

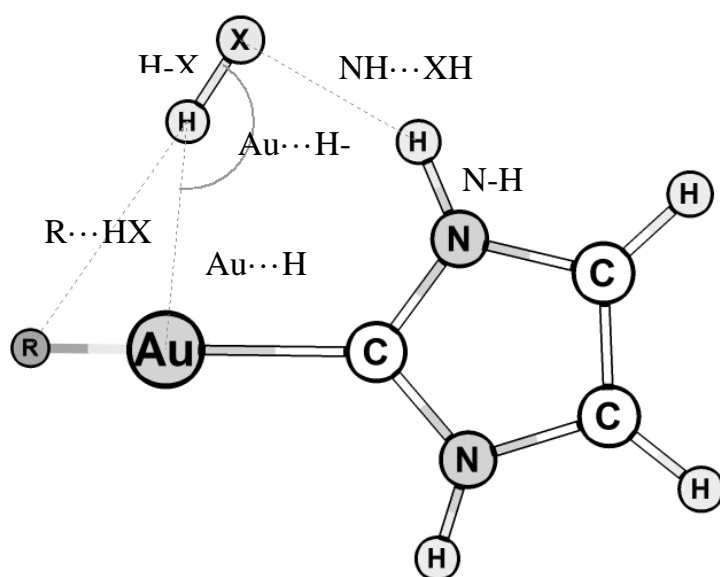
Computational investigation of Au^I⋯H hydrogen bonds involving neutral Au^I N-heterocyclic carbene complexes

Ferdinand Groenewald, Helgard G. Raubenheimer, Jan Dillen and Catharine Esterhuysen*

Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag XI, Matieland, Stellenbosch, 7602, South Africa. E-mail: ce@sun.ac.za

Supplementary Information

S1. Selected geometrical parameters at different levels of theory



Scheme S1 – Schematic representation defining the geometric parameters listed for the hydrogen bonded Au(I)NHC complexes.

Table S1 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol, various intermolecular geometrical parameters [$\text{Au}\cdots\text{H}$ (Å), $\text{Au}\cdots\text{H-X}$ angle (°), $\text{R}\cdots\text{HX}$ (Å), $\text{NH}\cdots\text{XH}$ (Å)], the H-N (Å), H-X (Å) distances of the H-bond donors of the H-bonded adducts of complex **1** to H_2O , HF and NH_3 at two levels of theory.

R = H			Intermolecular Geometrical Parameters					H-Bond Donors	
Method	H-Bond Donor	E_{INT} (kcal/mol)	$\text{Au}\cdots\text{H}$ (Å)	$\text{Au}\cdots\text{H-X}$ (deg)	$\text{H}\cdots\text{HX}$ (Å)	$\text{NH}\cdots\text{XH}$ (Å)	$\text{N-H}\cdots\text{X}$ (deg)	H-N (Å)	H-X (Å)
TPSS	H_2O	-10.70	2.39	149.7	3.01	1.88		1.03	0.99
MP2		-12.07	2.45	146.0	3.03	1.89		1.02	0.98
TPSS	HF	-12.39	2.16	156.0	2.77	1.97		1.02	0.97
MP2		-11.89	2.25	151.8	2.82	1.98		1.01	0.95
TPSS	NH_3	-11.38	2.73	139.2	3.34	1.87		1.04	1.03
MP2		-13.28	2.67	139.6	3.24	1.87		1.03	1.02

Table S2 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol, various intermolecular geometrical parameters [$\text{Au}\cdots\text{H}$ (Å), $\text{Au}\cdots\text{H-X}$ angle (°), $\text{R}\cdots\text{HX}$ (Å), $\text{NH}\cdots\text{XH}$ (Å)], the H-N (Å), H-X (Å) distances of the H-bond donors of the H-bonded adducts of complex **2** to H_2O , HF and NH_3 at two levels of theory.

R = CH₃			Intermolecular Distances (Å)				H-Bond Donors	
Method	H-Bond Donor	E_{INT} (kcal/mol)	$\text{Au}\cdots\text{H}$ (Å)	$\text{Au}\cdots\text{H-X}$ (deg)	$\text{C}\cdots\text{H}$ (Å)	$\text{NH}\cdots\text{XH}$ (Å)	H-N (Å)	H-X (Å)
TPSS	H_2O	-10.36	2.39	151.8	3.38	1.89	1.03	0.99
MP2		-11.78	2.44	148.1	3.36	1.89	1.02	0.98
TPSS	HF	-12.38	2.15	158.8	3.14	1.97	1.02	0.97
MP2		-11.78	2.24	154.8	3.17	1.98	1.01	0.95
TPSS	NH_3	-10.95	2.76	139.6	3.67	1.87	1.04	1.03
MP2		-12.89	2.68	140.7	3.55	1.88	1.03	1.02

Table S3 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol, various intermolecular geometrical parameters [$\text{Au}\cdots\text{H}$ (Å), $\text{Au}\cdots\text{H-X}$ angle ($^\circ$), $\text{R}\cdots\text{HX}$ (Å), $\text{NH}\cdots\text{XH}$ (Å)], the H-N (Å), H-X (Å) distances of the H-bond donors of the H-bonded adducts of complex **3** to H_2O , HF and NH_3 at two levels of theory.

R = Cl			Intermolecular Distances (Å)				H-Bond Donors	
Method	H-Bond Donor	E_{INT} (kcal/mol)	$\text{Au}\cdots\text{H}$ (Å)	$\text{Au}\cdots\text{H-X}$ (deg)	$\text{Cl}\cdots\text{HX}$ (Å)	$\text{NH}\cdots\text{XH}$ (Å)	H-N (Å)	H-X (Å)
TPSS	H_2O	-9.93	2.60	139.3	3.58	1.86	1.03	0.98
MP2		-11.68	2.64	134.6	3.52	1.87	1.02	0.97
TPSS	HF	-9.57	2.27	152.0	3.35	1.95	1.02	0.96
MP2		-9.76	2.44	141.9	3.33	1.98	1.01	0.94
TPSS	NH_3	-12.01	3.03	126.6	3.96	1.85	1.04	1.02
MP2		-13.91	2.85	129.9	3.71	1.85	1.02	1.04

Table S4 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol, various intermolecular geometrical parameters [$\text{Au}\cdots\text{H}$ (Å), $\text{Au}\cdots\text{H-X}$ angle ($^\circ$), $\text{R}\cdots\text{HX}$ (Å), $\text{NH}\cdots\text{XH}$ (Å)], the H-N (Å), H-X (Å) distances of the H-bond donors of the H-bonded adducts of complex **4** to H_2O , HF and NH_3 at two levels of theory.

R = OH			Intermolecular Distances (Å)				H-Bond Donors	
Method	H-Bond Donor	E_{INT} (kcal/mol)	$\text{Au}\cdots\text{H}$ (Å)	$\text{Au}\cdots\text{H-X}$ (deg)	$\text{O}\cdots\text{H}$ (Å)	$\text{NH}\cdots\text{XH}$ (Å)	H-N (Å)	H-X (Å)
TPSS	H_2O	-9.76	2.53	143.3	3.29	1.89	1.03	0.98
MP2		-11.59	2.57	139.7	3.28	1.89	1.02	0.97
TPSS	HF	-10.88	2.18	160.1	3.23	1.97	1.02	0.97
MP2		-10.64	2.32	152.2	3.19	1.97	1.01	0.94
TPSS	NH_3	-11.16	2.93	130.0	3.58	1.87	1.04	1.02
MP2		-13.14	2.81	132.3	3.43	1.87	1.03	1.02

Table S5 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol and various geometrical parameters [$\text{Au}\cdots\text{H}$ (Å), $\text{Au}\cdots\text{H-X}$ angle ($^\circ$), $\text{R}\cdots\text{HX}$ (Å), $\text{NH}\cdots\text{XH}$ (Å)], the H-N (Å), H-X (Å)] for the H-bonded adducts of complexes **5**, **6**, **7** and **8** with H_2O , HF and NH_3 at the MP2/aug-cc-pVTZ-pp level of theory (E_{INT} at the B3LYP-D3/aug-cc-pVTZ-pp level of theory given in parenthesis).

	R	H-bond donor	Intermolecular Geometrical Parameters				H-bond Donors		E_{INT} (kcal/mol)
			$\text{Au}\cdots\text{H}$ (Å)	$\text{Au}\cdots\text{H-X}$ ($^\circ$)	$\text{R}\cdots\text{HX}$ (Å)	$\text{NH}\cdots\text{XH}$ (Å)	H-N (Å)	H-X (Å)	
5	H	H_2O	2.43	145.2	3.00	1.90	1.02	0.98	-11.70
		HF	2.29	150.2	2.84	1.99	1.02	0.94	-10.69* (-12.60)
		NH_3	2.65	138.4	3.20	1.90	1.03	1.02	-12.54
6	CH_3	H_2O	2.43	147.4	3.34	1.91	1.02	0.98	-11.32
		HF	2.24	154.5	3.15	1.99	1.02	0.95	-11.56 (-12.61)
		NH_3	2.71	138.7	3.56	1.91	1.03	1.02	-11.76*
7	Cl	H_2O	2.24	133.4	3.48	1.89	1.02	0.97	-11.22
		HF	2.44	141.1	3.30	1.99	1.02	0.94	-9.54 (-10.40)
		NH_3	2.82	128.5	3.65	1.88	1.04	1.02	-13.09
8	OH	H_2O	2.58	137.5	3.24	1.92	1.02	0.97	-10.57
		HF	2.39	146.3	3.07	2.00	1.02	0.94	-9.31 (-10.36)
		NH_3	3.01	128.8	3.65	1.92	1.03	1.02	-13.14

* MP2/cc-pVTZ-pp value as MP2/aug-cc-pVTZ calculation did not complete owing to computational expense.

Table S6 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol and various geometrical parameters [Au...H (Å), Au...H-X angle (°), R...HX (Å), NH...XH (Å)], the H-N (Å), H-X (Å)] for the alternate conformations of H-bonded adducts of complexes **5**, **6**, **7** and **8** with H₂O, HF and NH₃ without NH...X interactions at the MP2/aug-cc-pVTZ-pp level of theory (E_{INT} at the B3LYP-D3/aug-cc-pVTZ-pp level of theory given in parenthesis).

	R	H-bond donor	Intermolecular Geometrical Parameters				H-bond Donors		E_{INT} (kcal/mol)
			Au...H (Å)	Au...H-X (°)	R...HX (Å)	NH...XH (Å)	H-N (Å)	H-X (Å)	
5	H	H ₂ O_alt	2.61	152.8	3.49	3.84	1.01	0.97	-6.65*
		HF_alt	2.32	158.3	2.80	5.05	1.01	0.94	-7.17* (-8.88)
		NH ₃ _alt	2.72	153.0	3.23	5.57	1.01	1.02	-4.96*
6	CH₃	H ₂ O_alt	2.56	158.5	3.67	4.38	1.01	0.97	-4.78**
		HF_alt	2.33	162.3	3.50	3.62	1.01	0.94	-8.59 (-9.12)
		NH ₃ _alt	2.72	155.3	3.53	5.54	1.01	1.02	-4.80*
7	Cl	H ₂ O_alt	2.23	146.2	4.10	3.75	1.01	0.97	-6.84
		HF_alt	2.47	153.4	3.84	3.94	1.01	0.93	-6.63 (-6.95)
		NH ₃ _alt	3.02	144.4	4.44	3.59	1.01	1.02	-6.17
8	OH	H ₂ O_alt	2.63	152.7	3.85	3.83	1.01	0.97	-6.91
		HF_alt	2.40	161.7	3.58	3.63	1.01	0.94	-7.67 (-8.16)
		NH ₃ _alt	2.97	151.9	3.94	5.01	1.01	1.02	-5.55

* B3LYP/aug-cc-pVTZ-pp value as the alternative geometry could not be found as a minimum on the MP2/aug-cc-pVTZ or MP2/cc-pVTZ-pp energy surfaces.

Table S7 – Counterpoise corrected values for the interaction energies (E_{INT}) in kcal/mol and various geometrical parameters [Au...H (Å), Au...H-X angle (°), R...HX (Å), NH...XH (Å)], the H-N (Å), H-X (Å)] for the alternate conformations of H-bonded adducts of complexes **9** and **10** with H₂O, HF and NH₃ at the B3LYP/aug-cc-pVTZ-pp level of theory (MP2/aug-cc-pVTZ calculations did not complete owing to computational expense).

			Intermolecular Geometrical Parameters				H-bond Donors		E_{INT} (kcal/mol)
	R	H-bond donor	Au...H (Å)	Au...H-X (°)	R...HX (Å)	CH...XH (Å)	H-N (Å)	H-X (Å)	
9	CH₃	H ₂ O	2.52	164.2	3.39	2.63	1.09	0.97	-4.90
		HF	2.30	164.2	3.08	2.82	1.09	0.95	-7.55
		NH ₃	2.86	157.1	3.54	2.56	1.09	1.02	-3.28

S2. Energy Decomposition Analysis (EDA) results for adducts of HF with complexes 1-9

Table S8 – EDA results (kcal/mol) at the BP86-D3/def2-TZVP level of theory for adducts of complexes **1** – **9** with HF.

	1	2	3	4	5	6	7	8	5alt	6alt	7alt	8alt	9
Electrostatic	-14.77	-14.83	-11.82	-13.95	-14.75	-14.74	-11.72	-11.55	-8.51	-8.7	-6.21	-7.82	-9.05
Pauli	15.31	15.83	11.48	14.76	15.54	16.02	11.5	11.93	8.69	9.26	6.6	8.45	9.47
Orbital	-12.43	-12.85	-8.83	-11.78	-12.57	-12.97	-8.78	-9.32	-8.11	-8.53	-5.79	-7.59	-8.86
Dispersion	-2.26	-2.45	-2.44	-2.34	-2.23	-2.43	-2.44	-2.31	-1.97	-2.25	-2.32	-2.25	-2.51
Total Bonding Energy	-14.15	-14.3	-11.61	-13.31	-14.01	-14.13	-11.44	-11.25	-9.91	-10.21	-7.71	-9.2	-10.95

Table S9 – EDA results (kcal/mol) at the BP86-D3/def2-TZVP level of theory for interactions involving ligands NHC1 and NHC3 with HF.

	NHC1	NHC3	1-NHC1	9-NHC3
Electrostatic	-8.37	-4.31	-6.4	-4.74
Pauli	5.82	1.73	9.49	7.74
Orbital	-3.2	-1.28	-9.23	-7.58
Dispersion	-1.29	-1.28	-0.97	-1.23
Total Bonding Energy	-7.04	-5.14	-7.11	-5.81

S3. AIM plots

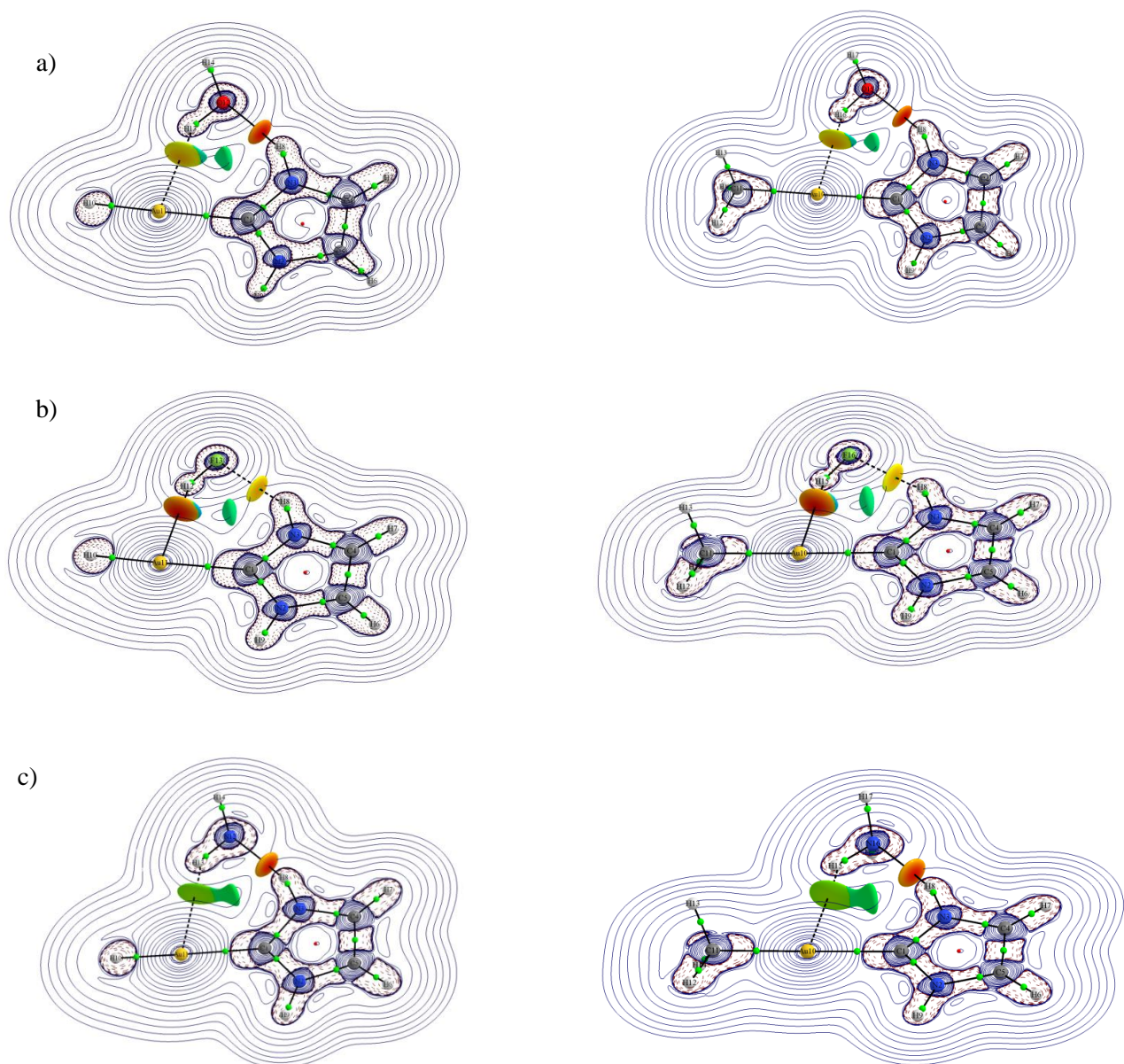


Figure S1a – The two-dimensional contour plot of $\nabla^2(\rho_b)$ (ea_0^{-5}) with the NCI plots shown as green to red areas on the images for complexes **1** (left) and **2** (right) with (a) H₂O, (b) HF and (c) NH₃.

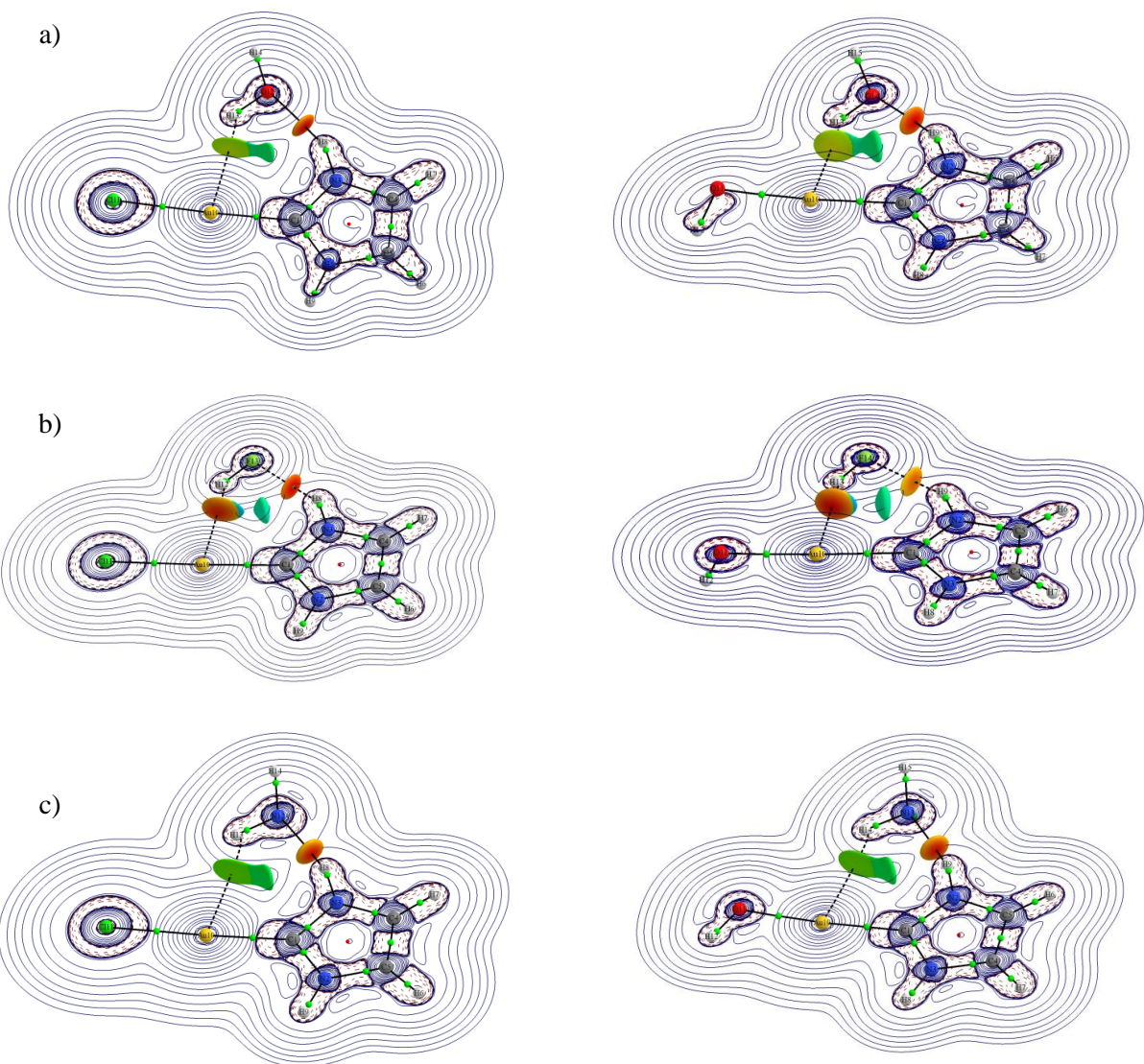


Figure S1b – The two-dimensional contour plot of $\nabla^2(\rho_b)$ (ea_0^{-5}) with the NCI plots shown as green to red areas on the images for complexes **3** (left) and **4** (right) with (a) H_2O , (b) HF and (c) NH_3 .

S4. Optimised geometries of adducts at various levels of theory

Cartesian coordinates (Å) and three lowest frequencies (cm⁻¹) of optimised geometries.

S4.1 Adducts with H-Au(I)-NHC1

S4.1.1 H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

71.9442 95.1630 135.5109

Optimised Coordinates

6	2.456069	-1.939848	4.223441
7	2.268585	-1.047195	5.224048
7	1.268524	-1.943701	3.582355
6	0.361263	-1.078067	4.160343
6	0.994993	-0.504383	5.208734
1	0.659518	0.222620	5.924085
1	-0.636549	-0.943362	3.787052
1	1.119851	-2.533346	2.765162
1	2.988805	-0.821272	5.886866
1	5.411760	-3.946126	3.287042
79	4.139739	-3.063386	3.718889
8	1.783654	-3.711703	1.390255
1	2.686790	-3.733889	1.755756
1	1.552752	-4.632238	1.232525

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

73.6357 111.2012 130.5374

Optimised Coordinates

6	2.457226000	-1.954369000	4.205766000
7	2.265744000	-1.062209000	5.218841000
7	1.261658000	-1.944879000	3.561327000
6	0.354451000	-1.078560000	4.145024000
6	0.991261000	-0.512698000	5.205247000

1	0.658937000	0.212318000	5.929962000
1	-0.645026000	-0.938134000	3.767065000
1	1.122454000	-2.536812000	2.731756000
1	2.987577000	-0.841431000	5.889168000
1	5.367511000	-3.978590000	3.215018000
79	4.109942000	-3.081700000	3.676947000
8	1.816279000	-3.679409000	1.405659000
1	2.711961000	-3.656909000	1.824286000
1	1.595780000	-4.622513000	1.370487000

MP2/cc-pVTZ-pp

Low Frequencies

72.0509	102.5695	145.9322
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Optimised Coordinates

6	2.463436000	-1.955118000	4.210180000
7	2.280559000	-1.052998000	5.206670000
7	1.266075000	-1.958884000	3.581083000
6	0.367875000	-1.095374000	4.154818000
6	1.017865000	-0.510114000	5.203292000
1	0.689053000	0.221623000	5.916517000
1	-0.632987000	-0.961376000	3.790492000
1	1.115065000	-2.556804000	2.768735000
1	3.011616000	-0.827224000	5.859494000
1	5.346260000	-3.907971000	3.321049000
79	4.092270000	-3.041421000	3.731579000
8	1.778342000	-3.694031000	1.416444000
1	2.669097000	-3.730023000	1.802444000
1	1.591229000	-4.606179000	1.183757000

MP2/aug-cc-pVTZ-pp

Low Frequencies

72.0056	108.5868	148.9143
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Optimised Coordinates

6	2.457611000	-1.959196000	4.204486000
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7	2.278746000	-1.059070000	5.204179000
7	1.259563000	-1.957466000	3.575775000
6	0.364155000	-1.092336000	4.152806000
6	1.017125000	-0.511998000	5.203073000
1	0.690902000	0.219261000	5.919219000
1	-0.637283000	-0.953894000	3.789312000
1	1.108706000	-2.554085000	2.760820000
1	3.012089000	-0.837692000	5.857309000
1	5.327579000	-3.920374000	3.296139000
79	4.078360000	-3.048920000	3.717301000
8	1.797504000	-3.688222000	1.419259000
1	2.691552000	-3.697631000	1.809938000
1	1.609143000	-4.614270000	1.236938000

S4.1.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

62.8027 108.3444 135.6637

Optimised Coordinates

6	2.509020000	-1.917074000	4.262148000
7	2.271943000	-1.032720000	5.257898000
7	1.340645000	-1.944346000	3.586960000
6	0.395853000	-1.102520000	4.140477000
6	0.987033000	-0.518850000	5.207424000
1	0.615068000	0.197744000	5.915119000
1	-0.593860000	-0.991372000	3.739206000
1	1.221801000	-2.532815000	2.771960000
1	2.965602000	-0.792607000	5.943905000
1	5.500836000	-3.894586000	3.377218000
79	4.221832000	-3.020245000	3.793486000
1	2.971018000	-3.823349000	2.083603000
9	2.160395000	-3.866347000	1.586223000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

64.8935 115.1577 130.2480

Optimised Coordinates

6	2.518144000	-1.926256000	4.254040000
7	2.274248000	-1.035734000	5.255532000
7	1.340673000	-1.950261000	3.577466000
6	0.392768000	-1.107822000	4.131501000
6	0.986033000	-0.521084000	5.204869000
1	0.615058000	0.197541000	5.916957000
1	-0.599629000	-0.998701000	3.725957000
1	1.229259000	-2.545605000	2.757218000
1	2.969331000	-0.792847000	5.946385000
1	5.479400000	-3.913945000	3.339814000
79	4.207101000	-3.029743000	3.772110000
1	2.979675000	-3.768743000	2.161575000
9	2.175125000	-3.845886000	1.622203000

MP2/cc-pVTZ-pp

Low Frequencies

60.7562 111.9015 145.0099

Optimised Coordinates

6	2.523381000	-1.929272000	4.252544000
7	2.282777000	-1.043160000	5.249608000
7	1.349213000	-1.951862000	3.580781000
6	0.409131000	-1.116703000	4.129899000
6	1.008437000	-0.529341000	5.206328000
1	0.637528000	0.186415000	5.915027000
1	-0.581166000	-1.003825000	3.731400000
1	1.233137000	-2.541876000	2.765587000
1	2.982737000	-0.807816000	5.932717000
1	5.455261000	-3.837336000	3.427431000
79	4.185678000	-2.987396000	3.814908000
1	2.941548000	-3.818585000	2.074617000
9	2.139523000	-3.858328000	1.584781000

MP2/aug-cc-pVTZ-pp*Low Frequencies*

61.0408 114.3286 148.9128

Optimised Coordinates

6	2.520997000	-1.931221000	4.248754000
7	2.282903000	-1.045134000	5.247184000
7	1.345863000	-1.952580000	3.578007000
6	0.407041000	-1.116449000	4.129057000
6	1.008454000	-0.529921000	5.205607000
1	0.638894000	0.186360000	5.915720000
1	-0.584382000	-1.002324000	3.731513000
1	1.228685000	-2.542974000	2.761713000
1	2.984965000	-0.811066000	5.929840000
1	5.445636000	-3.844419000	3.413077000
79	4.178991000	-2.990573000	3.807172000
1	2.955477000	-3.804268000	2.100546000
9	2.153660000	-3.854513000	1.597439000

S4.1.3. NH₃ adduct**B3LYP/aug-cc-pVTZ-pp***Low Frequencies*

66.7222 76.1693 106.7823

Optimised Coordinates

6	2.542686000	-1.845913000	4.353927000
7	2.276425000	-0.983619000	5.365099000
7	1.394153000	-1.864462000	3.646122000
6	0.433912000	-1.038401000	4.195648000
6	0.991476000	-0.474328000	5.291961000
1	0.596647000	0.224657000	6.005076000
1	-0.546128000	-0.920846000	3.772299000
1	1.301936000	-2.446347000	2.801616000
1	2.952968000	-0.758506000	6.072583000
1	5.626144000	-3.740617000	3.620649000
79	4.289194000	-2.907956000	3.952728000

7	1.754808000	-3.678362000	1.398109000
1	2.698463000	-3.840338000	1.745868000
1	1.292761000	-4.579543000	1.356053000
1	1.840943000	-3.339808000	0.446612000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

70.3252	77.6988	127.4396
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Optimised Coordinates

6	2.537248000	-1.857419000	4.334819000
7	2.275605000	-0.990425000	5.356122000
7	1.374531000	-1.864870000	3.632731000
6	0.419880000	-1.034227000	4.192263000
6	0.989594000	-0.473169000	5.292931000
1	0.604401000	0.227991000	6.015142000
1	-0.565213000	-0.911702000	3.771939000
1	1.282558000	-2.454025000	2.778484000
1	2.959738000	-0.768443000	6.064431000
1	5.579817000	-3.772531000	3.548375000
79	4.253644000	-2.924474000	3.908677000
7	1.776806000	-3.658542000	1.438709000
1	2.720292000	-3.795601000	1.820404000
1	1.343809000	-4.579967000	1.390690000
1	1.893679000	-3.336987000	0.478631000

MP2/cc-pVTZ-pp

Low Frequencies

74.4633	82.1821	97.8977
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Optimised Coordinates

6	2.534285000	-1.862262000	4.327474000
7	2.281678000	-1.000881000	5.346145000
7	1.374005000	-1.864482000	3.633143000
6	0.430549000	-1.039584000	4.190675000
6	1.010557000	-0.481224000	5.294134000

1	0.629207000	0.217117000	6.014798000
1	-0.552960000	-0.910632000	3.779712000
1	1.279070000	-2.446494000	2.786600000
1	2.972448000	-0.788786000	6.045602000
1	5.510382000	-3.727877000	3.568431000
79	4.209670000	-2.900440000	3.916550000
7	1.777607000	-3.660400000	1.435965000
1	2.711637000	-3.786391000	1.821439000
1	1.369478000	-4.585332000	1.384429000
1	1.908775000	-3.356724000	0.479251000

MP2/aug-cc-pVTZ-pp

Low Frequencies

75.8014 87.6950 104.8272

Optimised Coordinates

6	2.529454000	-1.864557000	4.321479000
7	2.280678000	-1.003473000	5.342027000
7	1.367494000	-1.864656000	3.629032000
6	0.426016000	-1.038466000	4.189495000
6	1.009534000	-0.481724000	5.292844000
1	0.630398000	0.217090000	6.015470000
1	-0.558951000	-0.907420000	3.780507000
1	1.274138000	-2.448383000	2.781100000
1	2.974305000	-0.793333000	6.040531000
1	5.492908000	-3.739625000	3.542068000
79	4.196782000	-2.906256000	3.900972000
7	1.795340000	-3.658608000	1.448963000
1	2.728686000	-3.777850000	1.843218000
1	1.378694000	-4.581176000	1.403336000
1	1.920911000	-3.345955000	0.493303000

S4.2. H₃C-Au(I)-NHC adducts

S4.2.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

44.9851 69.6168 83.6960

Optimised Coordinates

6	2.422143000	-1.930920000	4.212537000
7	2.241792000	-1.039982000	5.217211000
7	1.230090000	-1.928377000	3.578035000
6	0.328727000	-1.061348000	4.163829000
6	0.969833000	-0.493028000	5.210338000
1	0.640451000	0.232869000	5.929640000
1	-0.670657000	-0.922278000	3.796373000
1	1.073528000	-2.513981000	2.760060000
1	2.966644000	-0.818908000	5.876490000
79	4.102430000	-3.038940000	3.724490000
6	5.771225000	-4.152299000	3.215900000
1	6.547222000	-4.051153000	3.979691000
1	5.538385000	-5.216461000	3.124581000
1	6.200057000	-3.823703000	2.265781000
8	1.736140000	-3.693603000	1.382760000
1	2.628742000	-3.712822000	1.773599000
1	1.509186000	-4.614815000	1.223530000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

47.8100 70.6197 81.9547

Optimised Coordinates

6	2.424859000	-1.939179000	4.202809000
7	2.231216000	-1.048609000	5.218277000
7	1.228078000	-1.928317000	3.558617000
6	0.319994000	-1.063848000	4.144561000

6	0.956226000	-0.500035000	5.205923000
1	0.623149000	0.223063000	5.932245000
1	-0.679641000	-0.923303000	3.766991000
1	1.087647000	-2.517623000	2.728333000
1	2.953179000	-0.829296000	5.888853000
79	4.087663000	-3.048096000	3.704412000
6	5.741702000	-4.166941000	3.183075000
1	6.531362000	-4.058799000	3.938653000
1	5.503562000	-5.235661000	3.104869000
1	6.158460000	-3.846443000	2.219691000
8	1.799912000	-3.662097000	1.407381000
1	2.681627000	-3.627562000	1.854406000
1	1.586942000	-4.607003000	1.375749000

MP2/cc-pVTZ-pp

Low Frequencies

27.0123 69.3314 84.8413

Optimised Coordinates

6	2.443527000	-1.955890000	4.200573000
7	2.264143000	-1.061424000	5.205828000
7	1.244125000	-1.948364000	3.573441000
6	0.349911000	-1.086323000	4.156488000
6	1.003434000	-0.513414000	5.209158000
1	0.678392000	0.213085000	5.929459000
1	-0.650866000	-0.945106000	3.794609000
1	1.087757000	-2.536997000	2.756083000
1	2.997189000	-0.844877000	5.859442000
79	4.068921000	-3.028890000	3.731825000
6	5.699843000	-4.122456000	3.236056000
1	6.519267000	-3.936581000	3.934103000
1	5.493817000	-5.194745000	3.257737000
1	6.064859000	-3.878586000	2.236197000
8	1.755902000	-3.665235000	1.392141000
1	2.636613000	-3.694301000	1.801466000

1 1.579101000 -4.579644000 1.160240000

MP2/aug-cc-pVTZ-pp

Low Frequencies

22.5024 69.4358 85.8980

Optimised Coordinates

6 2.439669000 -1.958038000 4.198138000
7 2.260836000 -1.065270000 5.205606000
7 1.240876000 -1.947486000 3.569103000
6 0.346840000 -1.085006000 4.153142000
6 1.000282000 -0.515218000 5.208443000
1 0.675169000 0.210695000 5.930529000
1 -0.654038000 -0.941308000 3.790115000
1 1.086961000 -2.535524000 2.749346000
1 2.994482000 -0.851492000 5.860789000
79 4.060749000 -3.032080000 3.725807000
6 5.687175000 -4.128145000 3.223578000
1 6.508804000 -3.935794000 3.918796000
1 5.475543000 -5.200023000 3.252699000
1 6.042149000 -3.885277000 2.218949000
8 1.788186000 -3.660343000 1.398671000
1 2.669650000 -3.661102000 1.817573000
1 1.612603000 -4.588337000 1.213560000

S4.2.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

31.2238 60.3873 83.0106

Optimised Coordinates

6 2.491651000 -1.720924000 2.301164000
7 1.247467000 -2.237187000 2.434649000
7 2.285851000 -0.390096000 2.403341000
6 0.953778000 -0.078321000 2.595190000
6 0.288189000 -1.254989000 2.615697000

1	-0.755870000	-1.472355000	2.739835000
1	0.599153000	0.929881000	2.698548000
1	3.055220000	0.264215000	2.340057000
1	1.067422000	-3.225026000	2.403033000
79	4.307616000	-2.685375000	2.009454000
6	6.130264000	-3.614794000	1.718711000
1	5.993353000	-4.697704000	1.652180000
1	6.610001000	-3.284409000	0.794713000
1	6.819975000	-3.417964000	2.542502000
1	5.113743000	-0.580975000	2.025249000
9	5.047472000	0.367738000	2.087770000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

42.5826 62.2727 80.4972

Optimised Coordinates

6	2.499579000	-1.731511000	2.299930000
7	1.241665000	-2.237819000	2.439304000
7	2.296267000	-0.391219000	2.398867000
6	0.964422000	-0.068046000	2.592690000
6	0.286855000	-1.246224000	2.619144000
1	-0.761545000	-1.460206000	2.746410000
1	0.618529000	0.947587000	2.693041000
1	3.080631000	0.256086000	2.330369000
1	1.051381000	-3.228923000	2.412072000
79	4.311879000	-2.679739000	2.009994000
6	6.137733000	-3.590764000	1.720366000
1	6.005935000	-4.677144000	1.627595000
1	6.627423000	-3.234207000	0.806109000
1	6.817985000	-3.406544000	2.560717000
1	5.047193000	-0.660488000	2.025422000
9	5.029353000	0.310876000	2.080062000

MP2/cc-pVTZ-pp

Low Frequencies

30.6711 58.2724 84.2138

Optimised Coordinates

6	2.530223000	-1.730900000	2.295150000
7	1.283815000	-2.249865000	2.426057000
7	2.311349000	-0.399157000	2.401918000
6	0.986972000	-0.092754000	2.591524000
6	0.322120000	-1.284252000	2.607495000
1	-0.720805000	-1.506984000	2.729485000
1	0.625863000	0.912554000	2.697498000
1	3.080431000	0.256728000	2.340908000
1	1.115060000	-3.240837000	2.389568000
79	4.281242000	-2.670584000	2.012987000
6	6.058539000	-3.594058000	1.728374000
1	5.923111000	-4.677035000	1.682146000
1	6.532799000	-3.284416000	0.795399000
1	6.758748000	-3.387126000	2.539625000
1	5.120294000	-0.542766000	2.029582000
9	5.045525000	0.393168000	2.094377000

MP2/aug-cc-pVTZ-pp

Low Frequencies

25.5819 58.8276 85.5004

Optimised Coordinates

6	2.531587000	-1.729312000	2.295067000
7	1.284845000	-2.248770000	2.425988000
7	2.313401000	-0.397207000	2.401768000
6	0.988547000	-0.090551000	2.591451000
6	0.323019000	-1.282439000	2.607485000
1	-0.720736000	-1.505148000	2.729583000
1	0.627388000	0.915594000	2.697480000
1	3.083865000	0.258899000	2.340592000
1	1.116448000	-3.240654000	2.389399000
79	4.281676000	-2.666903000	2.013147000

6	6.061092000	-3.584647000	1.728597000
1	5.923474000	-4.668342000	1.682614000
1	6.530995000	-3.269630000	0.794256000
1	6.757518000	-3.372593000	2.542884000
1	5.104395000	-0.580780000	2.029404000
9	5.047772000	0.364197000	2.092381000

S4.2.3. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

41.7676 63.1726 73.5679

Optimised Coordinates

6	2.581941000	-1.808178000	2.299856000
7	1.314608000	-2.266328000	2.452021000
7	2.444626000	-0.468887000	2.401300000
6	1.131358000	-0.096751000	2.610624000
6	0.406939000	-1.238911000	2.643829000
1	-0.644842000	-1.404511000	2.782917000
1	0.825058000	0.927212000	2.716444000
1	3.259558000	0.154619000	2.323111000
1	1.090036000	-3.244856000	2.424405000
79	4.321731000	-2.879120000	1.983694000
6	6.074820000	-3.935526000	1.664711000
1	5.872463000	-5.004565000	1.555174000
1	6.586728000	-3.604921000	0.756674000
1	6.773026000	-3.818136000	2.498119000
1	5.424167000	-0.217374000	1.946550000
7	5.082231000	0.730207000	2.094758000
1	5.353369000	1.278890000	1.286839000
1	5.579286000	1.105082000	2.894717000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

42.6099 64.6906 73.2981

Optimised Coordinates

6	2.588618000	-1.803187000	2.297680000
7	1.310588000	-2.260118000	2.450927000
7	2.445165000	-0.455426000	2.402892000
6	1.129130000	-0.082782000	2.613509000
6	0.400281000	-1.230829000	2.645168000
1	-0.654828000	-1.400882000	2.784557000
1	0.824226000	0.945564000	2.721266000
1	3.273779000	0.168836000	2.323452000
1	1.082785000	-3.243041000	2.422280000
79	4.326106000	-2.854278000	1.981769000
6	6.084941000	-3.890185000	1.662935000
1	5.890371000	-4.963965000	1.539103000
1	6.602712000	-3.543353000	0.758578000
1	6.779409000	-3.776546000	2.506164000
1	5.375611000	-0.302577000	1.994924000
7	5.064731000	0.670280000	2.098271000
1	5.360954000	1.164023000	1.257333000
1	5.592524000	1.066410000	2.874935000

MP2/cc-pVTZ-pp

Low Frequencies

18.8968 71.7738 74.7677

Optimised Coordinates

6	2.607995000	-1.801546000	2.290875000
7	1.340556000	-2.267734000	2.439519000
7	2.454321000	-0.461763000	2.401393000
6	1.147287000	-0.100615000	2.610453000
6	0.426465000	-1.260210000	2.635736000
1	-0.623773000	-1.435389000	2.772894000
1	0.831083000	0.919304000	2.722809000
1	3.271703000	0.161491000	2.326975000
1	1.130184000	-3.250455000	2.404241000
79	4.298869000	-2.825907000	1.983503000

6	6.023595000	-3.843537000	1.671879000
1	5.841493000	-4.918892000	1.610528000
1	6.509326000	-3.545115000	0.740014000
1	6.741618000	-3.683538000	2.479455000
1	5.371442000	-0.310631000	1.999029000
7	5.080699000	0.659439000	2.104083000
1	5.398978000	1.139201000	1.271505000
1	5.625262000	1.033840000	2.870852000

MP2/aug-cc-pVTZ-pp

Low Frequencies

13.2620	73.2635	77.7563
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Optimised Coordinates

6	2.608043000	-1.796892000	2.291051000
7	1.340525000	-2.264347000	2.439328000
7	2.454190000	-0.456740000	2.401908000
6	1.146388000	-0.095988000	2.610934000
6	0.425703000	-1.256541000	2.635761000
1	-0.625317000	-1.432255000	2.772794000
1	0.829304000	0.924490000	2.723636000
1	3.275455000	0.164441000	2.327022000
1	1.131091000	-3.248145000	2.403566000
79	4.300220000	-2.814382000	1.983954000
6	6.029240000	-3.823617000	1.672191000
1	5.846605000	-4.900100000	1.615074000
1	6.508269000	-3.521976000	0.736868000
1	6.745119000	-3.654593000	2.481027000
1	5.359935000	-0.350408000	1.998160000
7	5.084428000	0.626240000	2.101912000
1	5.395253000	1.107713000	1.266272000
1	5.622652000	1.001044000	2.874285000

S4.3. Adducts of Cl-Au(I)-NHC

S4.3.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

54.9387 65.0751 74.6716

Optimised Coordinates

6	2.475489000	-1.929221000	4.247299000
7	2.274629000	-1.030886000	5.239570000
7	1.295941000	-1.956440000	3.593298000
6	0.376552000	-1.095402000	4.158323000
6	0.994792000	-0.505089000	5.206357000
1	0.645753000	0.224300000	5.912459000
1	-0.619351000	-0.975822000	3.775395000
1	1.159299000	-2.555115000	2.779263000
1	2.987703000	-0.791903000	5.905704000
79	4.111121000	-2.987530000	3.802625000
17	5.936070000	-4.241559000	3.211884000
8	1.701238000	-3.712213000	1.369723000
1	2.640755000	-3.798683000	1.589927000
1	1.402805000	-4.605168000	1.171216000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

58.7051 64.8792 75.2305

Optimised Coordinates

6	2.468995000	-1.948443000	4.219073000
7	2.273663000	-1.049772000	5.225408000
7	1.276614000	-1.958596000	3.569032000
6	0.364136000	-1.093556000	4.146217000
6	0.994314000	-0.513197000	5.202002000
1	0.655506000	0.215348000	5.919810000
1	-0.635513000	-0.964953000	3.765097000
1	1.141504000	-2.557947000	2.743215000
1	2.993708000	-0.818795000	5.894307000

79	4.079331000	-3.014358000	3.754846000
17	5.878300000	-4.273313000	3.153825000
8	1.735531000	-3.677675000	1.376783000
1	2.667960000	-3.692561000	1.678471000
1	1.488747000	-4.612913000	1.314958000

MP2/cc-pVTZ-pp

Low Frequencies

60.2819	68.7235	74.5542
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Optimised Coordinates

6	2.480994000	-1.941690000	4.234357000
7	2.286169000	-1.033594000	5.222305000
7	1.290327000	-1.969867000	3.594459000
6	0.380418000	-1.110839000	4.156652000
6	1.016323000	-0.508010000	5.203205000
1	0.674615000	0.226303000	5.907463000
1	-0.619461000	-0.992628000	3.784604000
1	1.150401000	-2.577066000	2.785925000
1	3.011343000	-0.794081000	5.877105000
79	4.062343000	-2.970609000	3.801421000
17	5.843346000	-4.203598000	3.222949000
8	1.713512000	-3.701902000	1.402864000
1	2.636295000	-3.807851000	1.670452000
1	1.456171000	-4.575298000	1.099281000

MP2/aug-cc-pVTZ-pp

Low Frequencies

60.4520	70.6424	75.1546
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Optimised Coordinates

6	2.472830000	-1.946141000	4.227835000
7	2.283699000	-1.040249000	5.219262000
7	1.281159000	-1.967581000	3.588931000
6	0.375163000	-1.106224000	4.155136000
6	1.015388000	-0.509190000	5.203319000

1	0.677489000	0.224831000	5.910959000
1	-0.625439000	-0.982543000	3.784487000
1	1.141041000	-2.573430000	2.777883000
1	3.011737000	-0.805908000	5.874090000
79	4.045814000	-2.981660000	3.784523000
17	5.808894000	-4.219071000	3.191359000
8	1.737118000	-3.695697000	1.405264000
1	2.666643000	-3.763146000	1.674775000
1	1.491261000	-4.594718000	1.165221000

S4.3.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

56.1825 61.1026 66.7528

Optimised Coordinates

6	2.506834000	-1.916765000	4.262397000
7	2.276946000	-1.033562000	5.260473000
7	1.339736000	-1.945255000	3.585702000
6	0.399250000	-1.101426000	4.143250000
6	0.992791000	-0.519612000	5.209462000
1	0.623639000	0.197062000	5.918302000
1	-0.590511000	-0.988810000	3.742927000
1	1.217663000	-2.532481000	2.770407000
1	2.973319000	-0.796051000	5.944915000
79	4.167370000	-2.953786000	3.847232000
17	6.024129000	-4.169774000	3.304831000
1	2.906873000	-3.885262000	1.969457000
9	2.067491000	-3.861089000	1.543502000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

59.9290 62.2153 67.7624

Optimised Coordinates

6	2.507874	-1.937704	4.235252
7	2.283471	-1.050303	5.244257
7	1.326812	-1.953492	3.564908
6	0.392487	-1.105152	4.132828
6	0.998858	-0.527830	5.203361
1	0.639963	0.190482	5.921610
1	-0.601957	-0.987205	3.735378
1	1.202117	-2.543935	2.743352
1	2.987633	-0.816881	5.929364
79	4.153557	-2.973930	3.811922
17	6.012863	-4.169049	3.295463
1	2.907440	-3.790635	2.096421
9	2.094413	-3.841175	1.588742

MP2/cc-pVTZ-pp

Low Frequencies

59.0482 59.3877 69.6115

Optimised Coordinates

6	2.525841000	-1.922073000	4.262168000
7	2.286439000	-1.036493000	5.259479000
7	1.355052000	-1.950816000	3.585308000
6	0.414443000	-1.115957000	4.134549000
6	1.010718000	-0.526917000	5.211055000
1	0.637721000	0.188633000	5.918693000
1	-0.575184000	-1.005606000	3.733962000
1	1.239954000	-2.541139000	2.770297000
1	2.986349000	-0.800542000	5.942822000
79	4.137132000	-2.923160000	3.867913000
17	5.955084000	-4.115918000	3.342479000
1	2.884798000	-3.898531000	1.940459000
9	2.047184000	-3.858295000	1.533673000

MP2/aug-cc-pVTZ-pp

Low Frequencies

57.9234 59.8789 71.7607

Optimised Coordinates

6	2.521836000	-1.925114000	4.256104000
7	2.286777000	-1.039934000	5.255280000
7	1.349576000	-1.951546000	3.581383000
6	0.411380000	-1.115258000	4.133765000
6	1.011314000	-0.527951000	5.210064000
1	0.640983000	0.188107000	5.919807000
1	-0.579652000	-1.002798000	3.735096000
1	1.232368000	-2.541858000	2.765232000
1	2.989615000	-0.806056000	5.937584000
79	4.129791000	-2.928408000	3.857212000
17	5.937159000	-4.120419000	3.326944000
1	2.905082000	-3.880201000	1.974902000
9	2.069303000	-3.855376000	1.549486000

S4.3.3. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

48.0999 65.6004 70.8095

Optimised Coordinates

6	2.532171000	-1.891845000	4.306724000
7	2.283725000	-1.017301000	5.311295000
7	1.374354000	-1.933093000	3.617086000
6	0.421068000	-1.104529000	4.174145000
6	0.994003000	-0.519981000	5.251309000
1	0.607997000	0.187062000	5.961020000
1	-0.567058000	-1.000346000	3.766835000
1	1.267171000	-2.528797000	2.780168000
1	2.972288000	-0.777423000	6.002275000
79	4.210857000	-2.897887000	3.909599000
17	6.110108000	-4.080354000	3.396152000

1	2.508181000	-3.999145000	1.551595000
1	1.005662000	-4.600009000	1.339105000
7	1.545871000	-3.742165000	1.347635000
1	1.532442000	-3.370786000	0.404384000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

47.7085	65.4450	76.4610
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Optimised Coordinates

6	2.533720000	-1.900927000	4.294988000
7	2.284182000	-1.020680000	5.307722000
7	1.363782000	-1.935384000	3.606777000
6	0.412309000	-1.103651000	4.169886000
6	0.992153000	-0.518999000	5.252306000
1	0.611507000	0.190225000	5.968686000
1	-0.579764000	-0.997686000	3.762185000
1	1.258138000	-2.538602000	2.760422000
1	2.977738000	-0.781494000	6.001146000
79	4.193742000	-2.907376000	3.887624000
17	6.070019000	-4.092515000	3.359673000
1	2.528328000	-3.973762000	1.592253000
1	1.034006000	-4.600179000	1.360511000
7	1.559760000	-3.726992000	1.374701000
1	1.559219000	-3.368577000	0.420447000

MP2/cc-pVTZ-pp

Low Frequencies

57.2999	60.1212	68.9563
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Optimised Coordinates

6	2.515490000	-1.903720000	4.278981000
7	2.284899000	-1.031149000	5.292425000
7	1.343835000	-1.926988000	3.606181000
6	0.409538000	-1.099367000	4.175073000
6	1.008899000	-0.522115000	5.257783000

1	0.638958000	0.183666000	5.976941000
1	-0.583225000	-0.982412000	3.783538000
1	1.233430000	-2.522735000	2.767394000
1	2.989965000	-0.805731000	5.973477000
79	4.121667000	-2.898337000	3.860317000
17	5.942818000	-4.087787000	3.304994000
7	1.592548000	-3.727213000	1.390786000
1	2.553187000	-3.929804000	1.653026000
1	1.117534000	-4.620931000	1.365681000
1	1.629296000	-3.401976000	0.432729000

MP2/aug-cc-pVTZ-pp

Low Frequencies

58.5628 65.8400 71.3492

Optimised Coordinates

6	2.509701000	-1.905396000	4.273655000
7	2.283093000	-1.033254000	5.288755000
7	1.336658000	-1.926709000	3.602577000
6	0.404320000	-1.097817000	4.174188000
6	1.007114000	-0.522135000	5.256795000
1	0.639421000	0.184149000	5.977854000
1	-0.589826000	-0.978807000	3.784521000
1	1.228644000	-2.524507000	2.762386000
1	2.990820000	-0.809660000	5.968937000
79	4.108856000	-2.904709000	3.845038000
17	5.913349000	-4.098046000	3.275514000
7	1.614041000	-3.726376000	1.403613000
1	2.575444000	-3.923781000	1.673029000
1	1.131419000	-4.617367000	1.385115000
1	1.645784000	-3.392183000	0.447349000

S4.4. Adducts with HO-Au(I)-NHC

S4.4.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

71.9571 77.1073 101.5482

Optimised Coordinates

6	-1.672044000	-0.841666000	-1.178972000
7	-2.077398000	-1.722515000	-0.237273000
7	-2.833112000	-0.335501000	-1.661898000
6	-3.938401000	-0.888459000	-1.037140000
6	-3.453676000	-1.769298000	-0.133352000
1	-3.962787000	-2.412453000	0.559439000
1	-4.946309000	-0.613651000	-1.284145000
1	-2.858040000	0.360798000	-2.385177000
1	-1.402490000	-2.274786000	0.288947000
79	0.200213000	-0.432663000	-1.696214000
8	2.122535000	-0.098896000	-2.065753000
1	2.255241000	0.171515000	-2.978794000
1	0.795070000	-2.498267000	-0.092800000
8	0.351605000	-2.994270000	0.613555000
1	0.907910000	-2.878151000	1.390004000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

68.8716 88.0596 106.0585

Optimised Coordinates

6	-1.650478000	-0.858379000	-1.163647000
7	-2.074494000	-1.734770000	-0.212026000
7	-2.817022000	-0.348774000	-1.658286000
6	-3.931848000	-0.893038000	-1.034687000
6	-3.454606000	-1.774235000	-0.116705000
1	-3.970866000	-2.413096000	0.580781000
1	-4.939138000	-0.611432000	-1.293326000
1	-2.836549000	0.346293000	-2.389711000

1	-1.393131000	-2.293959000	0.316024000
79	0.220376000	-0.469136000	-1.663165000
8	2.141191000	-0.146908000	-2.021704000
1	2.250144000	0.173452000	-2.930339000
1	0.698455000	-2.459787000	-0.184911000
8	0.341508000	-2.991291000	0.560100000
1	0.904775000	-2.753204000	1.312031000

MP2/cc-pVTZ-pp

Low Frequencies

71.1291	82.0665	96.4753
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Optimised Coordinates

6	-1.650565000	-0.821100000	-1.159685000
7	-2.064933000	-1.721680000	-0.237128000
7	-2.814948000	-0.321293000	-1.647440000
6	-3.918453000	-0.887761000	-1.054258000
6	-3.432901000	-1.786406000	-0.149652000
1	-3.945676000	-2.444521000	0.525702000
1	-4.925685000	-0.619433000	-1.309995000
1	-2.829586000	0.387671000	-2.360461000
1	-1.385999000	-2.271960000	0.288301000
79	0.164505000	-0.393829000	-1.647520000
8	2.037406000	0.004784000	-2.011847000
1	2.184528000	-0.094275000	-2.958871000
1	0.767878000	-2.386910000	-0.084019000
8	0.349661000	-2.953363000	0.580867000
1	0.953084000	-2.918189000	1.326435000

MP2/aug-cc-pVTZ-pp

Low Frequencies

70.4522	79.6909	90.5477
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Optimised Coordinates

6	-1.652692000	-0.831725000	-1.156557000
7	-2.069716000	-1.725631000	-0.228594000

7	-2.814608000	-0.329145000	-1.647790000
6	-3.920707000	-0.888044000	-1.050533000
6	-3.438581000	-1.783972000	-0.140387000
1	-3.954320000	-2.436858000	0.539059000
1	-4.927607000	-0.616814000	-1.307976000
1	-2.826004000	0.376215000	-2.365711000
1	-1.390049000	-2.275849000	0.298401000
79	0.163573000	-0.412814000	-1.642068000
8	2.041701000	-0.026171000	-1.993722000
1	2.219887000	-0.061480000	-2.941469000
1	0.753379000	-2.402096000	-0.132925000
8	0.351405000	-2.949657000	0.562023000
1	0.952655000	-2.864224000	1.308678000

S4.4.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

52.3781 77.4634 103.9149

Optimised Coordinates

6	-1.251170000	-0.512654000	-1.672402000
7	-1.992618000	-1.194077000	-0.771810000
7	-2.173313000	0.188194000	-2.374240000
6	-3.460148000	-0.050793000	-1.924235000
6	-3.341732000	-0.930416000	-0.904603000
1	-4.086877000	-1.381411000	-0.276930000
1	-4.325366000	0.413942000	-2.357613000
1	-1.923717000	0.803008000	-3.128708000
1	-1.562844000	-1.824685000	-0.107049000
79	0.728541000	-0.539443000	-1.899066000
8	2.680331000	-0.621017000	-2.203941000
1	3.164858000	-0.240989000	-1.465299000
1	0.637455000	-2.117982000	-0.210784000
9	0.177976000	-2.622395000	0.448915000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

49.1072 89.0540 99.3508

Optimised Coordinates

6	-1.237745000	-0.486100000	-1.642012000
7	-1.988884000	-1.233890000	-0.788919000
7	-2.176097000	0.211339000	-2.347206000
6	-3.468868000	-0.092741000	-1.943855000
6	-3.345942000	-1.012827000	-0.952037000
1	-4.091756000	-1.518018000	-0.361041000
1	-4.338919000	0.361693000	-2.387903000
1	-1.931013000	0.865067000	-3.076354000
1	-1.546569000	-1.853963000	-0.112751000
79	0.733805000	-0.427458000	-1.823581000
8	2.680191000	-0.252438000	-2.076620000
1	3.139899000	-1.048951000	-1.770307000
1	0.610291000	-1.777048000	-0.118404000
9	0.232982000	-2.365382000	0.553224000

MP2/cc-pVTZ-pp

Low Frequencies

50.0332 78.3271 100.3555

Optimised Coordinates

6	-1.216661000	-0.458250000	-1.611388000
7	-1.977976000	-1.187678000	-0.761338000
7	-2.139462000	0.193959000	-2.362823000
6	-3.428471000	-0.113462000	-1.998213000
6	-3.321827000	-1.001846000	-0.968497000
1	-4.077610000	-1.496676000	-0.388905000
1	-4.291115000	0.306648000	-2.479080000
1	-1.872450000	0.827186000	-3.097511000

1	-1.549597000	-1.786933000	-0.066439000
79	0.710080000	-0.383223000	-1.731681000
8	2.649365000	-0.253472000	-1.781149000
1	2.980830000	-0.940855000	-2.369922000
1	0.648702000	-1.907525000	0.082395000
9	0.157567000	-2.428590000	0.686786000

MP2/aug-cc-pVTZ-pp

Low Frequencies

49.9000	78.3118	101.2737
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Optimised Coordinates

6	-1.220765000	-0.467206000	-1.614492000
7	-1.979915000	-1.202217000	-0.767465000
7	-2.144077000	0.196700000	-2.355641000
6	-3.432928000	-0.109088000	-1.986971000
6	-3.324574000	-1.008586000	-0.966284000
1	-4.079816000	-1.506814000	-0.387404000
1	-4.296813000	0.319527000	-2.459859000
1	-1.877531000	0.835132000	-3.087251000
1	-1.550156000	-1.807010000	-0.076508000
79	0.704393000	-0.388160000	-1.748435000
8	2.639488000	-0.228212000	-1.835732000
1	3.023738000	-1.004216000	-2.262310000
1	0.636969000	-1.858862000	0.041332000
9	0.173363000	-2.401705000	0.659256000

S4.4.3. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

59.6136	73.3740	82.6691
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Optimised Coordinates

6	-1.744611000	-0.738997000	-1.355370000
7	-2.087687000	-1.610104000	-0.380820000
7	-2.936675000	-0.259563000	-1.792082000

6	-4.000957000	-0.818437000	-1.104793000
6	-3.456597000	-1.674459000	-0.210676000
1	-3.921856000	-2.311257000	0.518184000
1	-5.024252000	-0.564336000	-1.306949000
1	-3.007505000	0.420878000	-2.527038000
1	-1.372557000	-2.137272000	0.140830000
79	0.089031000	-0.292451000	-1.961832000
8	1.986509000	0.053174000	-2.439969000
1	2.049111000	0.660239000	-3.182714000
7	0.304702000	-2.829701000	0.767970000
1	0.896292000	-2.297436000	0.134569000
1	0.600234000	-2.602264000	1.710624000
1	0.514555000	-3.809797000	0.616451000

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

58.8002 75.5658 90.7324

Optimised Coordinates

6	-1.731243000	-0.746855000	-1.354016000
7	-2.086097000	-1.620148000	-0.371382000
7	-2.932694000	-0.263283000	-1.792890000
6	-4.002406000	-0.818053000	-1.103379000
6	-3.458591000	-1.678551000	-0.202433000
1	-3.926369000	-2.315045000	0.530921000
1	-5.027248000	-0.557398000	-1.310344000
1	-3.002929000	0.419178000	-2.532763000
1	-1.361472000	-2.151638000	0.154733000
79	0.097274000	-0.312346000	-1.948305000
8	1.994570000	0.023574000	-2.413658000
1	2.039560000	0.651079000	-3.151240000
7	0.289014000	-2.808695000	0.745300000
1	0.869919000	-2.268992000	0.098196000
1	0.607513000	-2.574698000	1.684828000
1	0.518934000	-3.789913000	0.592815000

MP2/cc-pVTZ-pp*Low Frequencies*

42.8062 62.3539 70.9258

Optimised Coordinates

6	-1.721032000	-0.736047000	-1.315637000
7	-2.092973000	-1.621873000	-0.361820000
7	-2.905958000	-0.250404000	-1.770618000
6	-3.983175000	-0.811667000	-1.125386000
6	-3.456970000	-1.689732000	-0.223201000
1	-3.941272000	-2.336116000	0.484033000
1	-5.000941000	-0.553701000	-1.348279000
1	-2.951694000	0.443878000	-2.496253000
1	-1.381022000	-2.155908000	0.160041000
79	0.069134000	-0.299576000	-1.871415000
8	1.933392000	0.062596000	-2.316095000
1	1.960215000	0.483048000	-3.182247000
7	0.299459000	-2.796273000	0.724756000
1	0.832012000	-2.266084000	0.040259000
1	0.660271000	-2.519882000	1.629340000
1	0.568290000	-3.764043000	0.598906000

MP2/aug-cc-pVTZ-pp*Low Frequencies*

44.2076 68.7723 72.5999

Optimised Coordinates

6	-1.725205000	-0.762094000	-1.330122000
7	-2.096175000	-1.629666000	-0.359188000
7	-2.908706000	-0.268852000	-1.781218000
6	-3.985790000	-0.808582000	-1.115938000
6	-3.460052000	-1.679883000	-0.205841000
1	-3.944833000	-2.310963000	0.515978000
1	-5.003602000	-0.541985000	-1.332391000
1	-2.953882000	0.412947000	-2.519877000

1	-1.379710000	-2.159263000	0.165259000
79	0.064324000	-0.354132000	-1.903561000
8	1.933076000	-0.046900000	-2.373115000
1	2.000765000	0.601652000	-3.084116000
7	0.303194000	-2.774928000	0.713434000
1	0.837056000	-2.208277000	0.057589000
1	0.643460000	-2.542085000	1.639104000
1	0.563814000	-3.738772000	0.540388000

S4.5. Adducts with H-Au(I)-NHC2

S4.5.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

64.1874 99.1813 105.2458

Optimised Coordinates

1	1.442223	-7.011322	0.220929
6	1.279187	-5.936320	0.225187
6	0.668513	-5.450010	1.547607
1	-0.403887	-5.268254	1.496299
1	1.124933	-3.535892	2.524728
7	1.389481	-4.184566	1.781453
6	2.439177	-3.957554	1.046291
79	3.665800	-2.292851	1.233462
6	2.590379	-5.126134	0.106695
1	0.614293	-5.698784	-0.604263
1	0.857766	-6.130471	2.380250
1	2.810251	-4.789228	-0.905088
1	3.467839	-5.692194	0.434432
1	4.602484	-0.989828	1.407516
8	1.433057	-2.029374	3.714655
1	2.247822	-1.782520	3.239713
1	0.935646	-1.210903	3.805286

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

63.3587 104.1612 114.2785

Optimised Coordinates

1	1.422708	-6.998616	0.190789
6	1.270659	-5.918251	0.222779
6	0.668755	-5.458820	1.562494
1	-0.409678	-5.284965	1.528624
1	1.123403	-3.528569	2.556018
7	1.382679	-4.182847	1.802283
6	2.437862	-3.944529	1.061851
79	3.633498	-2.281430	1.268760
6	2.592415	-5.116526	0.117550
1	0.602055	-5.647930	-0.599066
1	0.881723	-6.147884	2.387852
1	2.824848	-4.781686	-0.896437
1	3.462742	-5.694337	0.457900
1	4.557869	-0.964232	1.458925
8	1.466182	-2.050798	3.699525
1	2.286383	-1.859758	3.180618
1	0.960862	-1.225026	3.654686

MP2/cc-pVTZ-pp

Low Frequencies

63.6501 105.7139 117.8682

Optimised Coordinates

1	1.375292	-6.964497	0.126179
6	1.270638	-5.886515	0.207857
6	0.696869	-5.459777	1.557634
1	-0.380713	-5.317553	1.558006
1	1.107112	-3.519263	2.514806
7	1.380006	-4.175982	1.779998
6	2.436672	-3.944901	1.053111
79	3.614380	-2.330342	1.209021
6	2.609669	-5.134469	0.143523

1	0.617392	-5.542965	-0.591984
1	0.960574	-6.144902	2.364056
1	2.902925	-4.830260	-0.857725
1	3.437765	-5.721047	0.551924
1	4.537091	-1.048441	1.351201
8	1.417954	-2.050716	3.676462
1	2.215975	-1.796715	3.183817
1	0.965365	-1.217859	3.827265

MP2/aug-cc-pVTZ-pp

Low Frequencies

63.1416 111.2601 117.3241

Optimised Coordinates

1	1.377216	-6.963365	0.122286
6	1.269294	-5.885162	0.207189
6	0.695244	-5.465191	1.559783
1	-0.383333	-5.324935	1.561924
1	1.103246	-3.523138	2.523366
7	1.375774	-4.179878	1.786795
6	2.432070	-3.944618	1.059237
79	3.602433	-2.328184	1.225108
6	2.607259	-5.129561	0.144894
1	0.614363	-5.539789	-0.591518
1	0.963306	-6.152890	2.363522
1	2.898569	-4.818867	-0.855863
1	3.437203	-5.716837	0.550690
1	4.521452	-1.042466	1.376667
8	1.434905	-2.046889	3.670168
1	2.242216	-1.815397	3.173021
1	0.973751	-1.209037	3.777881

S4.5.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

55.8395 104.6240 105.2635

Optimised Coordinates

6	1.279418	-5.932274	0.224929
6	0.650607	-5.461952	1.544510
1	-0.420095	-5.275875	1.480636
1	1.093250	-3.562151	2.542433
7	1.371136	-4.199841	1.801855
6	2.426986	-3.960735	1.080121
79	3.637733	-2.282982	1.301201
6	2.589540	-5.116807	0.128628
1	0.623654	-5.689547	-0.609984
1	0.828013	-6.151198	2.372172
1	2.817098	-4.766688	-0.877000
1	3.466049	-5.684126	0.456965
1	4.546085	-0.969015	1.507536
1	1.447112	-7.006335	0.212803
9	1.487705	-1.840292	3.525897
1	2.250456	-1.685344	2.976932

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

58.1642 103.8053 110.8842

Optimised Coordinates

6	1.274341	-5.919014	0.221524
6	0.650871	-5.465377	1.553034
1	-0.425435	-5.284612	1.501788
1	1.090680	-3.546600	2.554117
7	1.366761	-4.192929	1.809934
6	2.430885	-3.949551	1.085199
79	3.616504	-2.276274	1.314161
6	2.597429	-5.116204	0.137805
1	0.618360	-5.647083	-0.609605
1	0.847743	-6.157929	2.379107
1	2.842356	-4.775904	-0.871434

1	3.463858	-5.695206	0.486223
1	4.519980	-0.951935	1.524165
1	1.428717	-6.998833	0.189021
9	1.502561	-1.861380	3.490429
1	2.269135	-1.746331	2.904166

MP2/cc-pVTZ-pp

Low Frequencies

53.6501 108.9569 117.7447

Optimised Coordinates

6	1.267456	-5.880423	0.206805
6	0.687961	-5.474459	1.560496
1	-0.388840	-5.328159	1.558295
1	1.093861	-3.552231	2.539368
7	1.373795	-4.194990	1.803285
6	2.431049	-3.950346	1.081900
79	3.597480	-2.326373	1.264962
6	2.605879	-5.125728	0.156036
1	0.616180	-5.527272	-0.590214
1	0.947516	-6.171005	2.358111
1	2.900017	-4.806442	-0.840249
1	3.434374	-5.716958	0.556995
1	4.498807	-1.035855	1.433389
1	1.374878	-6.956786	0.110947
9	1.450671	-1.848531	3.505275
1	2.203663	-1.689604	2.964233

S4.5.3. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

66.5802 73.0753 98.3486

Optimised Coordinates

1	6.468954	2.536892	-0.392196
6	5.997837	1.922295	0.371321

6	4.465160	1.964095	0.283497
1	4.001559	2.623413	1.016077
1	3.112325	0.275296	0.699229
7	4.090815	0.563005	0.550112
6	5.049100	-0.317070	0.526267
79	4.797849	-2.355633	0.805582
6	6.331511	0.419539	0.229094
1	6.327467	2.290512	1.342169
1	4.103975	2.252568	-0.706100
1	7.136223	0.083561	0.881027
1	6.632576	0.148233	-0.787473
1	4.587330	-3.943053	1.025785
7	1.525779	-0.814780	1.018653
1	2.069991	-1.674989	1.061150
1	1.022358	-0.735165	1.894785
1	0.835700	-0.933351	0.285761

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

66.4830 77.6108 96.8753

Optimised Coordinates

1	6.487986	2.546636	-0.361229
6	5.997123	1.919225	0.385271
6	4.463273	1.977626	0.273345
1	3.991453	2.647889	0.996702
1	3.083029	0.285960	0.700052
7	4.072872	0.575911	0.548938
6	5.030063	-0.319522	0.527036
79	4.750830	-2.334499	0.815496
6	6.320281	0.412567	0.220586
1	6.312295	2.264117	1.374008
1	4.117899	2.256716	-0.729261
1	7.135778	0.064969	0.859623
1	6.604288	0.154184	-0.808833

1	4.515172	-3.923549	1.046956
7	1.573714	-0.817461	1.015718
1	2.154307	-1.663900	1.055237
1	1.067110	-0.768184	1.898781
1	0.879035	-0.973315	0.286312

MP2/cc-pVTZ-pp

Low Frequencies

67.4809 86.7471 97.8333

Optimised Coordinates

1	6.517107	2.559252	-0.253745
6	5.988986	1.896856	0.426254
6	4.473930	1.960806	0.241108
1	3.972844	2.652984	0.913228
1	3.092108	0.293393	0.695884
7	4.073226	0.578093	0.542502
6	5.021240	-0.315741	0.525324
79	4.766496	-2.280652	0.815057
6	6.304293	0.409302	0.202898
1	6.244302	2.177384	1.446494
1	4.185633	2.198895	-0.783698
1	7.133192	0.034763	0.797594
1	6.536957	0.184655	-0.842088
1	4.554444	-3.837125	1.045497
7	1.577379	-0.807709	1.031050
1	2.156198	-1.644684	1.066297
1	1.081877	-0.772924	1.913116
1	0.876294	-0.982177	0.321963

MP2/aug-cc-pVTZ-pp

Low Frequencies

67.7887 92.0408 104.1430

Optimised Coordinates

1	6.519837	2.558438	-0.252168
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6	5.988526	1.897210	0.427765
6	4.473387	1.965694	0.238814
1	3.971930	2.659625	0.910065
1	3.085773	0.296773	0.694236
7	4.067880	0.583465	0.540004
6	5.014971	-0.312771	0.524008
79	4.747264	-2.273398	0.814574
6	6.300318	0.408218	0.204067
1	6.242584	2.176534	1.449470
1	4.188910	2.202745	-0.788048
1	7.126774	0.030248	0.801544
1	6.534042	0.183876	-0.841601
1	4.523561	-3.830048	1.046450
7	1.592673	-0.821667	1.032640
1	2.182846	-1.653154	1.065489
1	1.102314	-0.777270	1.918311
1	0.892916	-0.989146	0.319116

S4.6. Adducts with CH₃-Au(I)-NHC2

S4.6.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

43.0464 62.7641 70.6963

Optimised Coordinates

1	1.458226	-6.965854	0.282222
6	1.312887	-5.888402	0.263945
6	0.668198	-5.370026	1.557434
1	-0.400461	-5.179708	1.470159
1	1.112390	-3.442119	2.508064
7	1.394485	-4.107762	1.787626
6	2.472459	-3.907562	1.083285
79	3.717144	-2.276088	1.246133
6	2.639531	-5.100626	0.175600
1	0.678938	-5.654006	-0.590390

1	0.825517	-6.036678	2.407867
1	2.901801	-4.790785	-0.834598
1	3.494661	-5.672277	0.549302
6	4.972940	-0.632110	1.407438
1	5.462184	-0.592826	2.384334
1	5.758148	-0.669363	0.647459
1	4.429931	0.307436	1.273768
1	2.238619	-1.708080	3.199633
8	1.412869	-1.911909	3.675897
1	0.936090	-1.077812	3.725033

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

45.2696 63.2066 65.6508

Optimised Coordinates

1	1.427473	-6.957314	0.255433
6	1.298363	-5.873437	0.262634
6	0.667556	-5.374664	1.574529
1	-0.406942	-5.186279	1.506785
1	1.122565	-3.430433	2.534444
7	1.394323	-4.105020	1.804668
6	2.477514	-3.901151	1.091718
79	3.702755	-2.270991	1.265213
6	2.639209	-5.101552	0.182770
1	0.660349	-5.604681	-0.583835
1	0.847247	-6.049095	2.419845
1	2.913519	-4.798727	-0.830714
1	3.483989	-5.688379	0.568949
6	4.944213	-0.623162	1.435317
1	5.434665	-0.587694	2.416896
1	5.732323	-0.649985	0.671157
1	4.391176	0.316954	1.309016
1	2.297953	-1.778489	3.123871
8	1.471445	-1.923753	3.647756

1 0.986862 -1.088705 3.563759

MP2/cc-pVTZ-pp

Low Frequencies

33.4332 61.3906 75.8406

Optimised Coordinates

1 1.405636 -6.904060 0.177196
6 1.315908 -5.823468 0.241267
6 0.704878 -5.368897 1.565228
1 -0.370630 -5.215353 1.528816
1 1.105175 -3.419609 2.503178
7 1.395365 -4.090056 1.788850
6 2.480993 -3.883303 1.094830
79 3.680390 -2.302428 1.239960
6 2.667514 -5.092933 0.212658
1 0.695175 -5.480280 -0.584320
1 0.934667 -6.045365 2.389344
1 3.001720 -4.811341 -0.782330
1 3.470314 -5.684892 0.661772
6 4.912675 -0.694730 1.383762
1 5.362561 -0.615688 2.375856
1 5.729031 -0.760613 0.661256
1 4.383340 0.241194 1.191335
1 2.221773 -1.716756 3.159179
8 1.410946 -1.928974 3.650742
1 0.979124 -1.079003 3.761634

MP2/aug-cc-pVTZ-pp

Low Frequencies

22.2803 60.7258 75.4723

Optimised Coordinates

1 1.406498 -6.905920 0.179534
6 1.315309 -5.824622 0.242837
6 0.702231 -5.371089 1.566990

1	-0.373970	-5.217531	1.529805
1	1.101972	-3.417673	2.505121
7	1.391951	-4.091058	1.791877
6	2.478804	-3.884474	1.098271
79	3.673622	-2.302411	1.248258
6	2.667244	-5.093137	0.216205
1	0.695033	-5.481335	-0.584029
1	0.933589	-6.047747	2.391418
1	3.002173	-4.809333	-0.778827
1	3.469926	-5.685792	0.666524
6	4.902097	-0.692698	1.398170
1	5.386533	-0.648908	2.377059
1	5.689478	-0.735013	0.641066
1	4.357598	0.244623	1.256825
1	2.253626	-1.733367	3.137439
8	1.434072	-1.917413	3.634544
1	0.998771	-1.061657	3.701125

S4.6.2. H₂O adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

13.5674 50.0641 50.9537

Optimised Coordinates

1	2.619798	-6.148674	-1.136625
6	2.832040	-5.084169	-1.196182
6	1.832928	-4.253685	-0.379843
1	1.045525	-3.797334	-0.977627
1	2.319104	-2.424754	0.700140
7	2.705032	-3.212439	0.200819
6	3.994842	-3.407339	0.137214
79	5.434879	-2.219712	0.989458
6	4.202801	-4.709489	-0.588422
1	2.790946	-4.793297	-2.245259
1	1.368543	-4.823050	0.427342

1	5.003834	-4.627185	-1.320915
1	4.541697	-5.428939	0.163536
6	6.902571	-1.054381	1.876842
1	6.634035	-0.772626	2.898151
1	7.863058	-1.574438	1.915065
1	7.051343	-0.129934	1.311301
1	5.282493	-4.292317	2.483558
8	5.017534	-5.180761	2.772248
1	5.582885	-5.376801	3.525016

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

17.9618 35.8571 54.6929

Optimised Coordinates

1	1.976441	-3.607925	-0.731511
6	2.839566	-3.147190	-1.215055
6	2.567744	-1.682531	-1.598970
1	2.319349	-1.538479	-2.653454
1	4.073412	-0.092749	-1.582235
7	3.872102	-1.044192	-1.292777
6	4.734548	-1.736796	-0.579586
79	6.589533	-1.115554	-0.006236
6	4.082174	-3.068894	-0.291032
1	3.078553	-3.729107	-2.108748
1	1.786376	-1.214611	-0.989147
1	4.792351	-3.885805	-0.440440
1	3.815819	-3.072987	0.775047
6	8.488152	-0.518109	0.558406
1	8.447815	0.436777	1.099727
1	8.969642	-1.253484	1.215516
1	9.137955	-0.371780	-0.314322
1	7.162817	-3.189814	-1.128850
8	7.148787	-4.083736	-1.537274
1	8.041524	-4.425004	-1.380334

S4.6.3. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

43.2414 53.7136 70.8208

Optimised Coordinates

1	1.476782	-6.999024	0.256200
6	1.316612	-5.923764	0.244353
6	0.646802	-5.426020	1.532983
1	-0.421224	-5.241186	1.430815
1	1.057699	-3.506847	2.503623
7	1.360203	-4.160058	1.787231
6	2.443209	-3.938335	1.098145
79	3.663561	-2.285225	1.293808
6	2.634352	-5.118203	0.179545
1	0.691385	-5.691082	-0.616572
1	0.796569	-6.099415	2.379114
1	2.902644	-4.793212	-0.824348
1	3.493147	-5.683114	0.555246
6	4.886752	-0.624570	1.489060
1	5.342718	-0.574795	2.480689
1	5.694742	-0.660536	0.753227
1	4.335139	0.305150	1.331280
1	2.218503	-1.663452	2.896207
9	1.444689	-1.764816	3.443728

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

44.0518 56.5706 65.8502

Optimised Coordinates

1	1.450195	-6.993971	0.233585
6	1.307611	-5.911985	0.240796
6	0.646731	-5.425437	1.541969
1	-0.426730	-5.241502	1.453653

1	1.064236	-3.487258	2.510610
7	1.361361	-4.151684	1.791618
6	2.453033	-3.931703	1.098002
79	3.656715	-2.281710	1.299572
6	2.641366	-5.124931	0.186130
1	0.682183	-5.648640	-0.616388
1	0.814571	-6.101414	2.388125
1	2.927300	-4.813377	-0.821496
1	3.486930	-5.704271	0.581900
6	4.869287	-0.619604	1.498933
1	5.319619	-0.568338	2.498043
1	5.684844	-0.652052	0.764338
1	4.309640	0.310129	1.338263
1	2.256880	-1.720704	2.822793
9	1.478513	-1.780051	3.403888

MP2/cc-pVTZ-pp

Low Frequencies

35.5121 51.3930 75.5107

Optimised Coordinates

1	1.422555	-6.931712	0.140139
6	1.319104	-5.853503	0.219058
6	0.689409	-5.426930	1.543503
1	-0.386408	-5.279762	1.497814
1	1.059201	-3.492364	2.507605
7	1.367917	-4.145724	1.793429
6	2.456419	-3.914291	1.112084
79	3.634538	-2.315937	1.286164
6	2.662846	-5.107631	0.213798
1	0.702521	-5.505332	-0.607328
1	0.916673	-6.113563	2.359567
1	3.002068	-4.807034	-0.773906
1	3.468634	-5.697306	0.660690
6	4.841193	-0.694144	1.453980

1	5.267677	-0.608030	2.455174
1	5.672091	-0.757165	0.747987
1	4.304241	0.233360	1.246215
1	2.175316	-1.661344	2.911881
9	1.408291	-1.770091	3.446481

MP2/aug-cc-pVTZ-pp

Low Frequencies

23.7827 51.4720 75.2929

Optimised Coordinates

1	1.423870	-6.933651	0.145196
6	1.320006	-5.854463	0.220893
6	0.686718	-5.425357	1.543544
1	-0.389569	-5.277154	1.495089
1	1.055006	-3.485784	2.504779
7	1.365269	-4.143124	1.793265
6	2.456131	-3.914632	1.113588
79	3.631855	-2.316162	1.289499
6	2.664809	-5.109103	0.218207
1	0.705588	-5.507256	-0.608485
1	0.913437	-6.110657	2.361793
1	3.006516	-4.808627	-0.769610
1	3.469157	-5.699462	0.668694
6	4.835438	-0.692940	1.461397
1	5.289696	-0.635797	2.453361
1	5.643296	-0.738202	0.726374
1	4.284309	0.235452	1.294408
1	2.196954	-1.670515	2.878377
9	1.425800	-1.761069	3.423968

S4.6.4. HF adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

14.6663 21.2794 36.3337

Optimised Coordinates

1	1.551310	-6.993463	0.361524
6	1.354767	-5.926002	0.302921
6	0.633304	-5.405886	1.553382
1	-0.438857	-5.271318	1.420491
1	0.947966	-3.446918	2.454216
7	1.290997	-4.099766	1.764787
6	2.390977	-3.868887	1.101765
79	3.604204	-2.220707	1.311912
6	2.646649	-5.079139	0.244244
1	0.745804	-5.747149	-0.582278
1	0.796213	-6.034575	2.430571
1	2.940745	-4.790515	-0.763367
1	3.508910	-5.592633	0.680589
6	4.864060	-0.594130	1.545709
1	4.993751	-0.329726	2.597559
1	5.852900	-0.785139	1.123028
1	4.448004	0.279398	1.035196
1	4.831121	-3.796420	2.480962
9	5.126626	-4.608821	2.860871

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

11.3825 42.3852 45.1583

Optimised Coordinates

1	1.879294	-3.562068	-0.703942
6	2.755542	-3.135990	-1.195278
6	2.523124	-1.674304	-1.615614
1	2.287379	-1.548671	-2.675226
1	4.065529	-0.120692	-1.622771
7	3.840558	-1.060562	-1.313053
6	4.680655	-1.757736	-0.579974
79	6.556265	-1.172920	-0.012062
6	3.996045	-3.067357	-0.267337

1	2.981201	-3.745735	-2.073717
1	1.749306	-1.172653	-1.023606
1	4.687569	-3.903499	-0.394557
1	3.725545	-3.044175	0.797396
6	8.469734	-0.620942	0.537844
1	8.448521	0.344711	1.061130
1	8.930562	-1.356761	1.207657
1	9.120873	-0.507869	-0.337874
1	7.190998	-3.126425	-0.847979
9	7.229119	-4.009148	-1.221543

MP2/cc-pVTZ-pp

Low Frequencies

24.8056 36.7033 47.9375

Optimised Coordinates

1	1.548264	-6.909259	0.203763
6	1.388907	-5.837057	0.267749
6	0.791279	-5.423006	1.610200
1	-0.292605	-5.343373	1.610468
1	1.095200	-3.465664	2.526812
7	1.403111	-4.097161	1.800484
6	2.458820	-3.825106	1.081159
79	3.616667	-2.219531	1.252403
6	2.690303	-5.022680	0.198548
1	0.721455	-5.537816	-0.538118
1	1.103084	-6.073389	2.427709
1	2.980996	-4.726423	-0.805638
1	3.538062	-5.557151	0.636767
6	4.841326	-0.614445	1.442309
1	5.003841	-0.346354	2.487618
1	5.817747	-0.795463	0.989814
1	4.406375	0.257082	0.946974
1	4.490425	-3.885767	2.687098
9	4.603890	-4.698819	3.131787

MP2/aug-cc-pVTZ-pp

Low Frequencies

24.1210 30.8315 47.1623

Optimised Coordinates

1	1.546179	-6.902372	0.179823
6	1.382483	-5.831243	0.261664
6	0.821663	-5.438039	1.626773
1	-0.262951	-5.365951	1.660484
1	1.143915	-3.489164	2.561111
7	1.430070	-4.109619	1.815436
6	2.465401	-3.824939	1.070736
79	3.624199	-2.222034	1.246371
6	2.677941	-5.008821	0.166417
1	0.690454	-5.524729	-0.521461
1	1.164844	-6.095359	2.426991
1	2.939209	-4.697012	-0.842064
1	3.540592	-5.545540	0.574475
6	4.852072	-0.620629	1.443433
1	4.910323	-0.280040	2.479388
1	5.865002	-0.850537	1.105766
1	4.481738	0.213351	0.840385
1	4.416362	-3.859271	2.696558
9	4.514573	-4.667417	3.167948

S4.6.5. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

39.9872 64.8299 67.5182

Optimised Coordinates

1	1.442646	-6.946184	0.235327
6	1.312618	-5.866487	0.246543
6	0.712747	-5.368998	1.569674
1	-0.355808	-5.164331	1.517680

1	1.197358	-3.460973	2.554733
7	1.460596	-4.121656	1.810253
6	2.518848	-3.918687	1.077306
79	3.784744	-2.307077	1.220893
6	2.646480	-5.094235	0.139008
1	0.657845	-5.603365	-0.583557
1	0.883959	-6.059700	2.398477
1	2.885132	-4.765253	-0.870935
1	3.503718	-5.685283	0.475910
6	5.066497	-0.678346	1.355956
1	5.575982	-0.646494	2.323340
1	5.836783	-0.718348	0.580945
1	4.530827	0.267914	1.237595
7	1.187503	-1.918037	3.760242
1	2.028834	-1.540002	3.328422
1	0.465303	-1.211469	3.680010
1	1.383848	-2.036364	4.747517

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

40.7982 63.1439 69.2145

Optimised Coordinates

1	1.416472	-6.942901	0.204181
6	1.302626	-5.857633	0.239822
6	0.704876	-5.380650	1.575098
1	-0.369237	-5.181080	1.533865
1	1.183931	-3.453352	2.572651
7	1.448035	-4.123725	1.821499
6	2.517507	-3.915787	1.088760
79	3.762946	-2.305212	1.241991
6	2.650676	-5.100468	0.152653
1	0.651708	-5.560394	-0.587299
1	0.893035	-6.078628	2.399825
1	2.911602	-4.780168	-0.858922

1	3.494516	-5.705401	0.512115
6	5.029238	-0.670914	1.383477
1	5.539091	-0.638691	2.356054
1	5.803965	-0.702126	0.605833
1	4.483800	0.275686	1.268553
7	1.232133	-1.928815	3.712168
1	2.080918	-1.584783	3.248046
1	0.533966	-1.190620	3.632175
1	1.454656	-2.017713	4.702793

MP2/cc-pVTZ-pp

Low Frequencies

28.7105 65.0959 76.3140

Optimised Coordinates

1	1.380406	-6.882599	0.122525
6	1.305854	-5.803564	0.224381
6	0.748267	-5.384272	1.583323
1	-0.326654	-5.221091	1.591053
1	1.192682	-3.457314	2.569448
7	1.458020	-4.119613	1.824338
6	2.518416	-3.901479	1.095805
79	3.731683	-2.333882	1.236239
6	2.663244	-5.085675	0.170499
1	0.659759	-5.427473	-0.566863
1	0.999495	-6.091097	2.375567
1	2.965306	-4.776459	-0.826549
1	3.474751	-5.699407	0.572248
6	4.978590	-0.734914	1.371970
1	5.442615	-0.665110	2.358672
1	5.785330	-0.796186	0.638305
1	4.451343	0.205749	1.195875
7	1.228130	-1.921616	3.707758
1	2.066995	-1.581337	3.242042
1	0.542732	-1.181012	3.627510

1 1.459496 -1.985026 4.691194

S4.6.6. NH₃ adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

11.7106 29.6799 51.7392

Optimised Coordinates

1 0.583669 -6.191616 0.522187
6 0.836678 -5.293108 -0.035439
6 -0.195320 -4.176591 0.177346
1 -0.901895 -4.068428 -0.644258
1 0.269874 -2.050590 0.282269
7 0.664182 -2.979534 0.273458
6 1.949714 -3.170740 0.418306
79 3.362576 -1.702240 0.625043
6 2.173224 -4.658716 0.414835
1 0.887144 -5.560678 -1.089990
1 -0.762483 -4.290188 1.103523
1 3.022218 -4.917075 -0.218211
1 2.452369 -4.941878 1.434803
6 4.807805 -0.226459 0.822257
1 4.507644 0.521039 1.561754
1 5.768419 -0.639461 1.141375
1 4.971555 0.298199 -0.123218
7 5.168135 -4.307908 -1.499830
1 5.312959 -4.096681 -2.480608
1 4.967251 -3.426501 -1.033773
1 6.055847 -4.636124 -1.136709

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

27.1163 30.7086 52.2923

Optimised Coordinates

1 0.577220 -6.208138 0.482735

6	0.834848	-5.294045	-0.055246
6	-0.199898	-4.180095	0.178438
1	-0.921362	-4.065702	-0.634691
1	0.272739	-2.044110	0.271824
7	0.666742	-2.978951	0.264374
6	1.962186	-3.173581	0.409908
79	3.371373	-1.718743	0.599583
6	2.173387	-4.669398	0.415640
1	0.890826	-5.534211	-1.120372
1	-0.750676	-4.294962	1.119294
1	3.033044	-4.940705	-0.205263
1	2.429016	-4.952949	1.446244
6	4.820534	-0.251322	0.778676
1	4.597596	0.417435	1.620990
1	5.818261	-0.676942	0.947821
1	4.872350	0.369173	-0.126060
7	5.157546	-4.289643	-1.435936
1	5.319154	-4.053328	-2.414855
1	4.911745	-3.411214	-0.968541
1	6.064936	-4.563847	-1.059444

MP2/cc-pVTZ-pp

Low Frequencies

20.5466 33.1974 63.8074

Optimised Coordinates

1	0.624234	-6.205657	0.390253
6	0.885730	-5.262866	-0.081341
6	-0.155429	-4.177555	0.183604
1	-0.901824	-4.075867	-0.600214
1	0.300802	-2.043133	0.229187
7	0.691558	-2.974521	0.242016
6	1.976177	-3.159335	0.410062
79	3.350987	-1.745802	0.592312
6	2.188218	-4.648923	0.457612

1	0.977891	-5.428168	-1.153039
1	-0.663012	-4.303565	1.140666
1	3.078714	-4.931163	-0.100191
1	2.364953	-4.900421	1.507825
6	4.787895	-0.320818	0.763277
1	4.552374	0.383011	1.564699
1	5.766962	-0.750908	0.984790
1	4.886101	0.259823	-0.156759
7	5.091745	-4.271817	-1.424157
1	5.235574	-4.039550	-2.399170
1	4.855639	-3.395082	-0.967140
1	6.006276	-4.522961	-1.069173

S4.7. Adducts with Cl-Au(I)-NHC2

S4.7.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

54.8513 60.5347 65.2169

Optimised Coordinates

1	1.420597	-7.009702	0.222313
6	1.276198	-5.932273	0.224059
6	0.680165	-5.431374	1.548322
1	-0.391233	-5.243431	1.503967
1	1.154133	-3.509498	2.504629
7	1.408462	-4.169783	1.767667
6	2.458557	-3.968069	1.022160
79	3.652926	-2.385838	1.162910
6	2.600055	-5.147474	0.095071
1	0.611438	-5.684760	-0.602405
1	0.872500	-6.106992	2.384108
1	2.825626	-4.824598	-0.919476
1	3.467375	-5.722971	0.432278
17	4.985612	-0.528575	1.383107
1	2.199803	-1.700570	3.390244

8	1.364159	-2.046463	3.737882
1	0.811504	-1.273486	3.888911

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

57.3991 59.9115 63.5122

Optimised Coordinates

1	1.404179	-6.993728	0.184660
6	1.270178	-5.911305	0.219688
6	0.675651	-5.445154	1.560948
1	-0.402576	-5.270778	1.530643
1	1.133124	-3.508142	2.540774
7	1.389053	-4.170289	1.793013
6	2.449056	-3.952119	1.047642
79	3.613441	-2.364686	1.202742
6	2.604311	-5.133501	0.115491
1	0.606302	-5.626220	-0.600868
1	0.892157	-6.132042	2.387211
1	2.850252	-4.811336	-0.898778
1	3.461611	-5.720185	0.472296
17	4.918794	-0.505423	1.418262
1	2.252179	-1.815064	3.315624
8	1.402703	-2.070183	3.733144
1	0.877462	-1.255702	3.723256

MP2/cc-pVTZ-pp

Low Frequencies

60.1642 64.4152 65.6371

Optimised Coordinates

1	1.359993	-6.964470	0.129161
6	1.269750	-5.884979	0.205664
6	0.705676	-5.444287	1.555518
1	-0.370914	-5.296064	1.559167
1	1.130602	-3.496540	2.495722

7	1.394598	-4.163272	1.766394
6	2.453026	-3.955578	1.031247
79	3.601745	-2.417097	1.151565
6	2.618363	-5.153492	0.132134
1	0.618722	-5.536096	-0.593528
1	0.969455	-6.125325	2.365316
1	2.914377	-4.859555	-0.870948
1	3.438677	-5.745843	0.547115
17	4.911342	-0.601938	1.339597
1	2.169356	-1.705695	3.304240
8	1.358298	-2.058475	3.694047
1	0.854811	-1.277149	3.933338

MP2/aug-cc-pVTZ-pp

Low Frequencies

59.9983 65.6260 66.2967

Optimised Coordinates

1	1.360809	-6.963883	0.123174
6	1.267878	-5.884186	0.204315
6	0.703530	-5.451569	1.557445
1	-0.374074	-5.305623	1.563307
1	1.126054	-3.501849	2.504144
7	1.389655	-4.168920	1.773396
6	2.447654	-3.956554	1.037646
79	3.586498	-2.412305	1.170263
6	2.615791	-5.149530	0.133880
1	0.615468	-5.531987	-0.593311
1	0.972162	-6.135567	2.364061
1	2.910693	-4.849450	-0.868608
1	3.437196	-5.743212	0.546876
17	4.876894	-0.594960	1.375717
1	2.206895	-1.727925	3.294400
8	1.380931	-2.052407	3.686348
1	0.873844	-1.255929	3.872696

S4.7.2. H₂O adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

16.1114 50.3599 61.0671

Optimised Coordinates

1	2.056334	-6.884028	0.231917
6	1.777477	-5.913055	0.633060
6	1.935656	-5.856655	2.159342
1	0.999220	-5.969464	2.702762
1	2.563876	-4.098205	3.285694
7	2.480321	-4.500043	2.363964
6	2.908420	-3.869391	1.301988
79	3.713194	-2.058714	1.255058
6	2.679644	-4.769057	0.118448
1	0.741583	-5.723234	0.356765
1	2.646274	-6.591136	2.543051
1	2.257601	-4.209309	-0.714642
1	3.662131	-5.120392	-0.212048
17	4.598800	0.051364	1.106667
1	2.228631	-1.565074	-0.972711
8	1.663115	-1.988588	-1.632924
1	1.620994	-1.361868	-2.361358

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

22.1018 53.5058 61.1258

Optimised Coordinates

1	2.118406	-6.908166	0.215175
6	1.835991	-5.915840	0.570122
6	1.893805	-5.817910	2.104489
1	0.921135	-5.917178	2.592055
1	2.433264	-4.008389	3.216627
7	2.420328	-4.446443	2.302012
6	2.935523	-3.849858	1.245722

79	3.739386	-2.052820	1.203400
6	2.799058	-4.804796	0.083311
1	0.822102	-5.705631	0.220816
1	2.587076	-6.536400	2.556325
1	2.450990	-4.279794	-0.809370
1	3.804180	-5.186219	-0.142806
17	4.647288	0.033058	1.085599
8	1.491175	-2.011805	-1.444018
1	2.094558	-1.717511	-0.733800
1	1.539008	-1.301146	-2.100625

MP2/cc-pVTZ-pp

Low Frequencies

27.2855 52.8427 71.5910

Optimised Coordinates

1	2.103590	-6.803174	0.164939
6	1.961517	-5.746906	0.373131
6	1.674399	-5.484820	1.850516
1	0.616256	-5.414492	2.087441
1	2.148262	-3.606680	2.861662
7	2.318776	-4.176547	2.045464
6	3.160593	-3.797043	1.121509
79	4.129410	-2.140704	1.077855
6	3.209926	-4.897649	0.095918
1	1.137850	-5.369571	-0.227190
1	2.141154	-6.214576	2.512743
1	3.250180	-4.491266	-0.909800
1	4.141671	-5.444470	0.268117
17	5.232866	-0.191558	0.967250
1	1.747435	-2.066069	-0.291560
8	0.996292	-2.584001	-0.604395
1	0.563094	-1.997325	-1.228567

MP2/aug-cc-pVTZ-pp

Low Frequencies

29.4436 55.4904 72.9129

Optimised Coordinates

1	2.103373	-6.807352	0.166450
6	1.959480	-5.749793	0.370868
6	1.671343	-5.483692	1.848111
1	0.612462	-5.412976	2.085069
1	2.140454	-3.596665	2.851181
7	2.314528	-4.173188	2.039349
6	3.156129	-3.796734	1.113146
79	4.114175	-2.134644	1.065032
6	3.208136	-4.900134	0.091700
1	1.135011	-5.375099	-0.231739
1	2.140477	-6.210935	2.512495
1	3.247698	-4.494716	-0.915511
1	4.140393	-5.446915	0.266174
17	5.204243	-0.186932	0.952056
1	1.774071	-2.072078	-0.256512
8	1.018404	-2.584484	-0.578533
1	0.592895	-2.000512	-1.214302

S4.7.3. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

53.1322 54.6114 61.0718

Optimised Coordinates

1	1.438584	-7.002775	0.199623
6	1.280179	-5.927713	0.221587
6	0.657303	-5.463666	1.546439
1	-0.414423	-5.282850	1.488992
1	1.093225	-3.560619	2.542578
7	1.370737	-4.199580	1.803875
6	2.428173	-3.967233	1.077914
79	3.605764	-2.373180	1.254924

6	2.596326	-5.124793	0.128857
1	0.625161	-5.670879	-0.609551
1	0.843653	-6.154414	2.370799
1	2.832347	-4.777802	-0.875315
1	3.465822	-5.696915	0.466489
17	4.920248	-0.514977	1.501892
1	2.176692	-1.620228	3.082580
9	1.408373	-1.862606	3.569910

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

55.5358 58.4785 61.1820

Optimised Coordinates

1	1.426810	-6.984002	0.165982
6	1.278861	-5.904272	0.218151
6	0.654555	-5.471127	1.556099
1	-0.423871	-5.303593	1.509221
1	1.068069	-3.552637	2.568521
7	1.352502	-4.193689	1.824192
6	2.421336	-3.947078	1.101403
79	3.581106	-2.354731	1.278625
6	2.606011	-5.110164	0.151862
1	0.626916	-5.611440	-0.608951
1	0.863190	-6.170027	2.373918
1	2.865964	-4.767385	-0.852106
1	3.463559	-5.693430	0.513913
17	4.908892	-0.518847	1.478956
1	2.199638	-1.735375	2.965480
9	1.434625	-1.882433	3.526328

MP2/cc-pVTZ-pp

Low Frequencies

52.2244 58.6729 64.4847

Optimised Coordinates

1	1.370081	-6.955769	0.103191
6	1.270140	-5.879130	0.202195
6	0.691698	-5.473651	1.556826
1	-0.385166	-5.329011	1.554716
1	1.094068	-3.548664	2.533942
7	1.373418	-4.193660	1.800391
6	2.434883	-3.959301	1.077249
79	3.573972	-2.414821	1.226995
6	2.613867	-5.136273	0.154479
1	0.622563	-5.518086	-0.594184
1	0.953049	-6.170344	2.353677
1	2.914663	-4.818619	-0.839912
1	3.435896	-5.731127	0.562615
17	4.874143	-0.601819	1.436561
1	2.126410	-1.606526	3.085828
9	1.364478	-1.863428	3.557025

MP2/aug-cc-pVTZ-pp

Low Frequencies

52.3711 57.7118 66.0464

Optimised Coordinates

1	1.370452	-6.954722	0.100710
6	1.269512	-5.877589	0.201818
6	0.689818	-5.476118	1.557809
1	-0.387885	-5.332305	1.556272
1	1.089283	-3.548566	2.537877
7	1.370047	-4.194908	1.804443
6	2.432237	-3.959407	1.081758
79	3.565899	-2.411798	1.237486
6	2.613748	-5.134006	0.157588
1	0.622253	-5.513865	-0.594633
1	0.954068	-6.174147	2.353474
1	2.915480	-4.813125	-0.836403
1	3.435231	-5.730549	0.566492

17	4.853469	-0.600271	1.454043
1	2.150062	-1.619909	3.053078
9	1.384488	-1.858945	3.539783

S4.7.4. HF adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

19.3002 43.0565 58.9720

Optimised Coordinates

1	1.676905	-7.112924	0.134199
6	1.379580	-6.069984	0.205096
6	0.706483	-5.755103	1.548671
1	-0.379265	-5.703408	1.493873
1	0.894211	-3.870218	2.627960
7	1.259620	-4.424413	1.867730
6	2.273327	-4.018689	1.152229
79	3.222683	-2.287450	1.369274
6	2.580057	-5.098531	0.150119
1	0.694726	-5.859088	-0.614092
1	0.978845	-6.456276	2.339517
1	2.751893	-4.671800	-0.835578
1	3.520520	-5.566822	0.456179
17	4.300704	-0.281987	1.581284
1	1.960325	-1.918624	-0.716640
9	1.413812	-2.198599	-1.424085

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

27.3340 44.3714 59.2291

Optimised Coordinates

1	1.710516	-7.123412	0.097578
6	1.418134	-6.076224	0.187352
6	0.771535	-5.774986	1.550666
1	-0.319996	-5.742598	1.525129

1	0.938886	-3.865213	2.610428
7	1.307113	-4.426220	1.849712
6	2.312600	-4.008326	1.111082
79	3.227390	-2.269447	1.295761
6	2.624118	-5.105855	0.120527
1	0.714951	-5.845873	-0.616264
1	1.084511	-6.467816	2.339769
1	2.799866	-4.694633	-0.875335
1	3.563832	-5.576604	0.440068
17	4.284443	-0.267831	1.495993
1	1.735902	-1.993532	-0.487839
9	1.094947	-2.187967	-1.162386

MP2/cc-pVTZ-pp

Low Frequencies

36.2152 54.9328 60.5598

Optimised Coordinates

1	1.686877	-7.004255	-0.081560
6	1.445850	-5.963114	0.110358
6	0.791135	-5.764530	1.475794
1	-0.295090	-5.762636	1.450298
1	0.891947	-3.894544	2.604359
7	1.288291	-4.428490	1.843770
6	2.317448	-3.985793	1.171149
79	3.194766	-2.294169	1.416379
6	2.680471	-5.053107	0.173750
1	0.776957	-5.606234	-0.669427
1	1.129455	-6.486982	2.218966
1	2.960704	-4.620531	-0.781639
1	3.561102	-5.565549	0.572192
17	4.219809	-0.319091	1.656032
1	1.605572	-2.149390	-0.535756
9	1.013454	-2.528124	-1.142422

MP2/aug-cc-pVTZ-pp

Low Frequencies

37.0232 56.4892 61.7945

Optimised Coordinates

1	1.685698	-7.004017	-0.082270
6	1.445724	-5.961322	0.106913
6	0.789694	-5.759477	1.472023
1	-0.297236	-5.755208	1.445853
1	0.889983	-3.882027	2.593881
7	1.288675	-4.422616	1.838123
6	2.319162	-3.983816	1.163948
79	3.190707	-2.288933	1.406093
6	2.682760	-5.053291	0.170227
1	0.778114	-5.603696	-0.674794
1	1.127993	-6.480894	2.217178
1	2.963859	-4.620833	-0.786112
1	3.562253	-5.567570	0.570993
17	4.209096	-0.319142	1.647469
1	1.614930	-2.174835	-0.496906
9	1.017336	-2.548861	-1.110376

S4.7.5. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

53.9319 61.4842 69.2905

Optimised Coordinates

1	6.447337	2.552289	-0.376380
6	5.985681	1.920190	0.378203
6	4.452426	1.932377	0.284631
1	3.974601	2.584452	1.014202
1	3.126687	0.219808	0.704669
7	4.100943	0.527708	0.552710
6	5.082278	-0.328708	0.522398
79	4.884898	-2.287437	0.789451

6	6.351583	0.427991	0.220773
1	6.303352	2.283322	1.354780
1	4.090226	2.212138	-0.707007
1	7.165829	0.102406	0.865272
1	6.649063	0.171248	-0.800324
17	4.596421	-4.547385	1.108190
1	0.808975	-0.816928	0.280268
7	1.502260	-0.778227	1.018972
1	1.923896	-1.701476	1.078701
1	1.003389	-0.624094	1.887978

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

54.6646 60.7197 69.5936

Optimised Coordinates

1	6.464289	2.564739	-0.343326
6	5.985071	1.916873	0.392836
6	4.450323	1.940985	0.275028
1	3.962692	2.603824	0.994449
1	3.101920	0.223867	0.708557
7	4.086625	0.535392	0.553875
6	5.070974	-0.333889	0.523520
79	4.857122	-2.275921	0.797945
6	6.345230	0.422267	0.210268
1	6.287191	2.255360	1.387713
1	4.104085	2.210049	-0.730038
1	7.172547	0.087180	0.839788
1	6.623812	0.180963	-0.824400
17	4.554046	-4.519048	1.124774
1	0.838234	-0.842217	0.278678
7	1.537276	-0.778731	1.017913
1	1.980074	-1.698958	1.079260
1	1.028335	-0.643063	1.890648

MP2/cc-pVTZ-pp*Low Frequencies*

56.7964 58.9429 64.4982

Optimised Coordinates

1	6.498904	2.571232	-0.244729
6	5.980780	1.896118	0.430143
6	4.464685	1.937047	0.243040
1	3.953859	2.623004	0.913927
1	3.103600	0.248253	0.701385
7	4.081169	0.551342	0.546004
6	5.049500	-0.322850	0.522204
79	4.839603	-2.214842	0.798018
6	6.322404	0.417107	0.196692
1	6.229749	2.173387	1.452720
1	4.174677	2.169885	-0.782440
1	7.157306	0.051683	0.787959
1	6.553330	0.201608	-0.850309
17	4.544536	-4.420344	1.124735
1	0.849279	-0.890189	0.314830
7	1.556533	-0.783040	1.031320
1	2.034317	-1.678049	1.086674
1	1.055615	-0.681680	1.905314

MP2/aug-cc-pVTZ-pp*Optimised Coordinates*

1	6.501886	2.572255	-0.241878
6	5.980465	1.897407	0.431981
6	4.464306	1.942402	0.240426
1	3.952431	2.629586	0.910443
1	3.098517	0.250375	0.699147
7	4.076725	0.556755	0.542597
6	5.044632	-0.319202	0.519945
79	4.818861	-2.208428	0.797669
6	6.319290	0.417192	0.197083

1	6.227462	2.172514	1.456428
1	4.178429	2.174345	-0.787140
1	7.152315	0.048661	0.790588
1	6.551166	0.203220	-0.850851
17	4.500553	-4.402367	1.127452
7	1.574183	-0.801081	1.033252
1	0.868854	-0.901305	0.312399
1	2.060857	-1.693171	1.087521
1	1.078913	-0.689486	1.910424

S4.7.6. NH₃ adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

19.9321 35.0648 61.3134

Optimised Coordinates

1	6.584107	2.552186	-0.024164
6	5.908693	1.994551	0.619581
6	4.488085	1.932969	0.040103
1	3.794630	2.636320	0.498047
1	3.141217	0.226015	0.203931
7	4.086423	0.547029	0.349904
6	5.033296	-0.270096	0.734442
79	4.820648	-2.204943	1.101526
6	6.315602	0.511637	0.768984
1	5.894246	2.484474	1.592200
1	4.463808	2.080561	-1.041128
1	6.876882	0.298667	1.677106
1	6.925747	0.143490	-0.064082
17	4.622170	-4.459138	1.483323
7	7.763579	-1.724832	-1.563361
1	7.148551	-2.360097	-1.063950
1	7.616784	-1.892251	-2.552338
1	8.712671	-2.015161	-1.356422

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

21.2419 30.3118 60.1776

Optimised Coordinates

1	6.602901	2.558594	0.018395
6	5.910987	1.984924	0.637144
6	4.506762	1.918824	0.012575
1	3.796914	2.633110	0.436836
1	3.144774	0.210295	0.182108
7	4.092385	0.534237	0.340987
6	5.040673	-0.287996	0.749496
79	4.822015	-2.204437	1.131132
6	6.326196	0.500074	0.781810
1	5.858932	2.461367	1.619847
1	4.517849	2.040194	-1.076487
1	6.895630	0.289076	1.689988
1	6.933587	0.137891	-0.062684
17	4.618650	-4.440842	1.531075
7	7.739002	-1.680463	-1.572200
1	7.120137	-2.321331	-1.072143
1	7.581313	-1.852937	-2.564881
1	8.688432	-1.999199	-1.379295

MP2/cc-pVTZ-pp

Low Frequencies

36.6140 57.7939 66.1197

Optimised Coordinates

1	6.769843	2.486700	0.424044
6	5.937514	1.878187	0.764495
6	4.973291	1.540256	-0.369602
1	4.138722	2.229716	-0.465288
1	3.717305	-0.244447	-0.407216
7	4.496265	0.212575	0.044526
6	5.244928	-0.430014	0.901328

79	5.022058	-2.249005	1.465801
6	6.369630	0.496787	1.278134
1	5.410241	2.417963	1.548920
1	5.482132	1.432492	-1.326949
1	6.575702	0.455819	2.344087
1	7.254379	0.125272	0.755776
17	4.818413	-4.391702	2.101075
7	6.906242	-1.091326	-1.836178
1	6.614692	-1.807371	-1.178573
1	6.553102	-1.396485	-2.735397
1	7.912680	-1.184035	-1.905278

MP2/aug-cc-pVTZ-pp

Low Frequencies

39.4550 61.6975 66.7527

Optimised Coordinates

1	6.765741	2.498374	0.419107
6	5.936853	1.885120	0.761916
6	4.964878	1.553502	-0.368346
1	4.126382	2.240857	-0.452366
1	3.713673	-0.237952	-0.410919
7	4.495013	0.219995	0.037718
6	5.253666	-0.426479	0.884155
79	5.039572	-2.252455	1.427137
6	6.377045	0.500179	1.261287
1	5.413375	2.417351	1.555020
1	5.467745	1.455752	-1.330991
1	6.589601	0.450775	2.326461
1	7.259590	0.136115	0.728082
17	4.844814	-4.395490	2.036294
7	6.905466	-1.117088	-1.792963
1	6.596881	-1.816043	-1.122552
1	6.535321	-1.409834	-2.690495
1	7.911521	-1.221299	-1.864841

S4.8. Adducts with HO-Au(I)-NHC2

S4.8.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

60.8015 72.3945 78.6209

Optimised Coordinates

1	1.399919	-6.964879	0.194377
6	1.286816	-5.884045	0.229547
6	0.699796	-5.406000	1.565756
1	-0.368900	-5.201183	1.526039
1	1.188783	-3.505133	2.547623
7	1.447493	-4.163386	1.812947
6	2.507493	-3.959638	1.072724
79	3.708596	-2.407001	1.216790
6	2.631280	-5.132152	0.130028
1	0.632358	-5.591383	-0.590687
1	0.880585	-6.108934	2.382124
1	2.878639	-4.803026	-0.877218
1	3.476362	-5.737098	0.472140
8	4.830773	-0.791369	1.463276
1	5.531829	-0.748793	0.806492
1	1.943930	-1.432419	2.985708
8	1.206801	-1.796880	3.499696
1	1.425954	-1.613310	4.418381

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

61.2123 72.4886 81.2332

Optimised Coordinates

1	1.379014	-6.945937	0.153840
6	1.282325	-5.860959	0.224406
6	0.694174	-5.416951	1.575294
1	-0.381120	-5.223558	1.546616
1	1.162438	-3.498871	2.574675

7	1.429383	-4.162996	1.836546
6	2.503045	-3.945757	1.099106
79	3.680812	-2.389277	1.252343
6	2.641034	-5.124344	0.155768
1	0.634397	-5.525157	-0.590050
1	0.895287	-6.132713	2.381640
1	2.916197	-4.801143	-0.850483
1	3.469207	-5.745181	0.523598
8	4.790585	-0.771573	1.492296
1	5.493039	-0.752345	0.823857
1	1.950564	-1.508649	2.864417
8	1.212231	-1.787400	3.447804
1	1.555895	-1.653818	4.344069

MP2/cc-pVTZ-pp

Low Frequencies

58.5264 81.5120 89.6380

Optimised Coordinates

1	1.344288	-6.897475	0.082602
6	1.281825	-5.820426	0.208683
6	0.742936	-5.425710	1.582497
1	-0.331674	-5.263906	1.606006
1	1.191338	-3.513973	2.572746
7	1.452346	-4.165605	1.831803
6	2.510504	-3.941559	1.091819
79	3.675988	-2.437639	1.224901
6	2.645585	-5.117620	0.154849
1	0.631321	-5.419395	-0.566333
1	1.006118	-6.146915	2.357647
1	2.945849	-4.801068	-0.839978
1	3.450625	-5.743652	0.549657
8	4.803354	-0.867634	1.451166
1	5.469417	-0.860640	0.755080
1	1.947729	-1.482210	2.967177

8	1.187847	-1.816776	3.463160
1	1.353110	-1.524427	4.362260

MP2/aug-cc-pVTZ-pp

Low Frequencies

58.5126 84.3991 90.2519

Optimised Coordinates

1	1.342529	-6.901243	0.083460
6	1.277774	-5.823597	0.209747
6	0.737731	-5.431423	1.584680
1	-0.337456	-5.268824	1.608377
1	1.186977	-3.516070	2.577204
7	1.447283	-4.170670	1.836875
6	2.505162	-3.946125	1.095980
79	3.666419	-2.439754	1.235658
6	2.641526	-5.118814	0.156487
1	0.626570	-5.422358	-0.565594
1	1.002673	-6.153560	2.359206
1	2.940063	-4.797433	-0.838210
1	3.447843	-5.745668	0.549507
8	4.786413	-0.865172	1.475209
1	5.469308	-0.821263	0.794781
1	1.948928	-1.479265	2.911909
8	1.203670	-1.806996	3.440418
1	1.415096	-1.538395	4.340049

S4.8.2. H₂O adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

13.0337 42.3866 78.1215

Optimised Coordinates

1	3.034338	-6.606017	-0.880923
6	2.756929	-5.647618	-0.449123
6	3.276292	-5.491845	0.986881

1	2.521773	-5.686849	1.747176
1	3.912733	-3.611541	1.882554
7	3.674253	-4.073230	1.018344
6	3.747672	-3.449561	-0.133070
79	4.236878	-1.568198	-0.413350
6	3.371671	-4.447031	-1.199823
1	1.671087	-5.572107	-0.462503
1	4.145339	-6.119186	1.196402
1	2.696709	-3.998956	-1.925300
1	4.288149	-4.708670	-1.737373
8	4.696457	0.343321	-0.631446
1	4.723391	0.588080	-1.561161
1	1.643039	-1.716685	-0.796213
8	0.796209	-2.161527	-0.951967
1	0.160740	-1.450741	-1.077771

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

20.5167 35.2627 81.1631

Optimised Coordinates

1	3.056840	-6.638100	-0.880696
6	2.778281	-5.662504	-0.478552
6	3.240559	-5.485914	0.977743
1	2.458003	-5.682782	1.714589
1	3.792012	-3.568782	1.875736
7	3.612683	-4.054443	1.004523
6	3.741363	-3.446277	-0.163863
79	4.194400	-1.569981	-0.458145
6	3.447840	-4.485015	-1.226626
1	1.691638	-5.563178	-0.536569
1	4.117254	-6.095839	1.226188
1	2.827636	-4.067310	-2.021788
1	4.406326	-4.768858	-1.682145
8	4.622108	0.340512	-0.696581

1	4.653889	0.551091	-1.642963
1	1.690860	-1.769002	-0.686414
8	0.776663	-2.105525	-0.791049
1	0.245304	-1.306453	-0.922055

MP2/cc-pVTZ-pp

Low Frequencies

24.7040 62.1559 87.8091

Optimised Coordinates

1	2.877059	-6.498661	-0.912214
6	2.699578	-5.501955	-0.518761
6	3.160507	-5.362352	0.930497
1	2.374309	-5.538020	1.660109
1	3.741161	-3.462441	1.833330
7	3.576790	-3.953799	0.967124
6	3.769955	-3.367094	-0.190418
79	4.286164	-1.558814	-0.480961
6	3.490762	-4.407105	-1.246244
1	1.638747	-5.272999	-0.584185
1	4.014503	-5.998432	1.167237
1	2.964989	-3.975217	-2.091947
1	4.462608	-4.758977	-1.604611
8	4.792999	0.300453	-0.715693
1	4.858362	0.485174	-1.659313
1	1.639533	-1.987923	-0.568179
8	0.862603	-2.561307	-0.586881
1	0.143030	-1.958890	-0.787558

MP2/aug-cc-pVTZ-pp

Low Frequencies

26.1761 65.1138 88.6618

Optimised Coordinates

1	2.875699	-6.505230	-0.908554
6	2.695232	-5.507167	-0.517821

6	3.155764	-5.363313	0.931998
1	2.368894	-5.535772	1.662711
1	3.733064	-3.456041	1.829325
7	3.572520	-3.953595	0.964901
6	3.763820	-3.371426	-0.195497
79	4.273562	-1.561425	-0.486750
6	3.485192	-4.412661	-1.248997
1	1.633065	-5.280529	-0.584470
1	4.011055	-5.998114	1.170213
1	2.956713	-3.980283	-2.094022
1	4.457342	-4.765231	-1.608186
8	4.777240	0.300332	-0.716576
1	4.848086	0.521533	-1.653485
1	1.677617	-1.983571	-0.562806
8	0.898325	-2.560069	-0.581859
1	0.170469	-1.965796	-0.788791

S4.8.3. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

42.4244 78.9546 84.3092

Optimised Coordinates

1	1.432450	-6.973451	0.183610
6	1.293699	-5.895825	0.219091
6	0.675082	-5.435781	1.546619
1	-0.397266	-5.256336	1.491786
1	1.109797	-3.535625	2.540425
7	1.389606	-4.174605	1.804091
6	2.457564	-3.945537	1.083314
79	3.637690	-2.374325	1.235516
6	2.622390	-5.113859	0.142258
1	0.645970	-5.615962	-0.610719
1	0.862749	-6.132656	2.366116
1	2.879326	-4.779170	-0.860776

1	3.474799	-5.699793	0.499125
8	4.741393	-0.750524	1.468157
1	5.483214	-0.738877	0.856028
1	2.243753	-1.647407	3.027008
9	1.482379	-1.822527	3.555417

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

41.5699 75.1045 88.1503

Optimised Coordinates

1	1.417193	-6.952835	0.144530
6	1.293259	-5.870736	0.213116
6	0.672647	-5.442376	1.553505
1	-0.406213	-5.275223	1.508141
1	1.085574	-3.528896	2.564300
7	1.372979	-4.169182	1.822803
6	2.455285	-3.927552	1.106819
79	3.618768	-2.356439	1.258081
6	2.635804	-5.103306	0.167182
1	0.651774	-5.549859	-0.612186
1	0.880837	-6.149357	2.365214
1	2.921425	-4.775695	-0.834737
1	3.471009	-5.704376	0.551621
8	4.726325	-0.738575	1.460387
1	5.462260	-0.760726	0.828579
1	2.264884	-1.747497	2.930581
9	1.510785	-1.839630	3.519131

MP2/cc-pVTZ-pp

Low Frequencies

32.4459 54.3788 85.3197

Optimised Coordinates

1	1.183235	-6.680899	-0.304179
6	1.101929	-5.664253	0.068470

6	1.142261	-5.604238	1.593305
1	0.163018	-5.622108	2.064276
1	1.831422	-3.870781	2.724544
7	1.793085	-4.305162	1.813751
6	2.459378	-3.806656	0.799191
79	3.525044	-2.226974	0.799899
6	2.278437	-4.769628	-0.346250
1	0.167222	-5.236955	-0.289652
1	1.763144	-6.389079	2.026278
1	2.133941	-4.246361	-1.287078
1	3.214436	-5.329557	-0.422320
8	4.580892	-0.604541	0.860787
1	4.992387	-0.466457	0.000086
1	4.898722	-4.147790	1.392122
9	5.154341	-5.027441	1.561929

MP2/aug-cc-pVTZ-pp

Low Frequencies

37.0304 88.1891 90.9910

Optimised Coordinates

1	1.382774	-6.917977	0.087317
6	1.291729	-5.840923	0.200164
6	0.710636	-5.447392	1.557338
1	-0.367887	-5.308183	1.554627
1	1.099750	-3.525460	2.542264
7	1.386977	-4.167312	1.809051
6	2.459075	-3.928051	1.093689
79	3.603291	-2.406503	1.227512
6	2.641465	-5.108450	0.172354
1	0.651378	-5.461667	-0.594888
1	0.974969	-6.152427	2.347262
1	2.958800	-4.793316	-0.818549
1	3.450084	-5.713439	0.594028
8	4.710855	-0.824404	1.437201

1	5.442283	-0.827824	0.807401
1	2.199178	-1.647799	3.003225
9	1.439238	-1.821131	3.527071

S4.8.4. HF adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

16.7793 44.1149 77.1524

Optimised Coordinates

1	1.249105	-6.770558	-0.211074
6	1.095115	-5.736374	0.085674
6	1.006416	-5.582865	1.610136
1	-0.012938	-5.516609	1.986461
1	1.719108	-3.859209	2.734298
7	1.716979	-4.310592	1.832195
6	2.434481	-3.851201	0.836111
79	3.554877	-2.234310	0.863287
6	2.271138	-4.817188	-0.309095
1	0.173012	-5.388772	-0.378516
1	1.521854	-6.381804	2.146452
1	2.124604	-4.291609	-1.250456
1	3.216001	-5.361146	-0.398884
8	4.630677	-0.586145	0.961930
1	5.095967	-0.417918	0.137005
1	5.103040	-4.016657	1.177871
9	5.483458	-4.875923	1.231762

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

17.7247 47.0303 76.6101

Optimised Coordinates

1	1.200735	-6.752293	-0.247418
6	1.083190	-5.717022	0.076307
6	1.026044	-5.596258	1.608349

1	0.011961	-5.536912	2.010919
1	1.758027	-3.878494	2.748099
7	1.740827	-4.320755	1.836054
6	2.460520	-3.853441	0.829539
79	3.574856	-2.245360	0.855367
6	2.282111	-4.821702	-0.319469
1	0.161067	-5.325544	-0.361999
1	1.561402	-6.404789	2.119011
1	2.146663	-4.296594	-1.267322
1	3.217376	-5.391331	-0.401714
8	4.626121	-0.587822	0.942695
1	5.083701	-0.436847	0.100636
1	5.005108	-3.994989	1.214444
9	5.443186	-4.838726	1.311661

MP2/cc-pVTZ-pp

Low Frequencies

32.4459 54.3788 85.3197

Optimised Coordinates

1	1.183235	-6.680899	-0.304179
6	1.101929	-5.664253	0.068470
6	1.142261	-5.604238	1.593305
1	0.163018	-5.622108	2.064276
1	1.831422	-3.870781	2.724544
7	1.793085	-4.305162	1.813751
6	2.459378	-3.806656	0.799191
79	3.525044	-2.226974	0.799899
6	2.278437	-4.769628	-0.346250
1	0.167222	-5.236955	-0.289652
1	1.763144	-6.389079	2.026278
1	2.133941	-4.246361	-1.287078
1	3.214436	-5.329557	-0.422320
8	4.580892	-0.604541	0.860787
1	4.992387	-0.466457	0.000086

1	4.898722	-4.147790	1.392122
9	5.154341	-5.027441	1.561929

MP2/aug-cc-pVTZ-pp

Low Frequencies

34.1613 55.1590 86.7517

Optimised Coordinates

1	1.180551	-6.683229	-0.305581
6	1.100923	-5.666245	0.068697
6	1.153348	-5.608483	1.593923
1	0.177619	-5.627076	2.073660
1	1.854482	-3.874317	2.722677
7	1.805669	-4.308455	1.811267
6	2.464431	-3.811052	0.791001
79	3.533063	-2.233075	0.790837
6	2.274788	-4.770706	-0.354452
1	0.162904	-5.238102	-0.281962
1	1.780843	-6.392540	2.020481
1	2.122710	-4.244034	-1.293156
1	3.210808	-5.331453	-0.438608
8	4.584310	-0.606834	0.853547
1	5.018835	-0.443550	0.007000
1	4.851095	-4.138352	1.404241
9	5.106514	-5.021376	1.591585

S4.8.5. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

58.1743 67.5327 76.7268

Optimised Coordinates

1	1.427276	-6.985978	0.255351
6	1.314154	-5.904502	0.240322
6	0.707523	-5.365842	1.544412
1	-0.362230	-5.171070	1.480881

1	1.174139	-3.418791	2.459397
7	1.444787	-4.109292	1.745228
6	2.517371	-3.940774	1.014919
79	3.724197	-2.390066	1.104897
6	2.659471	-5.156350	0.129239
1	0.672530	-5.649293	-0.602505
1	0.879661	-6.030381	2.394524
1	2.925091	-4.874745	-0.887708
1	3.498151	-5.743705	0.514883
8	4.862004	-0.773071	1.280491
1	5.597480	-0.798076	0.661655
7	1.085457	-1.856650	3.640338
1	1.922160	-1.410143	3.273451
1	1.227924	-1.980739	4.636253
1	0.323794	-1.197382	3.527341

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

58.7983 67.5320 77.3206

Optimised Coordinates

1	1.404791	-6.977258	0.216761
6	1.309683	-5.889724	0.230763
6	0.704563	-5.375227	1.549118
1	-0.371532	-5.188942	1.496706
1	1.157560	-3.410768	2.477253
7	1.432695	-4.107949	1.756651
6	2.519349	-3.932966	1.027010
79	3.705903	-2.381146	1.119867
6	2.670066	-5.158419	0.145528
1	0.673814	-5.595231	-0.609099
1	0.895582	-6.049647	2.393226
1	2.961748	-4.887005	-0.871347
1	3.491154	-5.760739	0.557329
8	4.825278	-0.757623	1.289779

1	5.563135	-0.802513	0.662134
7	1.101285	-1.872593	3.615485
1	1.946561	-1.440969	3.233019
1	1.257139	-1.977996	4.617261
1	0.352165	-1.190137	3.505924

MP2/cc-pVTZ-pp

Low Frequencies

54.3546 66.4914 71.9705

Optimised Coordinates

1	1.355086	-6.927199	0.151694
6	1.312306	-5.843514	0.214981
6	0.777554	-5.358711	1.561426
1	-0.295328	-5.182798	1.572832
1	1.256685	-3.394456	2.453690
7	1.503550	-4.096390	1.739612
6	2.568456	-3.937392	0.993000
79	3.761496	-2.450702	1.046314
6	2.688240	-5.169006	0.126585
1	0.671368	-5.476545	-0.584721
1	1.028221	-6.037833	2.378054
1	2.998470	-4.917205	-0.883597
1	3.480084	-5.784998	0.561807
8	4.918908	-0.889276	1.182766
1	5.622024	-0.970281	0.529168
7	1.273718	-1.821786	3.551599
1	2.111604	-1.442787	3.119189
1	1.473843	-1.877063	4.542391
1	0.562132	-1.109068	3.449342

MP2/aug-cc-pVTZ-pp

Low Frequencies

59.6436 66.9382 74.9619

Optimised Coordinates

1	1.350043	-6.931739	0.153257
6	1.306407	-5.847304	0.216227
6	0.772845	-5.363601	1.564462
1	-0.300458	-5.186039	1.577424
1	1.257354	-3.394311	2.457042
7	1.500347	-4.100996	1.743566
6	2.564199	-3.943256	0.994297
79	3.751875	-2.453135	1.054133
6	2.683048	-5.172442	0.126053
1	0.664091	-5.479746	-0.583105
1	1.025935	-6.043497	2.380526
1	2.990832	-4.917084	-0.884867
1	3.475945	-5.789866	0.559268
8	4.898012	-0.883060	1.205345
1	5.621436	-0.925464	0.568178
7	1.297758	-1.817387	3.532154
1	2.137679	-1.443871	3.095347
1	1.493127	-1.881580	4.524402
1	0.577941	-1.112633	3.422423

S4.8.6. NH₃ adduct in alternative geometry

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

24.5944 42.6736 77.3525

Optimised Coordinates

1	2.817697	-4.215937	-2.353403
6	3.349783	-3.287806	-2.160063
6	2.579731	-2.374031	-1.196920
1	2.017089	-1.585803	-1.694847
1	3.499803	-1.036354	0.254545
7	3.666915	-1.795073	-0.388113
6	4.843465	-2.373864	-0.472091
79	6.450425	-1.891636	0.543597
6	4.704034	-3.508974	-1.452268

1	3.498837	-2.782151	-3.113533
1	1.897027	-2.926136	-0.547619
1	5.553965	-3.549898	-2.130571
1	4.725952	-4.430797	-0.861007
8	8.030495	-1.364541	1.610995
1	8.808130	-1.866345	1.349741
7	5.404532	-5.605679	1.364261
1	5.874752	-4.718080	1.517397
1	6.128754	-6.301810	1.227822
1	4.931701	-5.842299	2.229110

TPSSTPSS/aug-cc-pVTZ-pp

Low Frequencies

21.9810 40.7221 72.8641

Optimised Coordinates

1	2.832923	-4.191791	-2.421585
6	3.362157	-3.268454	-2.179804
6	2.574799	-2.397809	-1.185975
1	1.990656	-1.604074	-1.658713
1	3.487184	-1.068189	0.291887
7	3.662123	-1.815851	-0.369311
6	4.854044	-2.389917	-0.462882
79	6.453376	-1.915310	0.545713
6	4.710638	-3.516749	-1.461783
1	3.525110	-2.715231	-3.109078
1	1.910225	-2.986126	-0.542259
1	5.567080	-3.561327	-2.138066
1	4.709918	-4.449765	-0.879475
8	8.036779	-1.392092	1.598337
1	8.802245	-1.918747	1.320043
7	5.387742	-5.573798	1.367039
1	5.838859	-4.662379	1.478730
1	6.143210	-6.253024	1.276605
1	4.934020	-5.776583	2.257611

S4.9. Adducts with H₃C-Au(I)-NHC3

S4.9.1. H₂O adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

17.1465 50.2367 53.8836

Optimised Coordinates

6	-0.385879	0.370697	-0.406299
7	-0.463992	1.495790	0.347416
7	-1.623411	0.245319	-0.950562
6	-2.456868	1.268068	-0.538819
6	-1.725516	2.053762	0.282573
1	-1.989832	2.948649	0.815037
1	-3.477773	1.350251	-0.863318
79	1.237685	-0.910792	-0.616540
8	0.983308	-0.933556	2.844083
1	1.566435	-1.554417	3.290440
1	1.113742	-1.109822	1.897259
6	-2.028214	-0.824740	-1.850041
1	-2.338596	-0.413050	-2.809819
1	-1.178387	-1.484061	-1.997034
1	-2.852296	-1.389060	-1.415095
6	0.619265	2.011914	1.177725
1	0.571861	1.581631	2.176565
1	1.566780	1.738195	0.724051
1	0.540922	3.095746	1.230901
6	2.847858	-2.199999	-0.803447
1	2.566146	-3.231621	-0.576739
1	3.239545	-2.183457	-1.824313
1	3.667228	-1.925437	-0.134010

S4.9.2. HF adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

16.3694 43.0865 47.4565

Optimised Coordinates

6	-0.342259	0.289202	-0.250536
7	-0.414362	1.460371	0.429470
7	-1.587844	0.120148	-0.762155
6	-2.421014	1.162823	-0.403149
6	-1.680989	2.005432	0.351205
1	-1.942242	2.931992	0.828202
1	-3.448294	1.216938	-0.713145
79	1.292252	-0.994894	-0.402922
9	1.322850	-0.923370	2.815050
1	1.404872	-1.103210	1.890681
6	-2.000586	-1.008142	-1.584208
1	-2.304853	-0.664129	-2.572110
1	-1.157467	-1.684915	-1.681245
1	-2.830714	-1.531729	-1.111880
6	0.678971	2.037956	1.203126
1	0.605572	1.740285	2.247719
1	1.619303	1.674733	0.801011
1	0.642545	3.122311	1.121353
6	2.909147	-2.279197	-0.527444
1	2.626739	-3.305036	-0.279606
1	3.310343	-2.281815	-1.544824
1	3.718028	-1.985777	0.145397

MP2/cc-pVTZ-pp

Optimised Coordinates

6	-0.263912	0.268922	-0.240423
7	-0.333217	1.446204	0.434550
7	-1.529919	0.081802	-0.700516
6	-2.361973	1.104832	-0.323902
6	-1.598132	1.972927	0.404798
1	-1.852482	2.898012	0.888836
1	-3.400505	1.140060	-0.597891

79	1.320874	-0.950805	-0.429141
9	0.598285	-0.834499	2.647011
1	0.853972	-1.012904	1.760750
6	-1.934806	-1.063107	-1.498628
1	-2.223670	-0.740079	-2.495886
1	-1.083323	-1.733365	-1.560482
1	-2.767914	-1.569591	-1.017907
6	0.785248	2.017485	1.170071
1	0.746640	1.695933	2.206901
1	1.702333	1.656139	0.716315
1	0.738305	3.100838	1.102123
6	2.915476	-2.187852	-0.589940
1	2.672838	-3.202220	-0.267927
1	3.260657	-2.245875	-1.624852
1	3.755222	-1.842881	0.016134

S4.8.5. NH₃ adduct

B3LYP/aug-cc-pVTZ-pp

Low Frequencies

15.1039 43.2003 51.4865

Optimised Coordinates

6	-0.453162	0.428335	-0.581700
7	-0.526854	1.517755	0.223465
7	-1.681437	0.354640	-1.157378
6	-2.503935	1.373869	-0.715606
6	-1.774953	2.104585	0.157585
1	-2.032800	2.979290	0.725493
1	-3.515478	1.492826	-1.057543
79	1.153873	-0.861844	-0.829077
7	1.148815	-0.944306	2.987494
1	0.518475	-1.622940	3.399299
1	1.259012	-1.198770	2.008475
1	2.051851	-1.078964	3.428073
6	-2.083707	-0.659869	-2.119716

1	-2.355041	-0.194858	-3.067003
1	-1.244614	-1.331338	-2.273918
1	-2.934056	-1.224131	-1.738140
6	0.555742	1.975459	1.090368
1	0.616408	1.354157	1.983203
1	1.495491	1.909094	0.549408
1	0.368891	3.011308	1.364391
6	2.753223	-2.159024	-1.058551
1	2.469065	-3.190769	-0.834085
1	3.129969	-2.138658	-2.084921
1	3.585232	-1.895847	-0.399594