3.325178 | 4.579262 |      |      |
| Au -1.550532 | 1.905008 | 1.426366 |      |      |
| Au 1.988424  | 2.602075 | 1.932564 |      |      |
| N -3.438684  | 3.089687 | 5.027069 |      |      |
| C -2.352157  | 2.911461 | 4.212505 |      |      |
| N -2.816913  | 2.384612 | 3.044612 |      |      |
| C -4.190218  | 2.241204 | 3.141064 |      |      |

|           |          |      |      |      |
|-----------|----------|------|------|------|
| Au -0.406798 | 3.325178 | 4.579262 |      |      |
| Au -1.550532 | 1.905008 | 1.426366 |      |      |
| Au 1.988424  | 2.602075 | 1.932564 |      |      |
| N -3.438684  | 3.089687 | 5.027069 |      |      |
| C -2.352157  | 2.911461 | 4.212505 |      |      |
| N -2.816913  | 2.384612 | 3.044612 |      |      |
| C -4.190218  | 2.241204 | 3.141064 |      |      |
C 5.021247 3.628842 3.376359  H 1.903110 4.502144 6.702834
N -0.317410 1.001130 -1.238427  H 4.584968 4.593630 5.965529
C  -0.153075 1.531148 0.013499  H 5.747903 3.021737 3.927909
N  1.177803 1.782900 0.164291  H 5.442436 4.623242 3.187917
C  1.831227 1.410090 -0.997785  H 2.901784 1.516578 -1.104436
C  0.906156 0.922683 -1.879502  H 1.001014 0.531624 -2.882663
C  -1.593119 0.613997 -1.836131  H -2.356465 0.624115 -1.053490
H  -4.775266 1.838471 2.325994  H -1.511383 -0.393630 -2.257895
H  -5.560596 2.735403 4.841360  H 4.786689 3.145167 2.424435
H  -3.873339 2.947133 7.079197  H -1.871313 1.321061 -2.626714
H  -3.947049 4.602554 6.401210  H -2.364455 3.810264 6.657577

HF=-1202.8418163
Zero-point vibrational energy   689445.4 (Joules/Mol)
Zero-point correction=          0.262596 (Hartree/Particle)
Thermal correction to Energy= 0.285927
Thermal correction to Enthalpy= 0.286871
Thermal correction to Gibbs Free Energy= 0.205070
Sum of electronic and zero-point Energies= -1202.579220
Sum of electronic and thermal Energies= -1202.555889
Sum of electronic and thermal Enthalpies= -1202.554945
Sum of electronic and thermal Free Energies= -1202.636747

Compound CTC\textsuperscript{Bz} in dichloromethane solution

Cartesian Coordinates

N  5.041979 1.862971 8.672419  
N  4.402015 -0.216667 8.938355  
N  3.737431 -5.310583 8.768541  
N  5.083677 -4.788132 7.119828  
N  8.041032 -2.461059 3.625587  
N  7.270020 -0.889526 4.945628  
C  5.134925 0.605362 8.138912  
C  4.268181 1.832349 9.819669  
H  4.076822 2.722177 10.402378  

C 3.868631 0.533673 9.973129  
C 3.250434 0.079711 10.734738  
C 5.782289 3.032832 8.190918  
C 5.129210 3.908725 8.267743  
C 5.995170 2.850533 7.131221  
C 7.067007 3.260767 8.964908  
C 8.047531 2.258055 9.026252  
C 7.873236 1.308725 8.523242  
C 9.234501 2.473975 9.731135
HF=-1895.6943855

Zero-point vibrational energy  1313604.8 (Joules/Mol)
Zero-point correction=  0.500326 (Hartree/Particle)
Thermal correction to Energy=  0.536682
Thermal correction to Enthalpy=  0.537626
Thermal correction to Gibbs Free Energy=  0.423831
Sum of electronic and zero-point Energies=  -1895.194060
Sum of electronic and thermal Energies=  -1895.157704

H 9.989067 1.690487 9.771722  C 2.481514 -3.195027 11.395765
C 9.454468 3.695037 10.383795  H 1.501761 -3.051955 10.943777
H 10.378685 3.861777 10.933842  C 7.273069 -2.234377 4.736264
C 8.480323 4.697292 10.327026  C 8.508159 -1.259832 3.121750
H 8.642299 5.646668 10.834105  H 9.130169 -1.214647 2.239124
C 7.290456 4.477981 9.621030  C 8.029093 -0.287455 3.955282
H 8.480323 5.256058 9.579599  H 8.174848 0.783391 3.926968
C 4.340915 -4.258312 8.131014  C 8.221393 -3.766121 2.986082
C 4.095395 -6.500317 8.157843  H 8.093715 -4.518710 3.773263
H 3.723868 -7.453170 8.507242  H 9.250099 -3.827114 2.615187
C 4.935280 -6.164974 7.132451  C 7.238287 -4.006877 1.855292
H 5.442565 -6.795634 6.415791  C 5.859394 -3.838165 2.056314
C 2.788566 -5.198048 9.890274  H 5.496748 -3.508073 3.027636
H 2.646345 -6.213888 10.277002  C 4.959152 -4.089608 1.017472
H 1.825257 -4.844275 9.504419  H 3.891738 -3.956108 1.183901
C 3.278564 -4.268910 10.980540  C 5.426641 -4.512625 -0.234364
C 4.554711 -4.432109 11.536878  H 4.724459 -4.706810 -1.042889
H 5.186487 -5.250764 11.197436  C 6.800040 -4.680981 -0.440605
C 5.032833 -3.524111 12.483717  H 7.171847 -5.004221 -1.411148
H 6.030637 -3.650155 12.899490  C 7.700764 -4.426047 0.601104
C 4.233483 -2.448151 12.892708  H 8.770702 -4.551630 0.439653
H 4.609624 -1.735720 13.624205  Au 6.212494 -0.003366 6.541202
C 2.953583 -2.290056 12.352492  Au 4.269961 -2.293166 8.605819
H 2.329061 -1.454103 12.661597  Au 6.251148 -3.583069 5.840126
Sum of electronic and thermal Enthalpies = -1895.156760
Sum of electronic and thermal Free Energies = -1895.270555

Compound I$_2$ in dichloromethane solution

**Cartesian Coordinates**

I 0.000000 0.000000 -0.006327
I 0.000000 0.000000 2.73632

HF = -22.9138694

Zero-point vibrational energy = 1168.4 (Joules/Mol)

Zero-point correction = 0.000445 (Hartree/Particle)

Thermal correction to Energy = 0.003374
Thermal correction to Enthalpy = 0.004318
Thermal correction to Gibbs Free Energy = -0.025389

Sum of electronic and zero-point Energies = -22.913424
Sum of electronic and thermal Energies = -22.910496
Sum of electronic and thermal Enthalpies = -22.909552
Sum of electronic and thermal Free Energies = -22.939259

Compound CTCMe*2I$_2$ in dichloromethane solution

**Cartesian Coordinates**

Au 0.380262 3.145327 4.594098
Au -0.806617 1.357367 1.644557
Au 2.328499 3.201509 1.527372
I -0.848385 5.082026 2.923366
N -2.276938 1.991087 5.577468
C -1.351985 2.097936 4.578472
N -1.795578 1.372237 3.520120
C -2.985730 0.776567 3.882902
C -3.293495 1.155093 5.165518
N 4.122929 4.749334 3.468997
H -3.527742 0.134962 3.202690
C 2.969080 4.057313 3.240852
C 2.265316 4.076440 4.409563
C 2.975460 4.804385 5.348071
C 4.138567 5.228393 4.767775
N 0.040555 1.018406 -1.286926
C 0.294932 1.524012 -0.040781
N 1.459633 2.225432 -0.127393
C 1.920373 2.153189 -1.430607
C 1.040436 1.403661 -2.161691
H -3.527742 0.134962 3.202690
H -4.123247 0.905853 5.811585  
H 2.604811 4.952620 6.352591  
H 4.963907 5.810499 5.151888  
H 2.837738 2.637591 -1.734841  
I -1.337900 7.260988 0.933994  
I 1.759973 8.194634 1.688824  
I 4.380216 9.011245 2.510951  
C 5.164251 4.995118 2.472424  
H 6.146602 4.894466 2.944817  
H 5.058137 4.254178 1.675733  
H 5.057322 6.002920 2.056641  
C -2.165277 2.602055 6.902112  
H -1.731389 1.890458 7.613552  
H -1.731389 1.890458 7.613552  
H -1.520579 3.481619 6.823991  
H -3.160650 2.904267 7.240158  
I -3.160650 2.904267 7.240158  
C 1.129486 0.227513 -1.661596  
H 1.670706 -0.038286 -0.749660  
C 5.164251 4.995118 2.472424  
H -1.784731 0.811052 -2.318897  
H -0.808600 -0.683399 -2.178639

HF= -1248.7201185
Zero-point vibrational energy  694659.9 (Joules/Mol)
Zero-point correction=  0.264582 (Hartree/Particle)
Thermal correction to Energy=  0.297625
Thermal correction to Enthalpy=  0.298569
Thermal correction to Gibbs Free Energy=  0.186018
Sum of electronic and zero-point Energies=  -1248.455537
Sum of electronic and thermal Energies=  -1248.422494
Sum of electronic and thermal Enthalpies=  -1248.421550
Sum of electronic and thermal Free Energies=  -1248.534101

Compound CTC\textsuperscript{Bz}\#2I\textsubscript{2} in dichloromethane solution

Cartesian Coordinates
Au 0.636646 3.210322 4.426554  
Au -0.741821 1.340623 1.621606  
Au 2.610162 2.757836 1.406682  
I -0.388855 5.089044 2.560439  
N -2.084725 2.322952 5.528919  
C -1.181544 2.315486 4.500376  
N -1.719281 1.592159 3.485504  
C -2.949387 1.122427 3.896704  
C -3.185200 1.570922 5.170549  
C -1.869592 2.906922 6.869713  
C -1.272655 4.293446 6.809144  
C -1.938536 5.324137 6.133276  
C -1.349668 6.583436 6.016459  
C -0.90855 6.828194 6.580558  
C 0.572588 5.808070 7.267466  
C -0.015582 4.542505 7.378817  
N 4.546769 4.269525 3.252262  
C 3.316759 3.709402 3.044376  
N 2.604575 3.914369 4.189243  
C 3.384993 4.615426 5.091560
C 4.601940 4.840561 4.513770
C 5.626533 4.367128 2.250236
C 5.737641 3.082732 0.081815
C 5.843251 1.886828
C 6.033962 0.679345 0.042212
C 6.136842 0.674816 1.439964
C 6.040344 1.871007 2.153640
N -0.034082 0.919962 -1.314744
C 0.368655 1.297494 -0.062792
N 1.634007 1.779335 -0.181275
C 2.010286 1.703741 -1.512670
C 0.971457 1.178164 -2.230145
C -1.399846 0.523275 -1.642183
C -2.324650 1.698910 -1.922935
C -2.136373 2.958871 -1.336190
C -3.050047 3.991917 -1.572465
C -4.160476 3.779334 -2.397144
C -4.350749 2.525106 -2.989681
C -3.435206 1.493826 -2.754924
H -3.564976 0.510065 3.253181
H -4.014729 1.420414 5.846624
H -1.215251 2.236803 7.438559
H -2.851273 2.921823 7.355321
H -2.903174 5.127095 5.669340

HF=-1941.5787287
Zero-point vibrational energy  1319176.1 (Joules/Mol)
Zero-point correction=        0.502448 (Hartree/Particle)
Thermal correction to Energy=  0.548497
Thermal correction to Enthalpy= 0.549442
Thermal correction to Gibbs Free Energy=  0.405533
Sum of electronic and zero-point Energies= -1941.076281
Sum of electronic and thermal Energies = -1941.030231
Sum of electronic and thermal Enthalpies = -1941.029287
Sum of electronic and thermal Free Energies = -1941.173195

Compound I$_3^+$ in dichloromethane solution

**Cartesian Coordinates**

|   |   |   |
|---|---|---|
| I | 0.292200 5.559900 2.404018 | I | 0.292200 5.559900 8.537532 |
| I | 0.292200 5.559900 5.469950 |

HF = -34.5770036

Zero-point vibrational energy = 1715.2 (Joules/Mol)

Zero-point correction = 0.000653 (Hartree/Particle)

Thermal correction to Energy = 0.006179

Thermal correction to Enthalpy = 0.007123

Thermal correction to Gibbs Free Energy = -0.032343

Sum of electronic and zero-point Energies = -34.576350

Sum of electronic and thermal Energies = -34.570824

Sum of electronic and thermal Enthalpies = -34.569880

Sum of electronic and thermal Free Energies = -34.609347

Compound CTC$_{Me}^+I^+$ in dichloromethane solution

**Cartesian Coordinates**

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Au | 1.052164 3.498161 3.892975 | C | 3.569189 3.331609 2.170178 |
| Au | -1.117762 2.168457 1.315735 | N | 3.100499 3.598996 3.436456 |
| Au | 2.409885 2.726866 0.641648 | C | 4.138775 4.057018 4.211989 |
| I | 0.368542 5.792604 2.639990 | C | 5.278022 4.040185 3.448062 |
| N | -1.634952 3.408191 5.335000 | C | 5.827305 3.429534 1.066570 |
| C | -0.902215 3.107197 4.222872 | N | -0.897309 1.411243 -1.641968 |
| N | -1.730801 2.565780 3.293792 | C | -0.298560 1.853919 -0.494332 |
| C | -2.972141 2.431983 3.874773 | N | 1.022520 2.066438 -0.791309 |
| C | -2.918044 2.955697 5.150911 | C | 1.226988 1.756778 -2.116595 |
| C | -1.099379 3.999044 6.565594 | C | 0.032703 1.348072 -2.657878 |
| N | 4.909243 3.581490 2.197604 | C | -2.318853 1.097807 -1.793600 |
H -3.803316 1.984897 3.348597  H 2.200602 1.842723 -2.577969
H -3.663900 3.020814 5.930492  H -0.229662 1.022987 -3.654671
H -0.300384 4.695402 6.297693  H -2.764247 1.030092 -0.797957
H -0.704518 3.213975 7.218668  H -2.426217 0.140125 -2.312474
H 4.004920 4.323707 5.250750  H -1.903736 4.538313 7.071539
H 6.303187 4.284730 3.687945  H 6.625003 2.728583 1.333441
H 6.258870 4.402402 0.808578  H -2.817764 1.887254 -2.366795
H 5.261823 3.039529 0.217091

HF=-1214.1030962
Zero-point vibrational energy  691479.2 (Joules/Mol)
Zero-point correction= 0.263371 (Hartree/Particle)
Thermal correction to Energy= 0.288924
Thermal correction to Enthalpy= 0.289868
Thermal correction to Gibbs Free Energy= 0.201614
Sum of electronic and zero-point Energies=-1213.839726
Sum of electronic and thermal Energies=-1213.814172
Sum of electronic and thermal Enthalpies=-1213.813228
Sum of electronic and thermal Free Energies=-1213.901483

Compound CTCBrI+ in dichloromethane solution

Cartesian Coordinates
Au 0.247718 3.509765 4.012141  C -2.130604 5.437969 5.827988
Au -0.832506 1.598641 1.119797  C -1.394905 6.619158 5.911991
Au 2.482189 3.057748 1.187985  C -0.182294 6.647266 6.618220
I -0.667113 5.410531 2.277560  C 0.294713 5.487663 7.231876
N -2.520995 2.503233 4.905828  C -0.429300 4.294079 7.127247
C -1.530605 2.534242 3.957364  N 4.206377 4.674144 3.133528
N -1.977038 1.855601 2.868106  C 3.023589 4.049343 2.852170
C -3.211577 1.334716 3.166184  N 2.227461 4.224384 3.956368
C -3.559569 1.732011 4.436123  C 2.894140 4.997650 4.877671
C -2.412566 2.971585 6.303365  C 4.137391 5.278155 4.374099
C -1.648654 4.265439 6.425815  C 5.344565 4.827943 2.200940
| C 5.653424 3.560070 1.439344 | H -1.762975 7.521238 5.429494 |
|-----------------------------|---------------------------------|
| C 5.650450 3.569357 0.035546 | H 0.384813 7.572869 6.686352   |
| C 5.870364 2.387952 -0.677445 | H 1.227900 5.506136 7.790363   |
| C 6.081280 0.869186 -1.652522  | H -0.057365 3.382394 7.589966   |
| C 6.088751 1.173234 1.406899  | H 2.454559 5.254903 5.828651   |
| C 5.882086 2.355613 2.119891  | H 4.973535 5.820865 4.791820   |
| N 0.253900 0.869186 -1.652522  | H 6.198716 5.136868 2.814200   |
| C 0.450776 1.447099 -0.426236  | H 5.113006 5.640624 1.503413   |
| N 1.715703 1.967063 -0.434725  | H 5.449094 4.499777 -0.489019   |
| C 2.294382 1.701753 -1.656664  | H 5.862983 2.404735 -1.765400   |
| C 1.388749 1.015401 -2.425079  | H 6.236723 0.263201 -0.548998   |
| C -0.955591 0.133599 -2.074282 | H 6.252433 0.239914 1.941808   |
| C -2.234208 0.831334 -1.664909  | H 5.864518 2.341405 3.208003   |
| C -3.185272 0.150991 -0.893333  | H 3.301255 2.019660 -1.886305   |
| C -4.334822 0.809362 -0.443141  | H 1.446007 0.628505 -3.432587   |
| C -4.533282 2.158452 -0.751986  | H -0.922311 -0.872929 -1.641904 |
| C -3.588390 2.840815 -1.530032  | H -0.891486 0.038124 -3.164186 |
| C -2.448524 2.178651 -1.989502  | H -3.008175 -0.888280 -0.622690 |
| H -3.754004 0.728320 2.455282  | H -5.065474 0.272864 0.159030   |
| H -4.425965 1.515362 5.044923  | H -5.417692 2.677710 -0.388513   |
| H -1.928123 2.183644 6.890287  | H -3.739146 3.890710 -1.772940   |
| H -3.439219 3.090641 6.665838  | H -1.701082 2.716719 -2.569277   |
| H -3.064013 5.412379 5.270175  |                                 |

HF= -1906.9671695

Zero-point vibrational energy = 1314823.5 (Joules/Mol)

Zero-point correction= 0.500790 (Hartree/Particle)

Thermal correction to Energy= 0.539484

Thermal correction to Enthalpy= 0.540428

Thermal correction to Gibbs Free Energy= 0.421706

Sum of electronic and zero-point Energies= -1906.466380

Sum of electronic and thermal Energies= -1906.427686

Sum of electronic and thermal Enthalpies= -1906.426742

Sum of electronic and thermal Free Energies= -1906.545463
Compound CTCMeI₂ in dichloromethane solution

Cartesian Coordinates

|    | X          | Y          | Z          |
|----|------------|------------|------------|
| Au | -0.414276  | 3.255373   | 4.549721   |
| Au | -1.560087  | 1.874382   | 1.412014   |
| Au | 1.981272   | 2.574521   | 1.936879   |
| I  | -0.901529  | 5.856406   | 3.932661   |
| N  | -3.414215  | 3.034016   | 5.039862   |
| C  | -2.378075  | 2.840400   | 4.188651   |
| N  | -2.841195  | 2.349826   | 3.028140   |
| C  | -4.218538  | 2.236849   | 3.148751   |
| C  | -4.584402  | 2.663047   | 4.396587   |
| C  | -3.304763  | 3.627664   | 6.372071   |
| N  | 3.763307   | 3.775133   | 4.144858   |
| C  | 2.529874   | 3.378700   | 3.706616   |
| N  | 1.664443   | 3.642991   | 4.718068   |
| C  | 2.348235   | 4.201215   | 5.779075   |
| C  | 3.667318   | 4.286030   | 5.427675   |
| C  | 5.003860   | 3.684337   | 3.377440   |
| N  | -0.313956  | 0.993103   | -1.248543  |
| C  | -0.153748  | 1.509428   | 0.008894   |
| N  | 1.176122   | 1.755507   | 0.170002   |

HF= -1225.8087469

Zero-point vibrational energy 694360.1 (Joules/Mol)

Zero-point correction= 0.264468 (Hartree/Particle)

Thermal correction to Energy= 0.292264

Thermal correction to Enthalpy= 0.293208

Thermal correction to Gibbs Free Energy= 0.198773

Sum of electronic and zero-point Energies= -1225.544279

Sum of electronic and thermal Energies= -1225.516483

Sum of electronic and thermal Enthalpies= -1225.515539
Sum of electronic and thermal Free Energies= -1225.609974

Compound CTC$_2$Bz$_2$ in dichloromethane solution

**Cartesian Coordinates**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Au      | 0.617887| 3.327555| 4.433440|
| Au      | -0.829147| 1.615095| 1.591386|
| Au      | 2.514829 | 3.045505| 1.364985|
| I       | -0.437540| 5.362229| 2.964597|
| N       | -0.437540| 5.362229| 2.964597|
| C       | 1.663434 | 1.129880| 5.661557|
| C       | -2.039814| 2.340732| 5.587849|
| C       | -1.219454| 2.438428| 4.508795|
| C       | -1.793965| 1.817544| 3.462564|
| C       | -3.011700| 1.313835| 3.896941|
| C       | -3.172232| 1.632625| 5.216685|
| C       | -1.713403| 2.769342| 6.960806|
| C       | -1.212243| 4.194468| 7.023984|
| C       | -2.006227| 5.251702| 6.561024|
| C       | -1.517350| 6.558774| 6.580065|
| C       | -0.230804| 6.821969| 7.067676|
| C       | 0.563770| 5.771641| 7.536331|
| C       | 0.073669 | 4.461286| 7.513953|
| N       | 4.509946 | 4.437763| 3.244865|
| C       | 3.254902 | 3.941082| 3.017882|
| C       | 3.377771 | 4.721901| 5.112808|
| C       | 4.599961 | 4.928961| 4.536504|
| C       | 5.59478 | 4.850353| 2.248042|
| C       | 5.758609 | 3.173101| 1.510519|
| C       | 5.721295 | 3.149279| 0.110889|
| C       | 5.784610 | 1.934031| -0.579556|
| C       | 5.874844 | 0.732185| 0.129123|
| C       | 5.921692 | 0.751685| 1.529633|
| C       | 5.869640 | 1.966441| 2.215712|
| N       | -0.066431| 1.041069| -1.311013|
HF=-1918.6679655
Zero-point vibrational energy  1318513.6 (Joules/Mol)
Zero-point correction=                           0.502195 (Hartree/Particle)
Thermal correction to Energy=                    0.542994
Thermal correction to Enthalpy=                  0.543939
Thermal correction to Gibbs Free Energy=         0.417562
Sum of electronic and zero-point Energies=       -1918.165770
Sum of electronic and thermal Energies=           -1918.124971
Sum of electronic and thermal Enthalpies=         -1918.124027
Sum of electronic and thermal Free Energies=      -1918.250404

Compound  CTCMeI2*2I2
Cartesian Coordinates
Au 0.455140 3.515768 4.368687                C 4.839589 4.132378 2.771190
Au -1.620602 1.796115 1.388810               N -0.381776 0.433230 -1.069406
Au 1.910812 2.480591 1.812283                C -0.223148 1.143658 0.084966
I -1.156883 6.121680 4.076836                N 1.119228 1.329273 0.245158
N -3.429554 3.167558 4.966317                C 1.784880 0.745647 -0.818329
C -2.408490 3.006995 4.089958                C 0.853412 0.176692 -1.641070
N -2.879029 2.474431 2.950128                C -1.658706 -0.034716 -1.605907
C -4.247053 2.305318 3.109541                H -4.854209 1.879493 2.323868
C -4.598054 2.735998 4.359226                H -5.547539 2.770580 4.873689
C -3.327100 3.765683 6.297416                H -4.097540 3.329220 6.938487
N 3.647953 4.261246 3.610234                H -3.458222 4.851229 6.232679
C 2.463075 3.620507 3.400063                C 1.804886 5.299257 6.096760
N 1.619402 4.003867 4.387874                H 4.392674 5.609892 5.118106
C 2.286833 4.860966 5.235215                H 5.514520 3.373843 3.183084
C 3.560356 5.023825 4.757069                H 5.348756 5.099429 2.729907
H 2.861437 0.780011 -0.902882
H 0.951488 -0.379949 -2.562154
H -2.463060 0.478416 -1.072619
H -1.754849 -1.116992 -1.460975
I 0.113745 0.887061 4.850513
H 4.526134 3.839311 1.765755

HF=-1271.684873
Zero-point vibrational energy 700282.5 (Joules/Mol)
Zero-point correction= 0.266724 (Hartree/Particle)
Thermal correction to Energy= 0.304049
Thermal correction to Enthalpy= 0.304994
Thermal correction to Gibbs Free Energy= 0.181700
Sum of electronic and zero-point Energies= -1271.418150
Sum of electronic and thermal Energies= -1271.380824
Sum of electronic and thermal Enthalpies= -1271.379880
Sum of electronic and thermal Free Energies= -1271.503173

Compound CTCMeI₃⁺
Cartesian Coordinates
Au -0.485352 3.463850 4.497157
Au -1.697534 2.285443 1.265618
Au 1.875002 2.473650 2.057303
I -1.263328 6.000277 4.836643
N -3.435154 2.923942 5.067848
C -2.435424 2.973455 4.152270
N -2.936962 2.743320 2.926430
C -4.296674 2.521857 3.078200
C -4.614727 2.637152 4.404879
C -3.302622 3.187551 6.502618
N 3.721776 3.853592 4.129598
C 2.480005 3.499977 3.725323
compound CTCMeI₄

Cartesian Coordinates

Au  -0.420151 3.281441 4.578650
Au  -1.539328 2.040847 1.357840
Au  2.016523 2.501656 1.954959
I   -0.883721 5.964994 4.753852
N   -3.442068 3.111959 4.994085
N   -2.388523 2.981887 4.152260
N   -2.828951 2.617277 2.937158
C   -4.212176 2.535635 3.010473
C   -4.601722 2.842818 4.285035
C   -3.369829 3.522921 6.395949
N   3.788964 3.734696 4.125563

H  -4.092085 2.647334 7.030713
H  -3.386792 4.262501 6.692659
H  1.771482 5.094264 6.446442
H  4.486534 4.947314 5.823473
H  5.736295 3.304187 4.190457
H  5.299806 4.416235 2.851342
H  2.817831 0.758863 -0.622139
H  0.983877 0.136826 -2.621545

HF=-1237.0734475
Zero-point vibrational energy  698765.0 (Joules/Mol)
Zero-point correction= 0.266146 (Hartree/Particle)
Thermal correction to Energy= 0.295717
Thermal correction to Enthalpy= 0.296661
Thermal correction to Gibbs Free Energy= 0.199060
Sum of electronic and zero-point Energies= -1236.807302
Sum of electronic and thermal Energies= -1236.777731
Sum of electronic and thermal Enthalpies= -1236.776787
Sum of electronic and thermal Free Energies= -1236.874387
HF=-1248.7700773

Zero-point vibrational energy   699663.4 (Joules/Mol)
Zero-point correction=          0.266488 (Hartree/Particle)
Thermal correction to Energy=   0.298570
Thermal correction to Enthalpy= 0.299514
Thermal correction to Gibbs Free Energy= 0.194821
Sum of electronic and zero-point Energies= -1248.503590
Sum of electronic and thermal Energies= -1248.471508
Sum of electronic and thermal Enthalpies= -1248.470563
Sum of electronic and thermal Free Energies= -1248.575256

CTCMeI_4*2I_2

Cartesian Coordinates
Au -0.250304 3.154259 4.831731   C -4.468277 3.249453 4.886220
Au -1.770844 2.553964 1.608567   C -3.008432 3.461803 6.949533
Au 1.851101 2.600136 1.881689   N 3.921639 3.267363 4.029968
I -0.352024 5.794903 5.477338   C 2.624313 3.038918 3.714449
N -3.232651 3.277603 5.514629   N 1.882094 3.173476 4.826570
C -2.269638 3.156168 4.572187   C 2.730723 3.488296 5.873660
N -2.850126 3.025429 3.366822   C 4.005052 3.550737 5.383649
C -4.222430 3.093568 3.550964   C 5.028661 3.318206 3.073438
N -0.908971 1.663267 -1.203266  H 2.355128 1.710317 -1.308200
C -0.565651 2.059096 0.055765  H 0.194419 1.160933 -2.982870
N 0.785078 2.125517 0.102456  H -2.955372 1.442697 -0.861263
C 1.291864 1.758035 -1.124687  H -2.302420 0.546268 -2.271983
C 0.235838 1.474319 -1.949846  I -0.356391 0.459009 4.447693
C -2.270321 1.483912 -1.710467  H 4.887267 2.530650 2.328963
H -4.904657 3.016008 2.717156  H -2.537480 2.325295 -2.358278
H -5.387713 3.336243 5.446688  H -2.093740 2.935116 7.232958
H -3.859287 3.041258 7.491482  I 1.194921 5.214987 1.600002
H -2.900598 4.527075 7.177458  I 2.941303 0.091000 1.954581
H 2.354715 3.648219 6.873214  I -2.805192 4.735605 0.129981
H 4.951718 3.760047 5.860110  I -3.824261 6.864052 -1.739529
H 5.964714 3.153142 3.612429  I -2.155304 5.045875 -3.985332
H 5.046595 4.295943 2.579681  I -0.675858 3.274532 -5.676011

HF=-1294.6411914
Zero-point vibrational energy  705370.3 (Joules/Mol)
Zero-point correction=  0.268661 (Hartree/Particle)
Thermal correction to Energy=  0.310390
Thermal correction to Enthalpy=  0.311334
Thermal correction to Gibbs Free Energy=  0.176146
Sum of electronic and zero-point Energies=  -1294.372530
Sum of electronic and thermal Energies=  -1294.330802
Sum of electronic and thermal Enthalpies=  -1294.329858
Sum of electronic and thermal Free Energies=  -1294.465046

Compound  **CTC**MeI$_5^+$

Cartesian Coordinates
Au -0.375024 3.161765 4.560471  C -2.374119 3.122756 4.127291
Au -1.502570 2.145661 1.351219  N -2.813758 2.877337 2.877879
Au 2.078265 2.789426 1.824502  C -4.195032 2.928650 2.892408
I -0.580981 5.711998 5.388210  C -4.593321 3.201698 4.171417
N -3.441555 3.315425 4.934030  C -3.408471 3.585557 6.374235
Compound $\text{CTC}^{\text{Me}}\text{I}_6$

Cartesian Coordinates

Au -0.425866 3.294618 4.559554  
Au -1.539209 1.905580 1.376858
Au 2.009966 2.553483 1.950999
I  0.858005 5.893967 3.898365
N -3.434824 3.105149 4.983537
C -2.378628 2.897494 4.163642

HF= -1260.0336785

Zero-point vibrational energy 704020.9 (Joules/Mol)

Zero-point correction= 0.268147 (Hartree/Particle)

Thermal correction to Energy= 0.302055
Thermal correction to Enthalpy= 0.302999
Thermal correction to Gibbs Free Energy= 0.194536

Sum of electronic and zero-point Energies= -1259.765531
Sum of electronic and thermal Energies= -1259.731623
Sum of electronic and thermal Enthalpies= -1259.730679
Sum of electronic and thermal Free Energies= -1259.839143
| Atom | X    | Y    | Z    |
|------|------|------|------|
| N    | 5.041562 | 1.862889 | 8.673338 |
| H    | -4.284451 | 3.511534 | 6.846914 |
| C    | -4.200557 | 2.282788 | 3.085023 |
| H    | -3.166825 | 4.774616 | 6.230624 |
| C    | -4.589912 | 2.762925 | 4.318791 |
| H    | 1.889871  | 4.448532 | 6.704908 |
| C    | -3.346690 | 3.697760 | 6.318629 |
| H    | 4.588672  | 4.476340 | 5.992516 |
| N    | 3.791122  | 3.637728 | 4.172134 |
| C    | 2.543200  | 3.324357 | 3.753403 |
| H    | 5.012858  | 4.247300 | 2.574222 |
| N    | 1.672356  | 3.619118 | 1.506112 |
| C    | 2.384248  | 4.138666 | 5.796104 |
| H    | 1.006013  | 0.609139 | -2.927214 |
| C    | 3.708600  | 4.155668 | 5.454393 |
| H    | -2.226207 | 0.233277 | -1.105835 |
| C    | 5.001770  | 3.488153 | 3.363569 |
| H    | -1.462849 | 0.068905 | -2.715675 |
| N    | -0.311113 | 1.049650 | -1.276861 |
| I    | -0.240969 | 0.929356 | 5.882916 |
| C    | -0.119161 | 1.534768 | -0.027989 |
| H    | 5.002570  | 2.490677 | 2.913575 |
| N    | 1.190626  | 1.759735 | 0.151353 |
| I    | -1.110216 | 1.656221 | -2.183149 |
| C    | 1.848753  | 1.414398 | -1.015973 |
| H    | -2.515903 | 3.229958 | 6.855519 |
| C    | 0.916758  | 0.972226 | -1.913718 |
| I    | 2.071881  | 5.060331 | 0.905871 |
| C    | -1.614755 | 0.733639 | -1.862105 |
| I    | 2.663289  | 0.077615 | 2.854520 |
| H    | -4.782845 | 1.893757 | 2.262927 |
| I    | -1.463356 | -0.706494 | 2.109150 |
| H    | -5.561613 | 2.804491 | 4.784378 |
| I    | -2.070178 | 4.268265 | 0.144239 |

HF=-1271.723155

Zero-point vibrational energy   703321.8 (Joules/Mol)
Zero-point correction=          0.267881 (Hartree/Particle)
Thermal correction to Energy=    0.304722
Thermal correction to Enthalpy=  0.305667
Thermal correction to Gibbs Free Energy= 0.186179
Sum of electronic and zero-point Energies= -1271.455274
Sum of electronic and thermal Energies= -1271.418433
Sum of electronic and thermal Enthalpies= -1271.417489
Sum of electronic and thermal Free Energies= -1271.536976

Compound **CTC** in iodomethane solution

**Cartesian Coordinates**

| Atom | X    | Y    | Z    |
|------|------|------|------|
| N    | 5.041562 | 1.862889 | 8.673338 |
| N    | 3.738126  | -5.310451 | 8.767958 |
| N    | 4.401782  | -0.216831 | 8.938648 |
| N    | 5.085346  | -4.787984 | 7.120155 |
HF=-1895.6935902

Zero-point vibrational energy  1313599.9 (Joules/Mol)
Zero-point correction= 0.500324 (Hartree/Particle)
Thermal correction to Energy= 0.536679
Thermal correction to Enthalpy= 0.537623
Thermal correction to Gibbs Free Energy= 0.423836
Sum of electronic and zero-point Energies= -1895.193266
Sum of electronic and thermal Energies= -1895.156911
Sum of electronic and thermal Enthalpies= -1895.155967
Sum of electronic and thermal Free Energies= -1895.269754

Compound CH$_3$I in iodomethane solution

**Cartesian Coordinates**

C -4.031762 1.708550 -0.036100  
H -3.644824 0.689174 0.006458  
H -3.645154 2.254498 -0.898057 
I -3.297140 2.746553 1.762511 

HF= -51.353084
Zero-point vibrational energy 93398.3 (Joules/Mol)
Zero-point correction= 0.035574 (Hartree/Particle)
Thermal correction to Energy= 0.038783
Thermal correction to Enthalpy= 0.039727
Thermal correction to Gibbs Free Energy= 0.009761
Sum of electronic and zero-point Energies= -51.17510
Sum of electronic and thermal Energies= -51.14301
Sum of electronic and thermal Enthalpies= -51.13357
Sum of electronic and thermal Free Energies= -51.343323

Transition State $^8$Br$_{TS}$

Imaginary Frequency at -424.5 cm$^{-1}$

**Cartesian Coordinates**

C 3.422185 10.523594 3.022435  C 2.885618 11.857672 4.774729 
C 3.257487 12.656449 3.748212  H 2.561200 12.103082 5.774840 
H 3.330046 13.731044 3.659389  C 0.026970 7.602002 4.961547
HF=-1947.0282326

Zero-point vibrational energy 1409786.2 (Joules/Mol)

Zero-point correction= 0.536959 (Hartree/Particle)

Thermal correction to Energy= 0.577689

Thermal correction to Enthalpy= 0.578633

Thermal correction to Gibbs Free Energy= 0.453015

Sum of electronic and zero-point Energies= -1946.491273

Sum of electronic and thermal Energies= -1946.450543

Sum of electronic and thermal Enthalpies= -1946.449599

Sum of electronic and thermal Free Energies= -1946.579217

Compound 8\text{Bz}

**Cartesian Coordinates**

C 3.470880 10.334076 3.490580  N 3.709502 11.664169 3.318098
C 3.302486 12.384017 4.429716  N 2.942192 10.236071 4.744454
H 3.388942 13.459537 4.474054  N -1.242715 7.938456 5.395557
C 2.823355 11.482865 5.329247  N -0.031466 6.595430 4.164564
H 2.421916 11.612848 6.323388  N 3.290072 4.921089 0.571988
C -0.419914 7.890076 4.302572  N 3.748268 6.996337 1.105961
C -1.375714 6.674191 5.944505  C 2.610915 3.615666 0.481951
H -1.988707 6.493914 6.816267  H 1.706577 3.728035 -0.127753
C -0.614290 5.842471 5.170216  H 3.297976 2.946463 -0.049052
H -0.440042 4.778488 5.251573  C -1.865551 9.164005 5.913702
C 2.904244 5.961081 1.373347  H -1.075957 9.827871 6.284558
C 4.372385 5.301486 -0.204435  H -2.486243 8.864306 6.766240
H 4.830976 4.624559 -0.911299  C 4.173107 12.339509 2.082309
C 4.652275 6.595732 0.137369  H 3.282309 12.650028 1.525202
H 5.421987 7.263052 -0.223317  H 4.708547 13.235389 2.417116
Au 3.681191 8.778347 2.225856  C -2.688969 9.887678 4.868008
Au 0.052034 9.442119 3.058165  C -2.510131 11.261682 4.669439
Au 1.411713 6.078643 2.730558  C -3.603614 9.190822 4.066656
C -3.238057 11.937145 3.684505 H 7.244918 9.116095 -0.970160
H -1.776010 11.796341 5.269757 C 2.251555 3.054552 1.840661
C -4.325560 9.860586 3.076431 C 0.917748 2.760230 2.148278
H -3.725497 8.117522 4.200291 C 3.234148 2.899845 2.828490
C -4.144807 11.236749 2.882886 C 0.564209 2.326365 3.430771
H -3.080186 13.002426 3.529000 H 0.151125 2.905691 1.389597
H -5.025213 9.309819 2.450535 C 2.883777 2.474913 4.111480
H -4.700520 11.755865 2.104506 H 4.268526 3.150003 2.599500
C 5.059488 11.484734 1.213465 C 1.545695 2.191082 4.417279
C 6.316317 11.062898 1.669491 H -0.477773 2.115086 3.662768
C 4.602108 11.057804 -0.039943 H 3.651082 2.371292 4.876319
C 7.098886 10.210654 0.888017 H 1.271704 1.869856 5.420339
H 6.666697 11.379834 2.650333 I 0.535590 11.335518 1.227329
C 5.388239 10.210983 -0.827941 C 2.599347 8.981745 5.421139
H 3.610839 11.358437 -0.372537 H 3.458724 8.625535 6.000562
C 6.635480 9.782948 -0.363188 H 1.748006 9.165285 6.080991
H 8.068704 9.878048 1.252709 H 2.312865 8.240370 4.673022
H 5.018408 9.872337 -1.793543

HF=-1947.1089215
Zero-point vibrational energy 1418388.0 (Joules/Mol)
Zero-point correction= 0.540235 (Hartree/Particle)
Thermal correction to Energy= 0.580980
Thermal correction to Enthalpy= 0.581924
Thermal correction to Gibbs Free Energy= 0.458734
Sum of electronic and zero-point Energies= -1946.568686
Sum of electronic and thermal Energies= -1946.527941
Sum of electronic and thermal Enthalpies= -1946.526997
Sum of electronic and thermal Free Energies= -1946.650187

Transition State 9^Bz\text{TS}
Imaginary Frequency at -426.8 cm^{-1}
Cartesian Coordinates
Au 0.482863 3.116169 4.493269
HF=-1998.4427635
Zero-point vibrational energy  1516864.1 (Joules/Mol)
Zero-point correction=  0.577743 (Hartree/Particle)
Thermal correction to Energy=  0.622627
Thermal correction to Enthalpy=  0.623571
Thermal correction to Gibbs Free Energy=  0.489122
Sum of electronic and zero-point Energies=  -1997.865020
Sum of electronic and thermal Energies=  -1997.820137
Sum of electronic and thermal Enthalpies=  -1997.819193
Sum of electronic and thermal Free Energies=  -1997.955642

Compound 9Bz

Cartesian Coordinates

C 0.872528 0.992691 -0.139432
Au 0.542193 3.687912 3.996405
Au -0.019695 0.909337 1.663715
N -1.358897 1.853043 5.523992
N -0.885361 1.022702 3.557253
C -1.779574 0.165148 4.178098
C -2.084024 0.679927 5.408072
C -1.422868 2.803270 6.644955
C -2.191804 4.055670 6.276888
C -3.558394 3.987643 5.969932
C -4.254075 5.137648 5.585556
C -3.587828 6.368213 5.507039
C -2.225250 6.441988 5.815368
C -1.531864 5.288406 6.197558
N 0.871821 0.071997 -1.144806
\[ HF = -1315.1836076 \]

Zero-point vibrational energy \[ \text{978633.3 (Joules/Mol)} \]

Zero-point correction = 0.372742 (Hartree/Particle)

Thermal correction to Energy = 0.401136

Thermal correction to Enthalpy = 0.402080

Thermal correction to Gibbs Free Energy = 0.304368

Sum of electronic and zero-point Energies = -1314.810866

Sum of electronic and thermal Energies = -1314.782472

Sum of electronic and thermal Enthalpies = -1314.781528

Sum of electronic and thermal Free Energies = -1314.885239

**Compound 4**

Cartesian Coordinates

N 3.579676 -5.440281 8.663932
N 5.070938 -4.848672 7.222370
C 4.346422 -4.384668 8.276114
C 3.825668 -6.548842 7.872764
H 3.318374 -7.489217 8.030089
H 4.762992 -6.173913 6.957546
H 5.231380 -6.721427 6.152897
C 2.682222 -5.407531 9.836471
H 2.066754 -6.311469 9.784115
H 4.304240 -6.385123 11.516821
H 4.381774 -7.272474 10.890196
C 5.056983 -6.291961 12.690608
C 3.458174 -5.334341 11.134372
C 4.304240 -6.385123 11.516821
H 5.712722 -7.110757 12.980346
C 4.968707 -5.145588 13.492311
C 4.968707 -5.145588 13.492311
H 5.558717 -5.071671 14.403694
C 4.123515 -4.096515 13.116218
H 4.056971 -3.198933 13.727450
C 3.370895 -4.192909 11.940900
H 2.732091 -3.368270 11.632288
Au 4.388362 -2.543504 9.138271
C 6.008188 -4.046597 6.431416

H 5.537993 -3.745746 5.488762
C 6.008188 -4.046597 6.431416
H 6.275383 -3.158992 7.009341
H 6.903015 -4.642011 6.226957
I 4.432787 -0.134707 10.266337

HF=-683.279163
Zero-point vibrational energy  540469.8 (Joules/Mol)
Zero-point correction=  0.205854 (Hartree/Particle)
Thermal correction to Energy=  0.221314
Thermal correction to Enthalpy=  0.222258
Thermal correction to Gibbs Free Energy=  0.157890
Sum of electronic and zero-point Energies=  -683.073309
Sum of electronic and thermal Energies=  -683.057849
Sum of electronic and thermal Enthalpies=  -683.056905
Sum of electronic and thermal Free Energies=  -683.121273

Transition State 4_{rs}
Imaginary Frequency at -390.2 cm^{-1}
Cartesian Coordinates
Au 0.597803 2.466993 5.071967
Au -0.148862 0.982542 1.900719
N -2.200268 1.317247 4.741187
C -0.734494 -0.005824 3.779271
C -2.005374 -0.592954 3.654171
C -2.914277 0.240270 4.222257
C -2.780898 2.614445 5.134396
C -2.417596 3.662741 4.095268
C -2.568388 3.389110 2.727892
C -2.124562 4.306779 1.773827
C -1.531580 5.509535 2.176727
C 8.37463 1.45318 0.286345
C -4.050963 0.332696 0.571540
C -2.302872 1.180909 -0.887286
C -2.787948 0.199243 -0.014200
C -4.837463 1.45318 0.286345
C -4.361362 2.433786 -0.593641  H -2.161927 -0.658826 0.221955
C -3.100132 2.296364 -1.179208  H -4.412281 -0.430106 1.257321
H -2.140188 -1.529351 3.132719  H -5.816909 1.564358 0.747008
H -3.989889 0.182785 4.309834  H -4.970363 3.307082 -0.817634
H -2.375952 2.893943 6.112119  H -2.728964 3.065054 -1.855245
H -3.862926 2.471556 5.225014  C 1.688283 3.789507 1.744934
H -2.992177 2.441398 2.402610  H 2.503889 4.480311 1.518118
H -2.236194 4.074937 0.718297  H 0.907537 4.295519 2.320374
H -1.174782 6.218038 1.431792  H 2.060226 2.942950 2.326180
H -0.904416 6.711309 3.861288  I 2.520744 4.173722 5.755218
H -1.658491 5.054702 5.552542  C 0.957517 -1.135728 4.256240
H 1.698376 4.893975 -0.849513  H 0.896471 -1.688485 3.330204
H 0.237040 3.364739 -2.667162  H 1.538252 -0.225018 4.304534
H -0.468762 0.094287 -1.201115  H 0.476425 -1.513879 5.146755
H -0.903606 1.173150 -2.549215  I 3.208287 -2.548769 4.913336

HF=-1366.5178347

Zero-point vibrational energy 1077087.1 (Joules/Mol)
Zero-point correction= 0.410241 (Hartree/Particle)
Thermal correction to Energy= 0.442523
Thermal correction to Enthalpy= 0.443467
Thermal correction to Gibbs Free Energy= 0.337941

Sum of electronic and zero-point Energies=-1366.107594
Sum of electronic and thermal Energies=-1366.075312
Sum of electronic and thermal Enthalpies=-1366.074367
Sum of electronic and thermal Free Energies=-1366.189894

Compound 5

Cartesian Coordinates
N 3.878842 -5.287332 7.773446  H 5.118417 1.945659 11.144899
N 2.723881 -4.170239 6.340201  C 3.610884 -4.018190 7.358119
C 5.272471 1.327209 10.273034  C 3.182483 -6.213855 7.021097
HF = -1366.6065089

Zero-point vibrational energy  1085538.7 (Joules/Mol)

Zero-point correction=  0.413460 (Hartree/Particle)

Thermal correction to Energy=  0.445945

Thermal correction to Enthalpy=  0.446889

Thermal correction to Gibbs Free Energy=  0.341884

Sum of electronic and zero-point Energies=  -1366.193049

Sum of electronic and thermal Energies=  -1366.160564
Sum of electronic and thermal Enthalpies: -1366.159620
Sum of electronic and thermal Free Energies: -1366.264625

Adduct between two molecules of 4
Cartesian Coordinates

\[
\begin{align*}
\text{N} & : -2.660267 12.944409 18.884830 & \text{H} & : -3.699795 10.306175 17.268857 \\
\text{N} & : -2.294043 10.819340 18.821942 & \text{H} & : -0.036893 12.262473 25.997478 \\
\text{C} & : -1.920098 11.959604 19.470846 & \text{H} & : 0.419431 9.516203 25.938404 \\
\text{C} & : -3.492642 12.427020 17.906976 & \text{H} & : -3.500046 14.723998 19.632310 \\
\text{C} & : -3.263990 11.087697 17.872595 & \text{H} & : -1.349801 7.646911 25.020179 \\
\text{C} & : -2.567656 14.375661 19.176720 & \text{C} & : -3.321089 13.250845 23.748760 \\
\text{H} & : -1.733760 14.540473 19.861991 & \text{C} & : -4.340410 12.889951 24.640823 \\
\text{H} & : -2.387369 14.921884 18.245388 & \text{C} & : -3.653999 13.704301 22.467876 \\
\text{C} & : -1.865814 9.438871 19.131687 & \text{C} & : -5.677460 12.973493 24.247702 \\
\text{H} & : -2.076188 8.854794 18.228722 & \text{H} & : -4.082629 12.521003 25.632105 \\
\text{H} & : -2.506730 9.063198 19.935863 & \text{C} & : -4.991446 13.796126 22.075070 \\
\text{C} & : -1.815702 10.609006 23.794821 & \text{H} & : -2.850920 13.940610 21.776731 \\
\text{C} & : -0.243501 10.141658 25.359029 & \text{C} & : -6.005279 13.427317 22.963442 \\
\text{C} & : -0.472407 11.480944 25.393532 & \text{H} & : -6.465129 12.681261 24.939303 \\
\text{N} & : -1.442191 11.749215 24.443981 & \text{H} & : -5.243928 14.127022 21.069896 \\
\text{N} & : -1.075527 9.624263 24.380872 & \text{H} & : -7.047003 13.480203 22.654282 \\
\text{C} & : -1.870353 13.129651 24.133998 & \text{C} & : -0.415007 9.317583 19.516665 \\
\text{H} & : -1.229319 13.505204 23.329873 & \text{C} & : -0.081866 8.864307 20.797560 \\
\text{H} & : -1.660119 13.713844 25.036917 & \text{C} & : 0.604176 9.678346 18.624355 \\
\text{C} & : -1.167907 8.192987 24.089066 & \text{C} & : 1.255648 8.772421 21.190105 \\
\text{H} & : -2.000729 8.028177 23.402502 & \text{H} & : -0.884845 8.628172 21.488876 \\
\text{H} & : -0.234832 7.844448 23.635049 & \text{C} & : 1.941294 9.594743 19.017247 \\
\text{Au} & : -0.460777 12.209708 20.881590 & \text{H} & : 0.346200 10.047185 17.630372 \\
\text{Au} & : -3.275051 10.358702 22.384159 & \text{C} & : 2.269314 9.141049 20.301498 \\
\text{I} & : -5.374920 9.860659 20.815273 & \text{H} & : 1.508272 8.441620 22.195257 \\
\text{I} & : 1.638859 12.707494 22.450848 & \text{H} & : 2.728848 9.886846 18.325460 \\
\text{H} & : -4.155597 13.052512 17.327676 & \text{H} & : 3.311088 9.088118 20.610440
\end{align*}
\]
HF=-1366.6055784

Zero-point vibrational energy 1085559.2 (Joules/Mol)
Zero-point correction= 0.413468 (Hartree/Particle)
Thermal correction to Energy= 0.445998
Thermal correction to Enthalpy= 0.446943
Thermal correction to Gibbs Free Energy= 0.343003
Sum of electronic and zero-point Energies= -1366.192111
Sum of electronic and thermal Energies= -1366.159580
Sum of electronic and thermal Enthalpies= -1366.158636
Sum of electronic and thermal Free Energies= -1366.262575

Compound CTC\textsuperscript{Me} in iodomethane solution

**Cartesian Coordinates**

C 4.068288 10.253720 1.745247  N 4.945538 11.224113 1.339079
C 4.966916 12.254239 2.262589  N 3.535836 10.673157 2.927486
H 5.595425 13.124086 2.133728  N 0.071239 8.450830 6.023377
C 4.086190 11.902109 3.247786  N 0.388696 7.101742 4.322271
H 3.808345 12.428478 4.150287  N 1.856243 4.742730 -0.017116
C 0.766724 8.298622 4.853119  N 2.940165 6.647001 0.093287
C -0.743737 7.352268 6.231507  C 0.969652 3.627099 0.303893
H -1.380641 7.270018 7.100949  H 1.55246 2.704946 0.412380
C -0.539284 6.518012 5.167310  H 0.463008 3.852245 1.246094
H -0.980685 5.556308 4.945689  H 0.226177 3.499121 -0.491196
C 2.030949 5.867888 0.744110  C 0.164632 9.594879 6.926752
C 2.653606 4.810762 -1.145862  H 0.879123 10.306935 6.505349
H 2.667516 4.021060 -1.883781  H -0.815985 10.074466 7.025589
C 3.324481 6.000008 -1.068265  H 0.512753 9.266038 7.912712
H 4.043791 6.436686 -1.747014  C 5.745417 11.191664 0.117258
Au 3.591679 8.509857 0.840177  H 6.812086 11.226056 0.367078
Au 2.111541 9.545708 4.001960  H 5.523815 10.261612 -0.412849
Au 1.159628 6.365678 2.499882  H 5.490724 12.046557 -0.519659

HF=-1202.8411966
Zero-point vibrational energy $688383.6$ (Joules/Mol)

Zero-point correction= $0.262191$ (Hartree/Particle)

Thermal correction to Energy= $0.284911$

Thermal correction to Enthalpy= $0.285855$

Thermal correction to Gibbs Free Energy= $0.203121$

Sum of electronic and zero-point Energies= $-1202.579005$

Sum of electronic and thermal Energies= $-1202.556286$

Sum of electronic and thermal Enthalpies= $-1202.555341$

Sum of electronic and thermal Free Energies= $-1202.638076$

Compound $10^{MeTS}$

Imaginary frequency -421.6 cm$^{-1}$

Cartesian Coordinates

C 3.370087 10.554086 2.992277
C 3.141510 12.678399 3.721094
H 3.162179 13.755135 3.629756
C 2.566417 12.101100 3.721094
C -1.579089 6.242427 5.748021
H -2.423275 5.952498 6.357450
C -0.929708 5.606892 4.763855
H -1.119229 4.641536 4.763855
C 2.890867 5.986342 1.276552
C 4.246425 5.308170 -0.390286
H 4.662330 4.622432 -1.114778
C 4.537967 6.610848 -0.395797
H 5.273598 7.273078 -0.530251
Au 3.627197 8.884475 1.901317
Au 1.409189 9.066946 4.790566
Au 1.486029 6.077898 2.727729
N 3.458032 11.850479 2.639234
N 3.703840 7.024968 0.928779
H -1.066946 8.051261 7.936623
N -0.937001 7.455414 5.920714

H 3.366064 2.846187 0.654795
H 1.872738 3.589812 1.298858
C -1.289103 8.444025 6.937697
H -2.355583 8.683154 6.865430
H -0.697232 9.345851 6.760352
C 3.843346 12.349136 1.317268
H 4.744479 12.964617 1.408849
H 4.041853 11.490150 0.672323
I 6.692196 8.311223 6.648779
C 4.504404 9.635811 5.297445
H 4.423510 8.706569 4.750559
H 4.059668 9.708574 6.280320
H 5.248854 10.361122 4.997163
H 3.025879 12.947885 0.902066
H 2.982994 10.530641 4.337899
H 2.096585 3.424766 -0.467804
HF=-1254.1710488

Zero-point vibrational energy    787049.5 (Joules/Mol)
Zero-point correction=                       0.299771 (Hartree/Particle)
Thermal correction to Energy=                 0.327332
Thermal correction to Enthalpy=               0.328276
Thermal correction to Gibbs Free Energy=      0.234390
Sum of electronic and zero-point Energies=     -1253.871277
Sum of electronic and thermal Energies=        -1253.843717
Sum of electronic and thermal Enthalpies=      -1253.842772
Sum of electronic and thermal Free Energies=   -1253.930956

Compound \textbf{11Me}

Cartesian Coordinates

\begin{verbatim}
C 3.323617 10.568418 1.851020  N 2.577841 11.009734 2.895410
C 2.808222 12.732319 1.481060  N 0.999024 8.177388 6.921860
H 2.794846 13.664679 0.950394  N 1.169325 6.903652 5.140357
C 2.254969 12.336824 2.671041  N 1.910354 6.802050 0.178731
H 1.660085 12.900349 3.375983  N 2.524040 4.736647 0.725540
C 1.321190 8.177347 5.591231  C 0.999427 9.350138 7.791886
C 0.639019 6.899923 7.312793  H 1.442796 10.183079 7.239276
H 0.343760 6.675009 8.328049  H -0.026410 9.607889 8.080937
C 0.749713 6.114753 6.196865  H 1.592798 9.146373 8.690171
H 0.562306 5.056864 6.074040  C 4.168424 11.565803 -0.300043
C 1.965879 5.917077 1.190077  C 4.757812 12.479238 -0.429354
C 2.465014 6.184907 -0.921185  H 4.831408 10.696311 -0.300752
H 2.541174 6.686557 -1.880158  H 3.445719 11.474059 -1.119434
C 2.855390 4.903719 -0.603641  I 5.473687 6.353280 1.960881
H 3.304496 4.107784 -1.183442  C 4.850098 6.193101 4.078142
Au 4.120617 8.703380 1.689877  H 4.217220 5.307587 4.129836
Au 1.925060 9.687178 4.402113  H 5.764662 6.112212 4.666935
Au 1.546586 6.327315 3.122032  H 4.283528 7.103311 4.273949
N 3.473426 11.615751 0.984787  C 2.804565 3.539501 1.505877
\end{verbatim}
HF=-1254.1742508

Zero-point vibrational energy  784362.2 (Joules/Mol)
Zero-point correction= 0.298748 (Hartree/Particle)
Thermal correction to Energy= 0.327070
Thermal correction to Enthalpy= 0.328014
Thermal correction to Gibbs Free Energy= 0.233413
Sum of electronic and zero-point Energies= -1253.875503
Sum of electronic and thermal Energies= -1253.847181
Sum of electronic and thermal Enthalpies= -1253.846237
Sum of electronic and thermal Free Energies= -1253.940838

Compound 12Me

Cartesian Coordinates

H 2.459233 2.650280 0.965660
H 3.881442 3.447885 1.701069

H 2.270239 3.615328 2.458629
H 3.479140 4.295337 2.319541

N 5.438577 10.833950 1.628695
N 4.136321 10.335522 3.325605

N 0.198870 8.060796 5.817012
N 1.273939 6.604757 4.586769

C 0.430319 3.923053 1.854563
H 0.191696 3.113977 1.158616

C 0.168579 5.973680 5.119869
H -0.042100 4.930952 4.926843

C 2.053644 5.826855 1.621730
C 0.808147 5.383347 -0.177593

H 0.066054 4.866858 -0.769666
C 1.620300 6.448790 -0.451845

H 1.708804 7.041549 -1.351100
C 3.591643 8.395320 1.137466

H 7.161448 10.609471 0.440517
H 5.637353 9.982090 -0.255771

Au 2.933465 5.681168 3.482527
H 5.935441 11.745896 -0.201209

C 4.469980 9.969286 2.054398
C 5.721192 11.747746 2.629040
H 6.461924 12.524475 2.500705

C 4.905031 11.428017 3.680797
H 4.813425 11.428017 3.680797

C 1.297341 7.888978 5.018107
C -0.514250 6.877179 5.889643

H 0.168579 5.973680 5.119869
H -0.185953 9.311914 6.464510

H 0.634160 10.024198 6.339647
H 1.708804 7.041549 -1.351100

H 1.106784 3.550299 2.628381
H 1.106784 3.550299 2.628381

C 0.808147 5.383347 -0.177593
C 0.808147 5.383347 -0.177593

H 0.066054 4.866858 -0.769666
C 1.620300 6.448790 -0.451845

H -1.419599 6.789225 6.473780
H -1.419599 6.789225 6.473780

C 6.087716 10.794559 0.321198
C 6.087716 10.794559 0.321198

Au 3.591643 8.395320 1.137466
Au 3.591643 8.395320 1.137466

Au 2.675785 9.218347 4.390448
Au 2.675785 9.218347 4.390448

Au 2.933465 5.681168 3.482527
Au 2.933465 5.681168 3.482527

C 4.721192 11.747746 2.629040
C 4.721192 11.747746 2.629040

N 0.198870 8.060796 5.817012
N 0.198870 8.060796 5.817012

N 1.273939 6.604757 4.586769
N 1.273939 6.604757 4.586769

N 1.097841 4.998985 1.122403
N 1.097841 4.998985 1.122403

N 2.398561 6.710938 0.665598
N 2.398561 6.710938 0.665598

N 0.430319 3.923053 1.854563
N 0.430319 3.923053 1.854563

H 0.191696 3.113977 1.158616
H 0.191696 3.113977 1.158616

H 0.168579 5.973680 5.119869
H 0.168579 5.973680 5.119869

H -0.042100 4.930952 4.926843
H -0.042100 4.930952 4.926843

H 0.066054 4.866858 -0.769666
H 0.066054 4.866858 -0.769666

H -1.094770 9.715433 6.002244
H -1.094770 9.715433 6.002244

H -0.364000 9.136973 7.531280
H -0.364000 9.136973 7.531280

H 1.708804 7.041549 -1.351100
H 1.708804 7.041549 -1.351100
HF= -1254.201774

Zero-point vibrational energy = 786112.2 (Joules/Mol)

Zero-point correction = 0.299414 (Hartree/Particle)

Thermal correction to Energy = 0.327461

Thermal correction to Enthalpy = 0.328405

Thermal correction to Gibbs Free Energy = 0.234814

Sum of electronic and zero-point Energies = -1253.902363

Sum of electronic and thermal Energies = -1253.874317

Sum of electronic and thermal Enthalpies = -1253.873372

Sum of electronic and thermal Free Energies = -1253.966964

Compound 3

Cartesian Coordinates

C 4.052124 10.289342 1.769221
C 4.933083 12.297235 2.290620
H 5.558390 13.169896 2.166509
C 4.032265 11.952978 3.260986
H 3.728675 12.485287 4.151459
C 0.754943 8.314959 4.889688
C -0.702913 7.406366 6.314459
H -1.334095 7.351872 7.189756
C -0.479413 6.530023 5.288352
H -0.890902 5.546164 5.113851
C 2.045300 5.878091 0.810470
C 2.651076 4.830528 -1.089255
H 2.662160 4.042334 -1.828819
C 3.309941 6.026911 -1.019776
H 4.014236 6.472481 -1.708285
Au 3.577711 8.537755 0.880725

C 4.555732 4.879077 2.387155
H 4.978527 5.722407 1.827813
H 5.283369 4.458263 3.085723
H 4.187709 4.115411 1.693899

H 4.978527 5.722407 1.827813
C 5.746817 11.221451 0.162125  C 3.576486 8.949157 5.320286
H 6.805467 11.342547 0.417322  H 3.148597 8.413231 6.171303
H 5.593593 10.253075 -0.321200  H 4.219707 8.294579 4.721620
H 5.439006 12.023531 -0.518607  H 4.111769 9.851100 5.635863
I 0.047586 10.325134 2.143644

HF= -1254.2147396
Zero-point vibrational energy  785715.7 (Joules/Mol)
Zero-point correction=    0.299263 (Hartree/Particle)
Thermal correction to Energy=    0.327458
Thermal correction to Enthalpy=    0.328402
Thermal correction to Gibbs Free Energy= 0.234015
Sum of electronic and zero-point Energies= -1253.915476
Sum of electronic and thermal Energies= -1253.887282
Sum of electronic and thermal Enthalpies= -1253.886338
Sum of electronic and thermal Free Energies= -1253.983724

Compound HCl
Cartesian Coordinates
H 0.000000 0.000000 0.004528  Cl 0.000000 0.000000 1.295472

HF= -460.8463191
Zero-point vibrational energy  17047.5 (Joules/Mol)
Zero-point correction=    0.006493 (Hartree/Particle)
Thermal correction to Energy=    0.008854
Thermal correction to Enthalpy=    0.009798
Thermal correction to Gibbs Free Energy= -0.011402
Sum of electronic and zero-point Energies= -460.839826
Sum of electronic and thermal Energies= -460.837466
Sum of electronic and thermal Enthalpies= -460.836321
Sum of electronic and thermal Free Energies= -460.857721
Transition State for the interaction of CTC\textsuperscript{Bz} and HCl

**Imaginary Frequency at -665.4 cm\textsuperscript{-1}**

**Cartesian Coordinates**

\[
\begin{array}{ll}
C & 3.067100 10.870700 2.663000 \\
C & 2.892800 13.085600 3.018600 \\
H & 3.092500 14.135100 2.855200 \\
C & 2.090200 12.433800 3.913300 \\
H & 1.449300 12.856000 4.690300 \\
C & 0.450000 7.802500 5.495700 \\
C & -0.798700 6.358000 6.696200 \\
H & -1.494800 6.049500 7.463200 \\
C & -0.111500 5.654400 5.746800 \\
H & -0.109000 4.596100 5.526400 \\
C & 3.107200 6.067300 1.758700 \\
C & 4.099200 5.587900 -0.213700 \\
H & 4.235000 5.041400 -1.136100 \\
C & 4.782100 6.619500 0.336000 \\
H & 5.646200 7.164700 -0.015000 \\
Au & 3.653700 9.055600 2.008700 \\
Au & 1.262700 9.481500 4.713900 \\
Au & 1.893500 6.167100 3.360800 \\
N & 3.495800 12.103800 2.250700 \\
N & 0.443000 7.685600 6.527100 \\
N & 0.654200 6.545000 5.013000 \\
N & 3.072800 5.260500 0.677800 \\
N & 4.177400 6.940300 1.566700 \\
C & 2.077300 4.193000 0.419900 \\
H & 1.179900 4.657500 -0.003600 \\
H & 2.520700 3.544500 -0.343700 \\
C & -0.907600 8.794000 7.379200 \\
H & -0.097800 9.078500 8.061100 \\
H & -1.733300 8.396200 7.980600 \\
C & 4.395900 12.373300 1.113000 \\
C & 3.067100 10.870700 2.663000 \\
C & 2.892800 13.085600 3.018600 \\
H & 3.092500 14.135100 2.855200 \\
C & 2.090200 12.433800 3.913300 \\
H & 1.449300 12.856000 4.690300 \\
C & 0.450000 7.802500 5.495700 \\
C & -0.798700 6.358000 6.696200 \\
H & -1.494800 6.049500 7.463200 \\
C & -0.111500 5.654400 5.746800 \\
H & -0.109000 4.596100 5.526400 \\
C & 3.107200 6.067300 1.758700 \\
C & 4.099200 5.587900 -0.213700 \\
H & 4.235000 5.041400 -1.136100 \\
C & 4.782100 6.619500 0.336000 \\
H & 5.646200 7.164700 -0.015000 \\
Au & 3.653700 9.055600 2.008700 \\
Au & 1.262700 9.481500 4.713900 \\
Au & 1.893500 6.167100 3.360800 \\
N & 3.495800 12.103800 2.250700 \\
N & 0.443000 7.685600 6.527100 \\
N & 0.654200 6.545000 5.013000 \\
N & 3.072800 5.260500 0.677800 \\
N & 4.177400 6.940300 1.566700 \\
C & 2.077300 4.193000 0.419900 \\
H & 1.179900 4.657500 -0.003600 \\
H & 2.520700 3.544500 -0.343700 \\
C & -0.907600 8.794000 7.379200 \\
H & -0.097800 9.078500 8.061100 \\
H & -1.733300 8.396200 7.980600 \\
C & 4.395900 12.373300 1.113000 \\
\end{array}
\]
HF = -2356.5498305

Zero-point vibrational energy = 1327670.2 (Joules/Mol)
Zero-point correction = 0.505683 (Hartree/Particle)
Thermal correction to Energy = 0.544418
Thermal correction to Enthalpy = 0.545362
Thermal correction to Gibbs Free Energy = 0.425182
Sum of electronic and zero-point Energies = -2356.044148
Sum of electronic and thermal Energies = -2356.005413
Sum of electronic and thermal Enthalpies = -2356.004469
Sum of electronic and thermal Free Energies = -2356.136904

Transition State for the interaction of CTCMe and HCl

**Imaginary Frequency at -693.9 cm⁻¹**

Cartesian Coordinates

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 2.919667   | 10.875668  | 2.549696   |
| C    | 2.530357   | 13.080562  | 2.734610   |
| H    | 2.631755   | 14.130586  | 2.499479   |
| C    | 1.770800   | 12.421275  | 3.661828   |
| H    | 1.073192   | 12.810106  | 4.390253   |
| C    | 0.495862   | 7.782064   | 5.534524   |
| C    | -0.521491  | 6.310951   | 6.904267   |
| H    | -1.136296  | 5.986171   | 7.731707   |
| C    | 0.181352   | 5.613656   | 5.961326   |
| H    | 0.285812   | 4.546848   | 5.821530   |
| C    | 3.210317   | 6.066888   | 1.828792   |
| C    | 4.139730   | 5.623264   | -0.179835  |
| C    | 4.252160   | 5.090516   | -1.113428  |
| C    | 4.828717   | 6.656754   | 0.359438   |
| H    | 5.674299   | 7.213159   | -0.018127  |
| Au   | 3.632082   | 9.076346   | 1.992342   |

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 0.844800   | 1.626800   | 5.010300   |
| Cl   | 5.894000   | 6.658100   | 3.851200   |
| H    | 4.987500   | 6.843200   | 2.629400   |
| Au   | 1.170909   | 9.467110   | 4.643400   |
| Au   | 2.028737   | 6.150136   | 3.453455   |
| N    | 3.235714   | 12.107997  | 2.048927   |
| N    | 2.012636   | 11.063301  | 3.545301   |
| N    | -0.318681  | 7.651219   | 6.626166   |
| N    | 0.805517   | 6.519930   | 5.121208   |
| N    | 3.146881   | 5.275598   | 0.740149   |
| N    | 4.258105   | 6.962230   | 1.610965   |
| C    | 2.183908   | 4.192380   | 0.531042   |
| H    | 2.722471   | 3.255653   | 0.353966   |
| H    | 1.567767   | 4.105558   | 1.428931   |
| C    | -0.875979  | 8.752571   | 7.408330   |
| H    | -1.963793  | 8.643053   | 7.478436   |
| C    | -0.632999  | 9.690564   | 6.902189   |
| H    | 4.212933   | 12.375131  | 0.995346   |
| Au   | 3.789014   | 13.082711  | 0.275285   |
HF=-1663.6931792

Zero-point vibrational energy  704912.1 (Joules/Mol)
Zero-point correction= 0.268487 (Hartree/Particle)
Thermal correction to Energy= 0.294045
Thermal correction to Enthalpy= 0.294989
Thermal correction to Gibbs Free Energy= 0.206920
Sum of electronic and zero-point Energies= -1663.424692
Sum of electronic and thermal Energies= -1663.399135
Sum of electronic and thermal Enthalpies= -1663.398190
Sum of electronic and thermal Free Energies= -1663.482260
5. Crystallographic files

**Figure S17.** ORTEP plot of the columnar packing in the crystal structure of the compound 2 corresponding to the platelets phase. The linear arrangement is based on the intermolecular iodine-iodine interactions.
Figure S18. Packing of compound 3 in the unit cell displaying neither aurophilic nor halogen contacts.

References

(1) Abdou, H. E.; Mohamed, A. A.; Fackler, J. P. Oxidative Addition of Methyl Iodide to Dinuclear Gold(I) Amidinate Complex: Schmidbaur’s Breakthrough Reaction Revisited with Amidinates. Zeitschrift fur Naturforsch. - Sect. B J. Chem. Sci. 2004, 59 (11–12), 1480–1482. https://doi.org/10.1515/znb-2004-11-1217.

(2) Muramatsu, S.; Wu, X.; Chen, M.; Zhou, M.; Tsukuda, T. Photoassisted Homocoupling of Methyl Iodide Mediated by Atomic Gold in Low-Temperature Neon Matrix. J. Phys. Chem. A 2017, 121 (44), 8408–8413. https://doi.org/10.1021/acs.jpca.7b08863.