Diversity of reactivity modes upon interplay between Au(III)-bound isocyanides and cyclic nitrones: a theoretical consideration

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Supporting Information

Nature of TS10-11,N1H$^+$

Due to very low imaginary frequency obtained for this structure (13i cm^{-1}), IRC calculations failed. To analyse the nature of this TS, the atoms were shifted from their equilibrium positions in **TS10-11,N1H**$^+$ along vectors corresponding to the imaginary frequency (at both directions), and resulting structures were optimized with small step size. These calculations led to associate **10•••N1H**$^+$, for one direction, and to associate **11•••Cl•••N1H**$^+$, for another direction. This indicates that **TS10-11,N1H**$^+$ indeed corresponds to the Cl$^-$ elimination from **10** assisted by the Cl•••H–O hydrogen bond between the Cl$^-$ ligand and **N1H**$^+$.

Mechanisms based on the reaction between isocyanate and imine

1. Reaction between isocyanate complex 6 and imine Im. The possibility of the reaction between isocyanate complex **6** and imine **Im** finally leading to metallacycle **3** was investigated in detail. Calculated possible pathways for this reaction are shown in Scheme S1. First group of the pathways is based on the direct interaction between **6** and **Im**. Five initial products of such an interaction may be drawn, each of them transforming then into **3**.

1) Acyclic intermediates **21** or **8** could be formed upon creation of the C–N bond. However, no minima were found for both these structures.

2) Imine molecule can be coordinated to the metal centre giving penta-coordinated complex **9**. However, the calculations demonstrated that only one isomer with both isocyanate and imine

ligands being in the mutual *trans*-position can exist for this complex (see Scheme 9). Thus, this complex cannot undergo cyclization to **13** or **24**. The PES scan of **13** with the C(5)–N(1) bond to be fixed and all other internal coordinated being relaxed indicated that the cleavage of this bond in **13** leads to the dissociation of OCN^{t}Bu and formation of **7** instead of **9**. No minimum for the deprotonated complex **27** was found. Hence, the pathway involving the **9** → **27** step may also be ruled out. Finally, complex **9** can undergo the elimination of Cl^- to give **29**. However, for the latter species also only one isomer with isocyanate and imine ligands in mutual *trans*-position was found. Therefore, **29** cannot cyclise to **26** or to **3**.

3) Complex **6** and **Im** can undergo cycloaddition to give **24** or **13**. However, no minimum for **24** and no transition state connecting **6** and **13** were found excluding these possibilities.

Second group of pathways is based on the initial deprotonation of imine **Im** → **Im-H**$^-$ which then reacts with **6**. Similarly, five initial products of such an interaction can be considered.

1) Acyclic intermediates **22** or **10** could be formed upon creation of the C–N bond. However, no TS connecting **6** + **Im-H**$^-$ and **10** was found. The PES scans of **10** and **22** with the N(1)–C(5) bond being fixed and all other internal coordinates being relaxed indicated that the cleavage of the N(1)–C(5) bond in **10** or **22** results in the liberation of OCN^{t}Bu.

2) Imine molecule **Im-H**$^-$ can be coordinated to the metal centre giving penta-coordinated complex **27**. However, no minimum was found for this species.

3) Complex **6** and **Im-H**$^-$ can undergo cycloaddition to give **25** or **12**. However, no minimum for both **25** and **12** were found excluding these possibilities.

Finally complex **6** may undergo Cl^- elimination and then react with **Im-H**$^-$ to give **29**, **23** or **3**. However, no minimum for **23** or TS connected **6** + **Im-H**$^-$ and **3** were found. Complex **29** has only *trans*-isomer (see above) and, hence, it cannot cyclise to **26** or **3**.

Thus, reaction between **6** and **Im** cannot lead to the formation of metallacycle **3**.

2. Reaction between the imino complex 7 and isocyanate OCN^{t}Bu. The possibility of the reaction between the imino complex **7** and isocyanate OCN^{t}Bu finally leading to metallacycle **3** was

investigated in detail. Calculated possible pathways for this reaction are shown in Scheme S2. First group of the pathways is based on the direct interaction between **7** and OCN^{t}Bu. Four initial products of such an interaction may be drawn, each of them transforming then into **3**.

1) Acyclic intermediate **30** could be formed upon creation of the C–N bond. However, no minima were found for this structure.

2) Imine molecule can be coordinated to the metal centre giving the penta-coordinated complex **9**. However, the calculations demonstrated that only one isomer with both isocyanate and imine ligands being in the mutual *trans*-position can exist for this complex, and this isomer cannot lead to **3** (see discussion above).

3) Complex **7** and OCN^{t}Bu can undergo cycloaddition to give **24** or **13**. However, no minimum for **24** and no transition state connecting **7** and **13** were found excluding these possibilities.

Second group of pathways is based on the initial deprotonation of imino complex **7** $\rightarrow$ **33** which then reacts with OCN^{t}Bu. Similarly, four initial products of such an interaction can be considered.

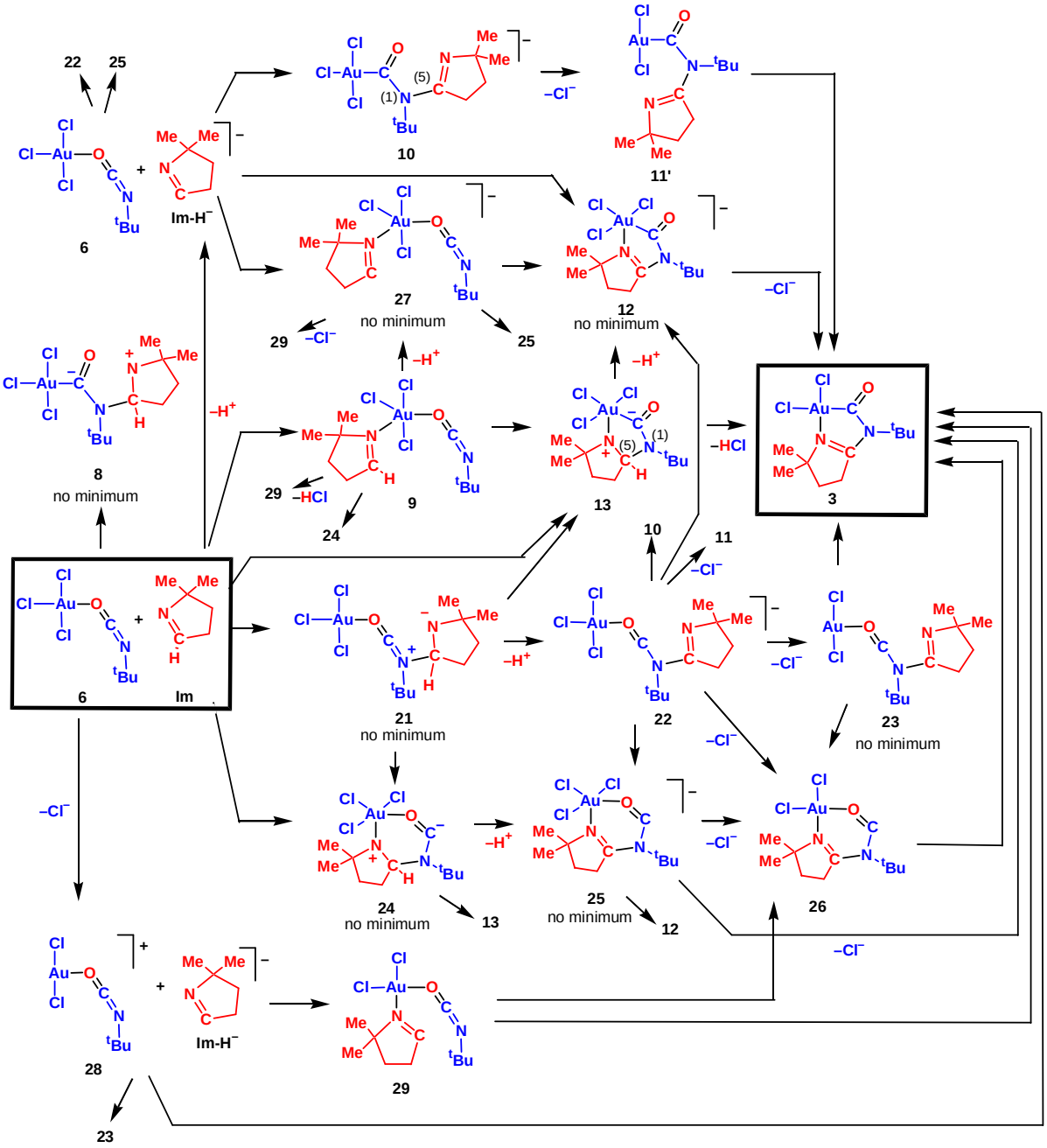
1) Acyclic intermediate **31** could be formed upon creation of the C–N bond. However, no minimum was found for this structure.

2) Isocyanate molecule OCN^{t}Bu can be coordinated to the metal centre giving the penta-coordinated complex **27**. However, no minimum was found for this species.

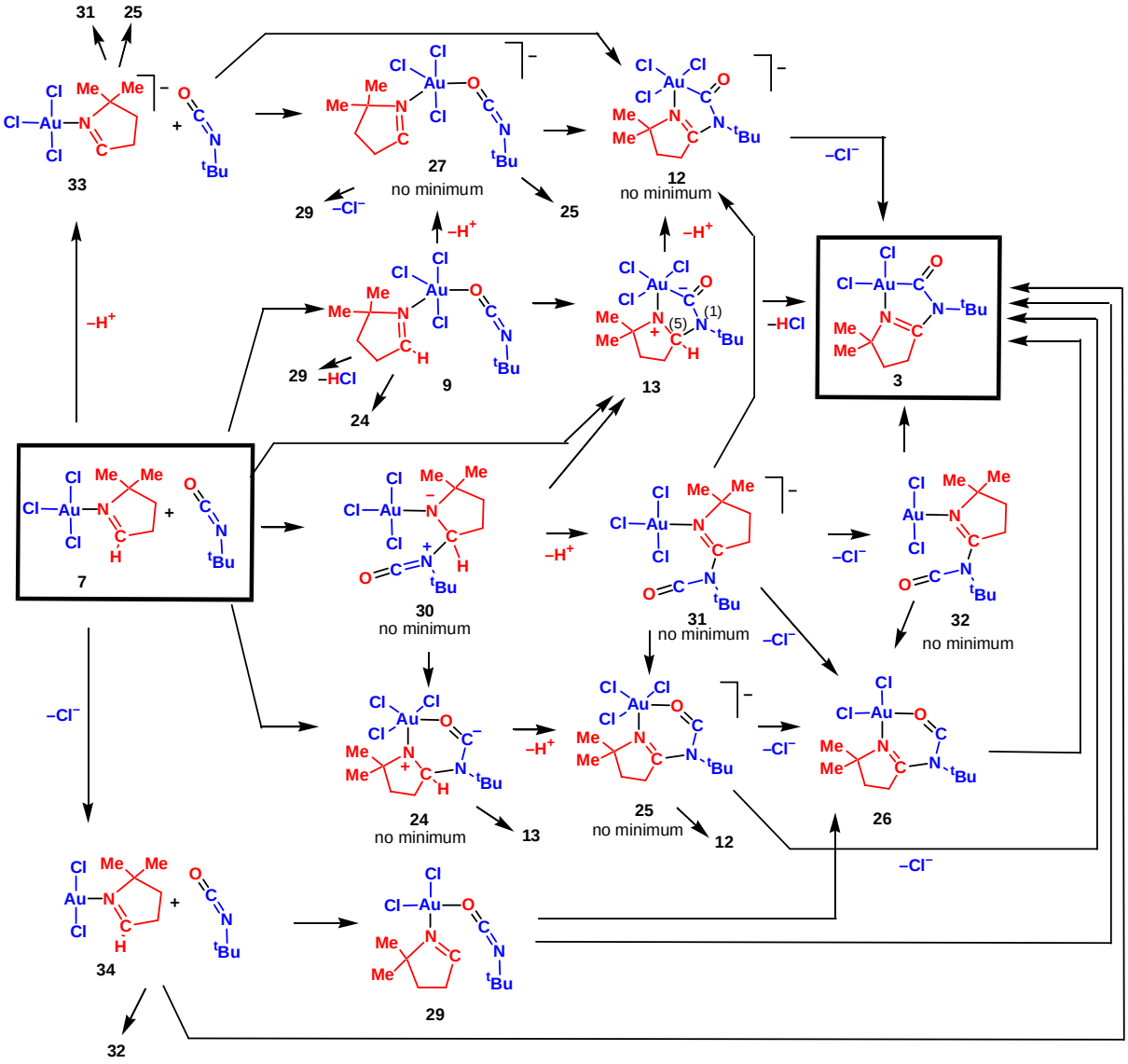
3) Complex **7** and OCN^{t}Bu can undergo cycloaddition to give **25** or **12**. However, no minimum for both **25** and **12** were found excluding these possibilities.

Finally complex **7** may undergo Cl^- elimination to give **34** and then react with OCN^{t}Bu to give **29**, **32** or **3**. However, no minimum for **32** or TS connected **7** + OCN^{t}Bu and **3** were found. Complex **29** has only *trans*-isomer and, hence, it cannot cyclise to **26** or **3** (see above).

Thus, reaction between **7** and OCN^{t}Bu also cannot lead to the formation of metallacycle **3**.



Scheme S1 Possible pathways of the reaction between **6** and **Im** leading to **3**.



Scheme S2 Possible pathways of the reaction between **7** and OCN^{t}Bu leading to **3**.

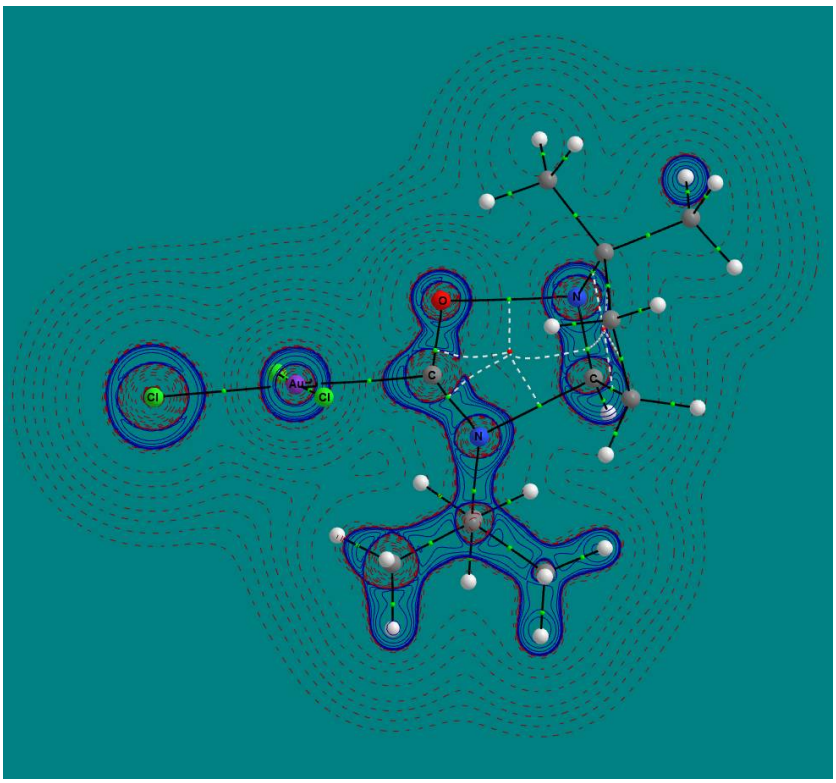


Fig. S1 Contour line diagram of the Laplacian distribution $\nabla^2\rho(\mathbf{r})$, bond paths and selected zero-flux surfaces in the plane of the oxadiazoline ring for **TS2-6**. Dashed lines indicate charge depletion ($\nabla^2\rho(\mathbf{r}) > 0$), solid lines indicate charge concentration ($\nabla^2\rho(\mathbf{r}) < 0$).

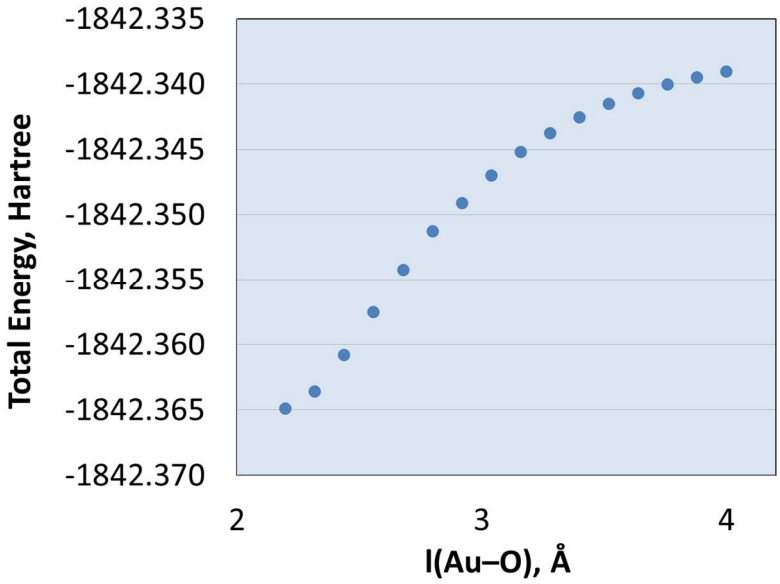


Fig. S2 Results of the PES scan of complex **6** with the fixed Au–O distance.

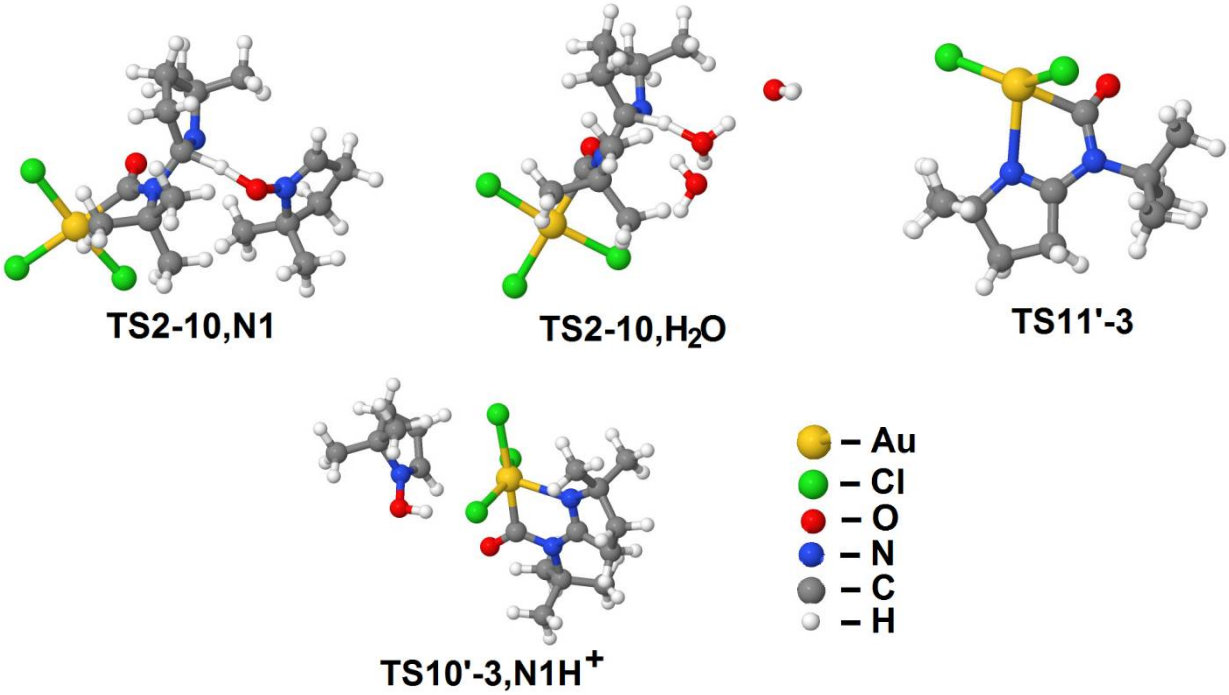


Fig. S3 Equilibrium structures of selected transition states.

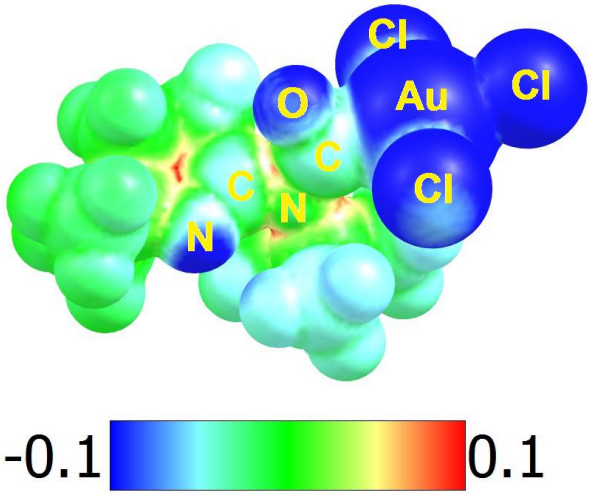


Fig. S4 ESP distribution in complex **10**.

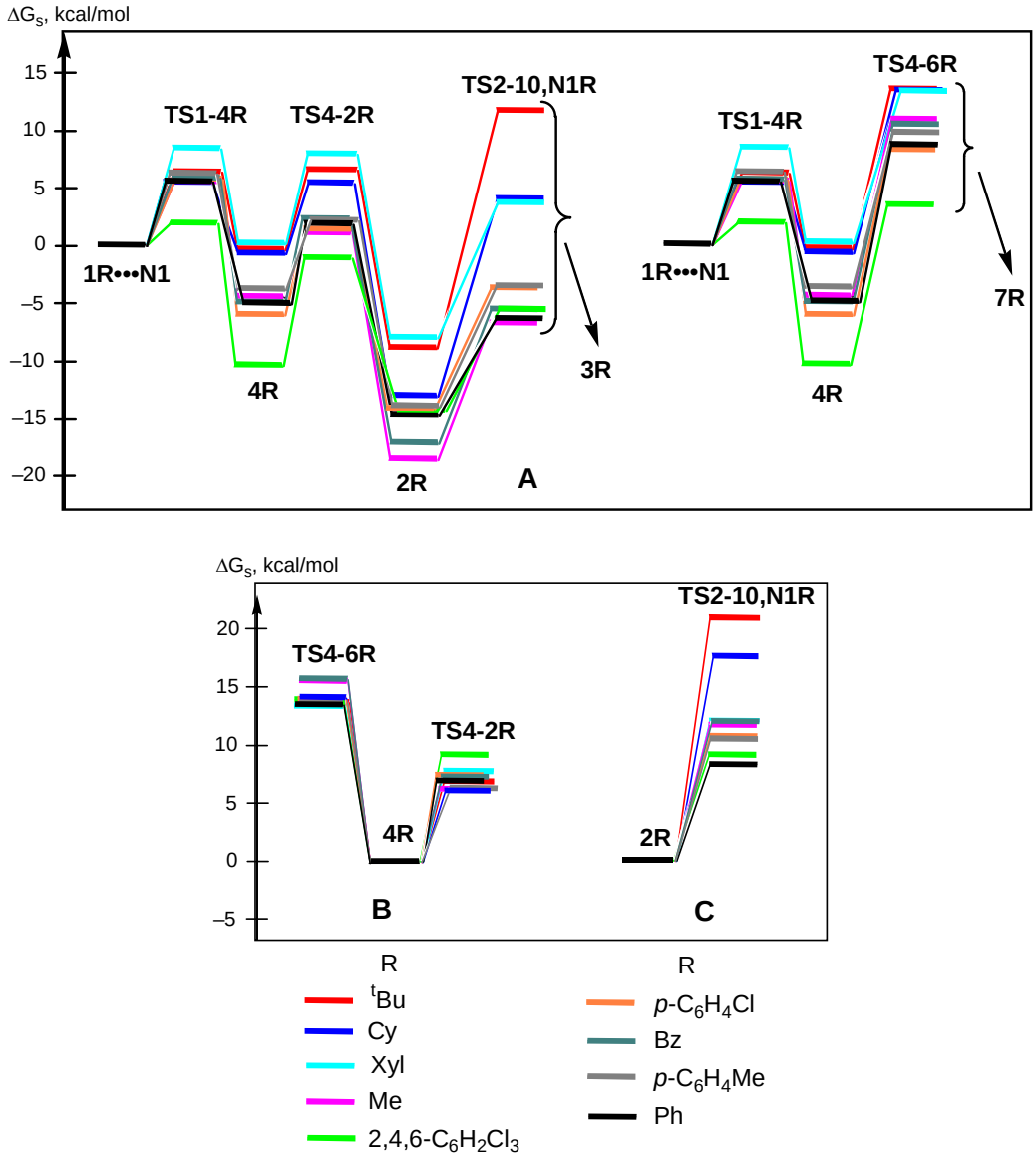


Fig. S5 Energy profiles of the rate limiting steps of the principal mechanisms for the reaction between [$AuCl_3$(C≡NR)] (**1R**) and **N1** (A), energies of **TS4-6R** and **TS4-2R** relative to **4R** (B) and energy of **TS2-10,N1R** relative to **2R** (C).

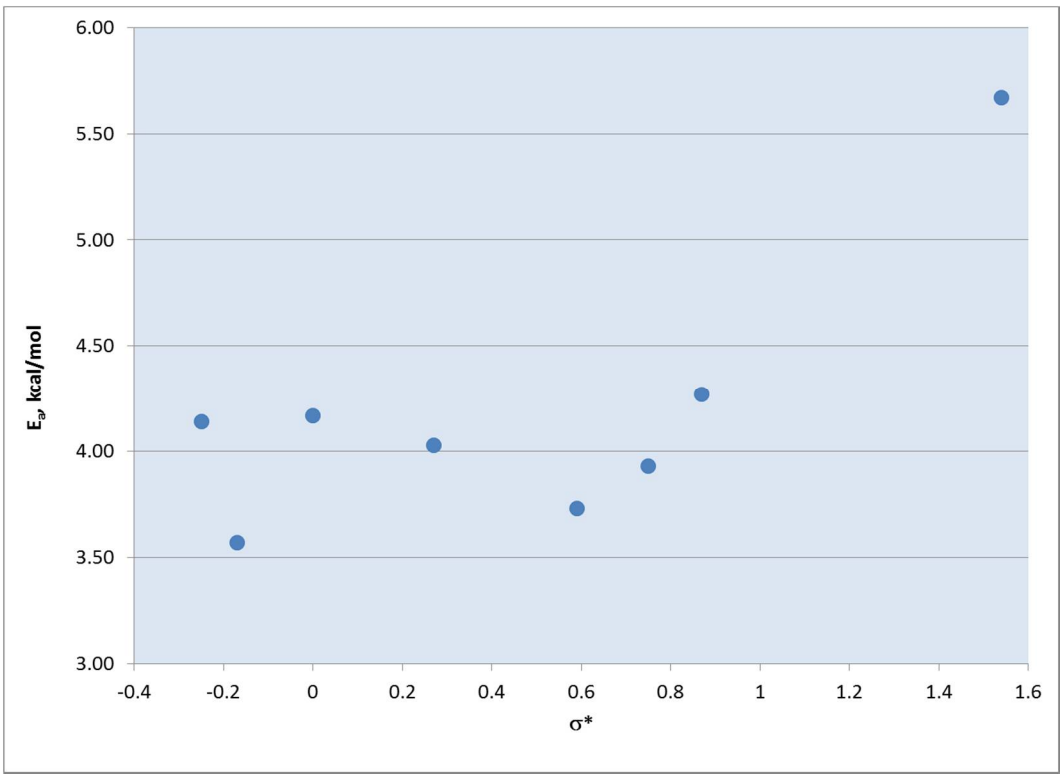


Fig. S6 Activation barrier of the cyclization **4** → **2** (E_a) *vs.* Taft constant of R (σ*).

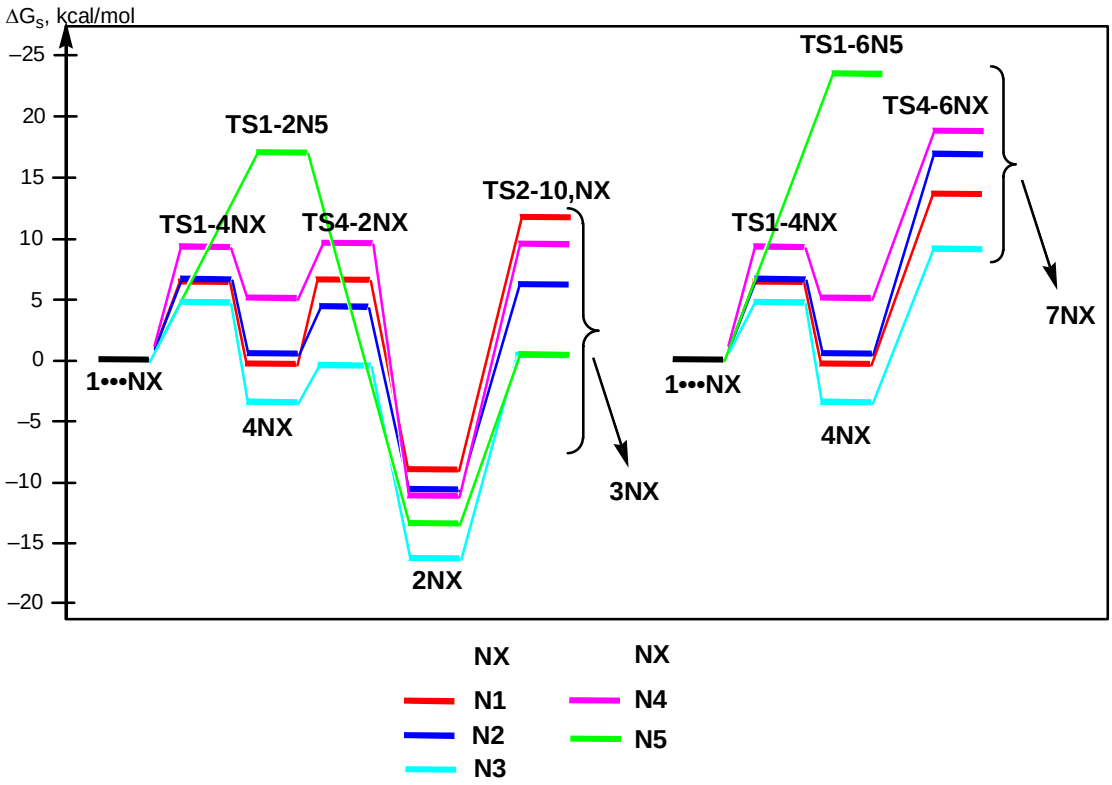


Fig. S7 Energy profiles of the rate limiting steps of the principal mechanisms for the reaction between [$AuCl_3$(C≡N^{t}Bu)] (**1**) and **N1**–**N5**.

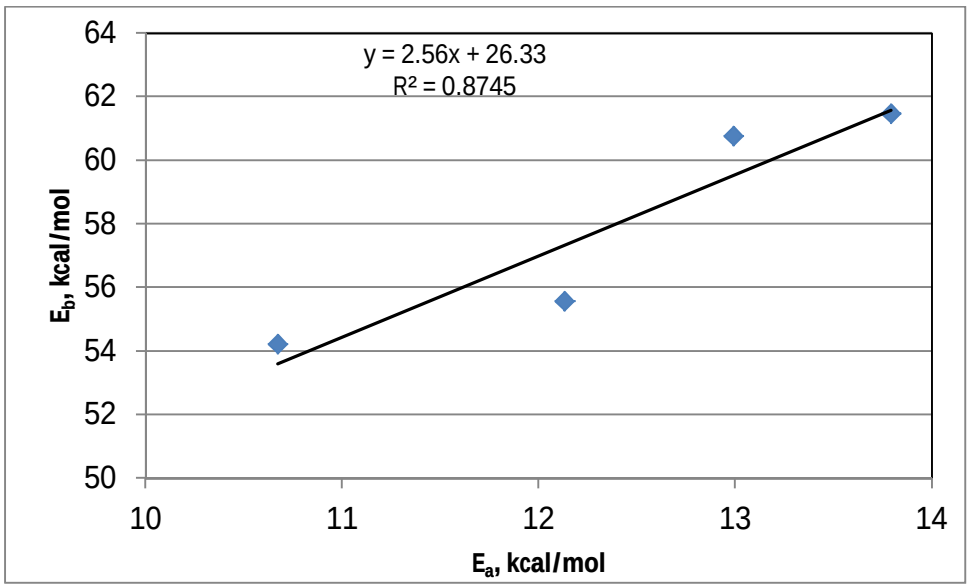


Fig. S8 Plot of the vertical N–O bond energy in **3** (E_b) *vs.* gas phase activation enthalpy at 0 K for the oxygen transfer step **3** → **6** + **I** (E_a) for various nitrones **N1**–**N4**.

Table S1 Calculated Gibbs free energies of activation and reaction in CH_2Cl_2 solution ($\Delta G_s^{\neq}$ and ΔG_s, in kcal/mol) for the calculated processes

Reaction		$\Delta G_s^{\neq}$	ΔG_s
1•••N1 → **4**	via **TS1-4**	6.3	–0.2
4 → **2**	via **TS4-2**	6.8	–8.9
1•••N1 → **4'**	via **TS1-4'**	15.2	12.5
C≡NtBu•••**N1** → OCNtBu + **Im**	via **TS1-6L**	32.3	–57.3
C≡NtBu•••**N1** → **2L**			6.9
2 → **6•••Im**	via **TS2-6**	33.6	–18.6
4 → **6•••Im**	via **TS4-6**	13.8	–27.5
6•••Im → **7**•••OCN^tBu	via **TS6-7**	0.6	–27.9
6 → $AuCl_3$ + OCN^tBu			9.1
6•••Im → **9**			2.2
2 → **14**	via **TS2-14**	33.2	24.6
2•••N1 → **10•••N1H**$^+$	via **TS2-10,N1**	20.9	–44.1
2•••$(H_2O)_3$ → **10**•••$(H_3O)(H_2O)_2^+$	via **TS2-10,H_2O**	21.2	
10•••N1H$^+$ → **11•••Cl**$^-$**•••N1H**$^+$	via **TS10-11,N1H**$^+$	11.4	11.4
11 → **11'**			–5.4
10 → **10'**			–2.6
11' → **3**	via **TS11'-3**	8.5	–16.9
10'•••N1H$^+$ → **3•••Cl**$^-$**•••N1**	via **TS10'-3,N1H**$^+$	5.9	
18 → **2**	via **TS18-2**	74.1	
18 → **19** + **Im'**	via **TS18-19**	73.7	
10 → **20**	via **TS10-20**	21.4	
1Cy•••N1 → **4Cy**	via **TS1-4Cy**	5.4	–0.9
1Xyl•••N1 → **4Xyl**	via **TS1-4Xyl**	8.2	0.0
1Me•••N1 → **4Me**	via **TS1-4Me**	5.4	–4.5

1PhCl$_3$•••N1 → 4PhCl$_3$	via **TS1-4PhCl$_3$**	1.9	–10.2
1PhCl•••N1 → 4PhCl	via **TS1-4PhCl**	5.5	–6.0
1Bz•••N1 → 4Bz	via **TS1-4Bz**	5.5	–5.1
1PhMe•••N1 → 4PhMe	via **TS1-4PhMe**	6.0	–3.9
1Ph•••N1 → 4Ph	via **TS1-4Ph**	5.2	–5.1
4Cy → 2Cy	via **TS4-2Cy**	6.0	–12.6
4Xyl → 2Xyl	via **TS4-2Xyl**	7.8	–8.1
4Me → 2Me	via **TS4-2Me**	6.1	–14.1
4PhCl$_3$ → 2PhCl$_3$	via **TS4-2PhCl$_3$**	9.0	–4.4
4PhCl → 2PhCl	via **TS4-2PhCl**	7.7	–8.4
4Bz → 2Bz	via **TS4-2Bz**	7.4	–12.2
4PhMe → 2PhMe	via **TS4-2PhMe**	6.2	–10.2
4Ph → 2Ph	via **TS4-2Ph**	7.1	–9.8
4Cy → 6Cy + Im	via **TS4-6Cy**	14.5	
4Xyl → 6Xyl + Im	via **TS4-6Xyl**	13.3	
4Me → 6Me + Im	via **TS4-6Me**	15.2	
4PhCl$_3$ → 6PhCl$_3$ + Im	via **TS4-6PhCl$_3$**	13.7	
4PhCl → 6PhCl + Im	via **TS4-6PhCl**	13.8	
4Bz → 6Bz	via **TS4-6Bz**	15.3	
4PhMe → 6PhMe + Im	via **TS4-6PhMe**	13.57	
4Ph → 6Ph + Im	via **TS4-6Ph**	13.4	
2Cy•••N1 → 10Cy•••N1H$^+$	via **TS2-10Cy,N1**	17.5	
2Xyl•••N1 → 10Xyl•••N1H$^+$	via **TS2-10Xyl,N1**	11.9	
2Me•••N1 → 10Me•••N1H$^+$	via **TS2-10Me,N1**	11.6	
2PhCl$_3$•••N1 → 10PhCl$_3$•••N1H$^+$	via **TS2-10PhCl$_3$,N1**	9.1	
2PhCl•••N1 → 10PhCl•••N1H$^+$	via **TS2-10PhCl,N1**	10.7	
2Bz•••N1 → 10Bz•••N1H$^+$	via **TS2-10Bz,N1**	11.8	
2PhMe•••N1 → 10PhMe•••N1H$^+$	via **TS2-10PhMe,N1**	10.4	
2Ph•••N1 → 10Ph•••N1H$^+$	via **TS2-10Ph,N1**	8.3	
1•••N2 → 4N2	via **TS1-4N2**	6.5	0.9
1•••N3 → 4N3	via **TS1-4N3**	4.8	–3.7
1•••N4 → 4N4	via **TS1-4N4**	9.0	9.8
1•••N5 → 2N5	via **TS1-2N5**	17.1	–13.6
4N2 → 2N2	via **TS4-2N2**	3.5	–11.6
4N3 → 2N3	via **TS4-2N3**	3.3	–12.7
4N4 → 2N4	via **TS4-2N4**	4.7	–16.0
4N2 → 6 + ImN2	via **TS4-6N2**	15.9	
4N2 → 6 + ImN3	via **TS4-6N3**	12.9	
4N2 → 6 + ImN4	via **TS4-6N4**	13.5	
1•••N5 → 6 + ImN5	via **TS1-6N5**	23.5	
2•••N2 → 10N2•••N2H$^+$	via **TS2-10N2,N2**	17.3	
2•••N3 → 10N3•••N3H$^+$	via **TS2-10N3,N3**	16.5	
2•••N4 → 10N4•••N4H$^+$	via **TS2-10N4,N4**	20.3	
2•••N5 → 10N5•••N5H$^+$	via **TS2-10N5,N5**	13.7	

Table S2 Total energies, enthalpies, Gibbs free energies (in Hartree) and entropies (in cal/mol•K) in gas phase (E_g, H_g, S_g, G_g) and in CH_2Cl_2 solution (E_s, H_s, S_s, G_s) of the calculated structures

Structure	E_g 6-31+G**	E_g 6-311+G**	E_s 6-311+G**	H_g	H_s	S_g	S_s	G_g	G_s
H_2O	-76.434048	-76.459142	-76.464414	-76.408983	-76.414255	46.48	32.85	-76.431066	-76.429862
$(H_2O)_3$	-229.318969	-229.393654	-229.404557	-229.238184	-229.249087	97.45	73.11	-229.284485	-229.283826
HCl	-460.803206	-460.834527	-460.834809	-460.793197	-460.793479	44.61	31.37	-460.814390	-460.808384
N1	-365.208050	-365.287952	-365.296853	-365.033483	-365.042384	85.84	63.94	-365.074267	-365.072765
N1H$^+$	-365.572755	-365.652588	-365.719948	-365.385377	-365.452737	87.76	65.46	-365.427075	-365.483838
CN^{t}Bu	-250.690812	-250.742327	-250.747500	-250.552794	-250.557967	81.11	60.20	-250.591334	-250.586572
CN^{t}Bu•••**N1**	-615.904180	-616.035806	-616.038232	-615.589474	-615.591900	140.30	106.97	-615.656133	-615.642723
$AuCl_3$	-1516.372741	-1516.460329	-1516.457584	-1516.362607	-1516.359862	86.15	64.19	-1516.403540	-1516.390359
TS1-6L	-615.851939	-615.982102	-615.989023	-615.539387	-615.546308	124.82	94.74	-615.598691	-615.591320
2L	-615.897812	-616.025973	-616.032812	-615.582425	-615.589264	117.97	89.32	-615.638478	-615.631705
^{3}1	-1767.091052								
1	-1767.140995	-1767.281155	-1767.284904	-1766.989721	-1766.993470	129.48	98.42	-1767.051241	-1767.040231
1•••N1	-2132.362530	-2132.583598	-2132.577140	-2132.034489	-2132.028031	178.96	137.51	-2132.119519	-2132.093365
TS1-4	-2132.341250	-2132.561802	-2132.568208	-2132.014681	-2132.021087	170.72	131.00	-2132.095793	-2132.083328
4	-2132.348225	-2132.566983	-2132.579678	-2132.020287	-2132.032982	166.78	127.88	-2132.099528	-2132.093744
TS1-4'	-2132.334228	-2132.554348	-2132.555054	-2132.007205	-2132.007911	167.90	128.77	-2132.086980	-2132.069093
4'	-2132.337479	-2132.557075	-2132.560754	-2132.009199	-2132.012878	166.15	127.39	-2132.088145	-2132.073403
TS4-2	-2132.341625	-2132.560163	-2132.569463	-2132.014529	-2132.023829	161.94	124.06	-2132.091470	-2132.082774
2	-2132.374641	-2132.591338	-2132.597187	-2132.044534	-2132.050383	157.97	120.92	-2132.119592	-2132.107838
2•••N1	-2497.594024	-2497.890798	-2497.890694	-2497.087108	-2497.087004	219.88	169.83	-2497.191578	-2497.167697
2•••$(H_2O)_3$	-2361.715293	-2362.006508	-2362.005647	-2361.301502	-2361.300641	210.43	162.37	-2361.401485	-2361.377787
TS2-10,N1	-2497.546988	-2497.846169	-2497.857626	-2497.047832	-2497.059289	204.95	158.04	-2497.145210	-2497.134378
TS2-10,H_2O	-2361.669688	-2361.962253	-2361.970829	-2361.263207	-2361.271783	197.43	152.10	-2361.357012	-2361.344050
10	-2131.946392	-2132.167409	-2132.217185	-2131.630119	-2131.679895	163.32	125.15	-2131.707716	-2131.739358
10'	-2131.951005	-2132.172458	-2132.221240	-2131.634833	-2131.683615	164.64	126.19	-2131.713057	-2131.743574
10•••N1H$^+$	-2497.668258	-2497.969787	-2497.966474	-2497.163144	-2497.159831	213.04	164.43	-2497.264365	-2497.237957
TS10-11	-2131.894594	-2132.116107	-2132.175349	-2131.579571	-2131.638813	168.56	129.29	-2131.659659	-2131.700243
TS10-11,N1H$^+$	-2497.642547	-2497.944540	-2497.942767	-2497.140540	-2497.138767	220.77	170.54	-2497.245436	-2497.219794
11	-1671.606196	-1671.797708	-1671.795461	-1671.292442	-1671.290195	156.79	119.99	-1671.366940	-1671.347207
11'	-1671.615289	-1671.807255	-1671.804157	-1671.301462	-1671.298364	158.09	121.02	-1671.376577	-1671.355864
11•••Cl$^-$•••N1H$^+$	-2497.645189	-2497.946971	-2497.941745	-2497.141947	-2497.136721	226.00	174.67	-2497.249327	-2497.219711
TS10'-3	-2131.926047	-2132.148048	-2132.210101	-2131.610043	-2131.672096	157.32	120.41	-2131.684790	-2131.729307
TS10'-3,N1H$^+$	-2497.662462	-2497.964453	-2497.963298	-2497.157625	-2497.156470	208.12	160.54	-2497.256507	-2497.232749
TS11'-3	-1671.59691	-1671.788292	-1671.791637	-1671.283350	-1671.286695	152.97	116.97	-1671.356030	-1671.342273
TS2-6	-2132.318194	-2132.539279	-2132.539949	-2131.992952	-2131.993622	166.60	127.74	-2132.072110	-2132.054316
TS4-6	-2132.326249	-2132.546428	-2132.553935	-2132.000803	-2132.008310	173.62	133.29	-2132.083295	-2132.071639
6	-1842.364892	-1842.529335	-1842.529050	-1842.208389	-1842.208104	138.63	105.65	-1842.274259	-1842.258300
6•••Im	-2132.397720	-2132.620926	-2132.616659	-2132.071272	-2132.067005	192.84	148.47	-2132.162898	-2132.137549
Im	-290.031223	-290.089436	-290.095266	-289.862355	-289.868185	82.16	61.03	-289.901392	-289.897184
TS6-7	-2132.403578	-2132.628093	-2132.622705	-2132.076883	-2132.071495	178.15	136.87	-2132.161530	-2132.136525
9	-2132.395188	-2132.618883	-2132.621118	-2132.067077	-2132.069312	177.35	136.23	-2132.151339	-2132.134041
7	-1806.477263	-1806.624478	-1806.631225	-1806.294928	-1806.301675	124.13	94.19	-1806.353907	-1806.346428
OCN^{t}Bu	-325.963014	-326.040548	-326.043448	-325.818974	-325.821874	89.07	66.49	-325.861293	-325.853467
TS2-14	-2132.313340	-2132.532922	-2132.543629	-2131.987180	-2131.997887	156.94	120.11	-2132.061749	-2132.054955

14	-2132.331401	-2132.550945	-2132.557785	-2132.003106	-2132.009946	161.22	123.49	-2132.079707	-2132.068621
18	-2132.439228	-2132.659837	-2132.671628	-2132.109016	-2132.120807	161.46	123.68	-2132.185729	-2132.179572
18•••H_2O	-2208.878692	-2209.124273	-2209.136090	-2208.521139	-2208.532956	186.82	143.72	-2208.609902	-2208.601240
TS18-2	-2132.311410	-2132.530708	-2132.545415	-2131.988013	-2132.002720	161.56	123.76	-2132.064775	-2132.061523
TS18-19	-2132.320843	-2132.543969	-2132.548105	-2131.995051	-2131.999187	172.55	132.44	-2132.077036	-2132.062115
3	-1671.632876	-1671.824289	-1671.835681	-1671.318004	-1671.329396	147.08	112.32	-1671.388360	-1671.382763
TSIm-Im-H^-,N1	-655.176258	-655.313484	-655.318079	-654.835997	-654.840592	124.00	94.09	-654.894914	-654.885296
De-H^-	-289.385188	-289.443990	-289.525764	-289.232082	-289.313856	82.16	61.03	-289.271119	-289.342855
13	-2132.348839	-2132.571174	-2132.575014	-2132.019996	-2132.023836	159.52	122.15	-2132.095789	-2132.081873
28	-1381.828828	-1381.962801	-1382.014899	-1381.675479	-1381.727577	129.90	98.75	-1381.737199	-1381.774496
***trans*-29**	-1671.544486	-1671.739827	-1671.739039	-1671.232749	-1671.231961	171.62	131.71	-1671.314291	-1671.294540
22	-2131.877041	-2132.097563	-2132.150742	-2131.562173	-2131.615352	171.53	131.64	-2131.643674	-2131.677897
22'	-2131.883955	-2132.104585	-2132.154144	-2131.569193	-2131.618752	171.34	131.49	-2131.650602	-2131.681226
TS22'-26	-2131.847732	-2132.068028	-2132.141848	-2131.533297	-2131.607117	158.72	121.52	-2131.608711	-2131.664854
26	-1671.565610	-1671.755284	-1671.764741	-1671.252327	-1671.261784	149.27	114.05	-1671.323251	-1671.315973
33	-1805.919263	-1806.067222	-1806.122862	-1805.751349	-1805.806989	124.42	94.42	-1805.810465	-1805.851851
34	-1345.575753	-1345.693992	-1345.697699	-1345.410149	-1345.413856	118.21	89.51	-1345.466315	-1345.456387
TS34-32	-1671.539030	-1671.735696	-1671.735949	-1671.228420	-1671.228673	174.87	134.28	-1671.311508	-1671.292472
TS10-20	-2131.911128	-2132.133353	-2132.182696	-2131.596310	-2131.645653	163.48	125.28	-2131.673984	-2131.705176
TS2-20	-2132.320433	-2132.538345	-2132.542232	-2131.992207	-2131.996094	155.17	118.71	-2132.065931	-2132.052498
19	-2132.366984	-2132.591961	-2132.585485	-2132.039597	-2132.033121	178.26	136.95	-2132.124295	-2132.098192
1Cy	-1844.565054	-1844.719994	-1844.725354	-1844.374625	-1844.379985	130.55	99.26	-1844.436655	-1844.427148
1Cy•••N1	-2209.787047	-2210.022576	-2210.017118	-2209.419956	-2209.414498	182.72	140.48	-2209.506774	-2209.481243
TS1-4Cy	-2209.766777	-2210.001824	-2210.010187	-2209.401069	-2209.409432	173.28	133.02	-2209.483398	-2209.472634
4Cy	-2209.773910	-2210.007360	-2210.021170	-2209.406820	-2209.420630	170.10	130.51	-2209.487641	-2209.482638
TS4-2Cy	-2209.768217	-2210.001396	-2210.012103	-2209.402160	-2209.412867	165.33	126.74	-2209.480712	-2209.473085
2Cy	-2209.806148	-2210.037513	-2210.043699	-2209.437266	-2209.443452	162.93	124.84	-2209.514680	-2209.502769
2Cy•••N1	-2575.027237	-2575.338539	-2575.336768	-2574.481241	-2574.479470	222.73	172.08	-2574.587069	-2574.561233
TS2-10Cy,N1	-2574.983988	-2575.297723	-2575.306797	-2574.445955	-2574.455029	213.40	164.71	-2574.547350	-2574.533290
10Cy	-2209.384003	-2209.619754	-2209.666438	-2209.028497	-2209.075181	169.58	130.10	-2209.109072	-2209.136994
TS4-6Cy	-2209.751902	-2209.986764	-2209.995099	-2209.387335	-2209.395670	175.19	134.53	-2209.470571	-2209.459589
1Xyl	-1919.574628	-1919.743178	-1919.744386	-1919.397242	-1919.398450	141.83	108.17	-1919.464631	-1919.449847
1Xyl•••N1	-2284.794312	-2285.043770	-2285.036449	-2284.440309	-2284.432988	195.34	150.45	-2284.533123	-2284.504470
TS1-4Xyl	-2284.773228	-2285.022279	-2285.026764	-2284.420664	-2284.425149	181.60	139.59	-2284.506946	-2284.491474
4Xyl	-2284.781266	-2285.029060	-2285.041045	-2284.427226	-2284.439211	178.64	137.25	-2284.512102	-2284.504425
TS4-2Xyl	-2284.775480	-2285.022935	-2285.030100	-2284.422246	-2284.429411	171.76	131.82	-2284.503856	-2284.492042
2Xyl	-2284.808403	-2285.054399	-2285.056439	-2284.452456	-2284.454496	172.23	132.19	-2284.534288	-2284.517304
2Xyl•••N1	-2650.026707	-2650.352698	-2650.349039	-2649.493865	-2649.490206	229.65	177.55	-2649.602980	-2649.574566
TS2-10Xyl,N1	-2649.988084	-2650.316384	-2650.327666	-2649.463335	-2649.474617	220.70	170.48	-2649.568198	-2649.555618
TS4-6Xyl	-2284.760614	-2285.009808	-2285.016670	-2284.408971	-2284.415833	184.27	141.70	-2284.496521	-2284.483160
10Xyl	-2284.393245	-2284.643374	-2284.688583	-2284.051045	-2284.096254	178.79	137.37	-2284.135991	-2284.161524
1Me	-1649.176516	-1649.294306	-1649.301938	-1649.113329	-1649.120961	110.46	83.39	-1649.165814	-1649.160583
1Me•••N1	-2014.399560	-2014.598237	-2014.596436	-2014.159591	-2014.157790	161.23	123.50	-2014.236198	-2014.216469
TS1-4Me	-2014.379472	-2014.577666	-2014.588736	-2014.140846	-2014.151916	154.17	117.92	-2014.214098	-2014.207945
4Me	-2014.392956	-2014.589166	-2014.605857	-2014.152749	-2014.169440	149.40	114.15	-2014.223733	-2014.223678
TS4-2Me	-2014.386315	-2014.582343	-2014.596132	-2014.147069	-2014.160858	146.48	111.85	-2014.216665	-2014.214000
2Me	-2014.425106	-2014.619273	-2014.629692	-2014.183148	-2014.193567	144.66	110.41	-2014.251879	-2014.246026
2Me•••N1	-2379.647371	-2379.922055	-2379.922107	-2379.228455	-2379.228507	196.95	151.72	-2379.322032	-2379.300593
TS4-6M2	-2014.370219	-2014.568197	-2014.577274	-2014.132598	-2014.141675	158.66	121.47	-2014.207984	-2014.199389

TS2-10Me,N1	-2379.619840	-2379.896361	-2379.900736	-2379.207488	-2379.211863	192.19	147.96	-2379.298805	-2379.282163
1PhCl$_3$	-3219.691370	-3219.933126	-3219.932454	-3219.598029	-3219.597357	147.14	112.37	-3219.667939	-3219.650747
1PhCl$_3$•••N1	-3584.911121	-3585.233994	-3585.222977	-3584.640972	-3584.629955	197.43	152.10	-3584.734778	-3584.702222
TS1-4PhCl$_3$	-3584.898149	-3585.220785	-3585.222074	-3584.629430	-3584.630719	187.27	144.07	-3584.718406	-3584.699172
4PhCl$_3$	-3584.913108	-3585.234526	-3585.242766	-3584.642771	-3584.651011	184.69	142.03	-3584.730524	-3584.718496
TS4-2PhCl$_3$	-3584.904070	-3585.225145	-3585.229370	-3584.634659	-3584.638884	178.95	137.50	-3584.719681	-3584.704214
2PhCl$_3$	-3584.933629	-3585.253404	-3585.252393	-3584.661769	-3584.660758	177.19	136.11	-3584.745956	-3584.725427
2PhCl$_3$•••N1	-3950.152001	-3950.552016	-3950.545388	-3949.703299	-3949.696671	234.21	181.15	-3949.814579	-3949.782743
TS4-6PhCl$_3$	-3584.891337	-3585.214567	-3585.217667	-3584.623500	-3584.626600	191.49	147.41	-3584.714484	-3584.696637
TS2-10PhCl$_3$,N1	-3950.116683	-3950.519074	-3950.527391	-3949.675993	-3949.684310	228.38	176.55	-3949.784506	-3949.768194
1PhCl	-2300.519632	-2300.702921	-2300.706520	-2300.409246	-2300.412845	133.21	101.36	-2300.472539	-2300.461006
1PhCl•••N1	-2665.741797	-2666.005895	-2666.001099	-2665.454669	-2665.449873	185.51	142.68	-2665.542812	-2665.517665
TS1-4PhCl	-2665.724171	-2665.987869	-2665.994176	-2665.438425	-2665.444732	175.88	135.07	-2665.521988	-2665.508910
2PhCl	-2665.763729	-2666.024081	-2666.029204	-2665.474835	-2665.479958	166.60	127.74	-2665.553994	-2665.540652
2PhCl•••N1	-3030.982953	-3031.323260	-3031.320505	-3030.517293	-3030.514538	226.39	174.98	-3030.624858	-3030.597675
4PhCl	-2665.737433	-2665.999579	-2666.013647	-2665.450133	-2665.464201	172.88	132.70	-2665.532271	-2665.527253
TS4-2PhCl	-2665.730627	-2665.992523	-2666.002363	-2665.444287	-2665.454127	167.22	128.23	-2665.523738	-2665.515054
TS4-6PhCl	-2665.716452	-2665.980191	-2665.988603	-2665.431727	-2665.440139	178.24	136.94	-2665.516415	-2665.505202
TS2-10PhCl,N1	-3030.951282	-3031.293887	-3031.302858	-3030.492567	-3030.501538	215.72	166.55	-3030.595064	-3030.580670
1Bz	-1880.242534	-1880.404808	-1880.412289	-1880.093626	-1880.101107	135.00	102.78	-1880.157767	-1880.149940
1Bz•••N1	-2245.465752	-2245.708852	-2245.704165	-2245.140041	-2245.135354	185.06	142.33	-2245.227967	-2245.202977
TS1-4Bz	-2245.446886	-2245.689561	-2245.696868	-2245.122449	-2245.129756	176.52	135.58	-2245.206319	-2245.194174
4Bz	-2245.460513	-2245.701284	-2245.714170	-2245.134514	-2245.147400	174.39	133.90	-2245.217374	-2245.211018
TS4-2Bz	-2245.454094	-2245.694701	-2245.703440	-2245.129055	-2245.137794	168.81	129.49	-2245.209261	-2245.199318
2Bz	-2245.492825	-2245.731538	-2245.736104	-2245.165069	-2245.169635	167.05	128.10	-2245.244438	-2245.230498
2Bz•••N1	-2610.712871	-2611.032084	-2611.026322	-2610.208169	-2610.202407	219.79	169.76	-2610.312599	-2610.283066
TS2-10Bz,N1	-2610.683432	-2611.004267	-2611.004132	-2610.185715	-2610.185580	214.44	165.54	-2610.287604	-2610.264231
TS4-6Bz	-2245.437125	-2245.679672	-2245.685903	-2245.113821	-2245.120052	182.32	140.16	-2245.200449	-2245.186647
1PhMe	-1880.250992	-1880.412335	-1880.416305	-1880.102972	-1880.106942	137.57	104.81	-1880.168335	-1880.156740
1PhMe•••N1	-2245.471725	-2245.713901	-2245.708949	-2245.146921	-2245.141969	191.66	147.54	-2245.237985	-2245.212070
TS1-4PhMe	-2245.453537	-2245.695267	-2245.702287	-2245.130176	-2245.137196	178.96	137.51	-2245.215205	-2245.202530
4PhMe	-2245.465049	-2245.705201	-2245.719421	-2245.140126	-2245.154346	175.27	134.59	-2245.223403	-2245.218295
TS4-2PhMe	-2245.459101	-2245.699001	-2245.709292	-2245.135281	-2245.145572	172.57	132.46	-2245.217275	-2245.208507
2PhMe	-2245.493766	-2245.732162	-2245.737395	-2245.167279	-2245.172512	170.14	130.54	-2245.248117	-2245.234535
2PhMe•••N1	-2610.714871	-2611.033578	-2611.029809	-2610.211378	-2610.207609	223.00	172.30	-2610.317333	-2610.289473
TS4-6PhMe	-2245.443661	-2245.685392	-2245.694321	-2245.121382	-2245.130311	181.69	139.66	-2245.207709	-2245.196669
TS2-10PhMe,N1	-2610.679346	-2610.999991	-2611.009398	-2610.183053	-2610.192460	219.30	169.38	-2610.287249	-2610.272936
1Ph	-1840.928390	-1841.082460	-1841.086355	-1840.809502	-1840.813397	126.10	95.75	-1840.869417	-1840.858889
1Ph•••N1	-2206.149567	-2206.384489	-2206.379636	-2205.853886	-2205.849033	179.44	137.89	-2205.939143	-2205.914547
TS1-4Ph	-2206.131828	-2206.366399	-2206.373366	-2205.837661	-2205.844628	169.29	129.87	-2205.918095	-2205.906332
2Ph	-2206.171721	-2206.402888	-2206.408447	-2205.874392	-2205.879951	160.39	122.84	-2205.950598	-2205.938314
2Ph•••N1	-2571.393648	-2571.705260	-2571.698945	-2570.919313	-2570.912998	210.20	162.19	-2571.019185	-2570.990058
4Ph	-2206.143992	-2206.376961	-2206.391231	-2205.848207	-2205.862477	165.24	126.67	-2205.926718	-2205.922661
TS4-2Ph	-2206.137734	-2206.370487	-2206.380734	-2205.842942	-2205.853189	160.00	122.53	-2205.918965	-2205.911406
TS4-6Ph	-2206.122643	-2206.357262	-2206.366196	-2205.829440	-2205.838374	172.72	132.58	-2205.911504	-2205.901366
TS2-10Ph,N1	-2571.357708	-2571.671119	-2571.681481	-2570.890460	-2570.900822	207.25	159.86	-2570.988931	-2570.976775
N3	-401.095217	-401.189035	-401.198734	-400.945135	-400.954834	86.12	64.16	-400.986053	-400.985320
1•••N3	-2168.249587	-2168.484453	-2168.479270	-2167.945904	-2167.940721	179.98	138.31	-2168.031418	-2168.006438
2N3	-2168.276508	-2168.506944	-2168.511903	-2167.970650	-2167.975609	156.82	120.02	-2168.045158	-2168.032632

2N3•••N3	-2569.384136	-2569.709085	-2569.706264	-2568.925932	-2568.923111	212.73	164.18	-2569.027007	-2569.001120
4N3	-2168.243549	-2168.476245	-2168.488522	-2167.939461	-2167.951738	166.29	127.50	-2168.018469	-2168.012316
TS1-4N3	-2168.233151	-2168.467698	-2168.473724	-2167.930718	-2167.936744	170.14	130.54	-2168.011557	-2167.998767
TS4-2N3	-2168.242272	-2168.474695	-2168.484706	-2167.938968	-2167.948979	159.60	122.21	-2168.014800	-2168.007046
TS4-6N3	-2168.226552	-2168.460311	-2168.466026	-2167.924805	-2167.930520	168.31	129.09	-2168.004775	-2167.991856
TS2-10N3,N3	-2569.342493	-2569.669510	-2569.678359	-2568.891652	-2568.900501	202.56	156.15	-2568.987892	-2568.974693
N4	-401.101816	-401.195346	-401.203506	-400.952098	-400.960258	87.20	65.02	-400.993528	-400.991149
1•••N4	-2168.255060	-2168.489643	-2168.483239	-2167.951883	-2167.945479	181.13	139.22	-2168.037946	-2168.011627
2N4	-2168.270438	-2168.500824	-2168.507790	-2167.964887	-2167.971853	157.18	120.30	-2168.039569	-2168.029012
2N4•••N4	-2569.383095	-2569.707221	-2569.708023	-2568.925576	-2568.926378	218.44	168.70	-2569.029365	-2569.006531
4N4	-2168.234937	-2168.467538	-2168.478169	-2167.932092	-2167.942723	166.94	128.01	-2168.011410	-2168.003545
TS1-4N4	-2168.231044	-2168.465136	-2168.471142	-2167.929412	-2167.935418	169.66	130.16	-2168.010021	-2167.997261
TS4-2N4	-2168.231900	-2168.463980	-2168.472460	-2167.929635	-2167.938115	159.09	121.81	-2168.005222	-2167.995990
TS4-6N4	-2168.215605	-2168.449126	-2168.454404	-2167.915024	-2167.920302	169.09	129.71	-2167.995362	-2167.981931
TS2-10N4,N4	-2569.336974	-2569.663561	-2569.675777	-2568.887418	-2568.899634	203.53	156.92	-2568.984120	-2568.974190
N5	-322.423056	-322.501721	-322.512190	-322.331963	-322.342432	72.45	53.36	-322.366386	-322.367787
1•••N5	-2089.577065	-2089.796676	-2089.792767	-2089.332410	-2089.328501	165.92	127.20	-2089.411241	-2089.388940
2N5	-2089.593115	-2089.808142	-2089.819253	-2089.346663	-2089.357774	145.64	111.18	-2089.415863	-2089.410601
2N5•••N5	-2412.029501	-2412.323541	-2412.329054	-2411.689595	-2411.695108	190.56	146.67	-2411.780138	-2411.764796
TS1-2N5	-2089.535758	-2089.752667	-2089.767290	-2089.292639	-2089.307262	149.98	114.61	-2089.363897	-2089.361718
TS1-6N5	-2089.519335	-2089.736922	-2089.752743	-2089.277136	-2089.292957	160.68	123.07	-2089.353482	-2089.351429
TS2-6N5	-2089.544960	-2089.764236	-2089.770003	-2089.302702	-2089.308469	154.17	117.92	-2089.375951	-2089.364498
TS2-10N5,N5	-2411.994876	-2412.290642	-2412.306505	-2411.661716	-2411.677579	178.97	137.51	-2411.746749	-2411.742916
N2	-286.565712	-286.630543	-286.642102	-286.449388	-286.460947	73.48	54.18	-286.484302	-286.486688
1•••N2	-2053.721202	-2053.927270	-2053.923313	-2053.451380	-2053.447423	168.16	128.97	-2053.531278	-2053.508703
2N2	-2053.735545	-2053.937247	-2053.946563	-2053.463799	-2053.473115	145.02	110.69	-2053.532700	-2053.525709
2N2•••N2	-2340.314800	-2340.581853	-2340.584961	-2339.924349	-2339.927457	189.21	145.60	-2340.014249	-2339.996638
4N2	-2053.704030	-2053.907733	-2053.923916	-2053.434316	-2053.450499	156.11	119.45	-2053.508489	-2053.507256
TS1-4N2	-2053.698733	-2053.903944	-2053.913749	-2053.430386	-2053.440191	159.88	122.43	-2053.506352	-2053.498363
TS4-2N2	-2053.702984	-2053.906365	-2053.919904	-2053.434051	-2053.447590	148.94	113.79	-2053.504815	-2053.501656
TS4-6N2	-2053.683331	-2053.888320	-2053.896616	-2053.416076	-2053.424372	158.14	121.06	-2053.491214	-2053.481891
TS2-10N2,N2	-2340.271360	-2340.540352	-2340.554436	-2339.888584	-2339.902668	181.88	139.81	-2339.975002	-2339.969098

Table S3 Cartesian atomic coordinates (Å) of the calculated equilibrium structures

1

N	2.235651	0.001044	-0.002115
C	1.078545	0.001030	-0.001726
Au	-0.923474	0.000186	-0.000661
Cl	-0.863890	-2.362845	0.024687
C	3.693286	0.000469	-0.001218
Cl	-3.238569	-0.001054	0.000727
Cl	-0.866536	2.363255	-0.026998
C	4.146561	-0.083907	1.467449
C	4.151474	1.313563	-0.660206
C	4.149759	-1.229394	-0.805927
H	3.782878	-2.153943	-0.352535
H	5.242890	-1.256532	-0.818079
H	3.792558	-1.177556	-1.837919
H	5.244648	1.340095	-0.669270
H	3.786131	2.180621	-0.103674
H	3.794082	1.381440	-1.691133
H	5.239626	-0.085559	1.499293
H	3.784101	-1.001987	1.937516
H	3.783868	0.774176	2.039608

10

C	-1.605063	0.839664	-0.101986
C	0.598195	1.580820	0.077059
C	0.327351	-0.871229	-0.533965
C	-0.542100	-2.068412	-0.110213
H	-1.456261	-2.155064	-0.699221
H	-0.803083	-2.028715	0.949959
H	0.038998	-2.979750	-0.290802
C	0.511010	-0.873409	-2.063929
H	1.167729	-0.057283	-2.372991
H	-0.457009	-0.760706	-2.560180
H	0.952291	-1.827033	-2.379910
C	1.688788	-1.042362	0.174882
H	2.417595	-0.294393	-0.137893
H	2.090237	-2.028767	-0.077351
H	1.567576	-0.996789	1.262984
C	0.570226	2.377322	1.372989
H	-0.439892	2.621042	1.700689
H	1.034005	1.765389	2.159609
C	1.424451	3.591517	0.982691
H	2.059555	3.959522	1.795349
H	0.773905	4.414558	0.666816
C	2.255217	3.078966	-0.236361
C	3.651379	2.589841	0.192365
H	3.583848	1.874407	1.019368
H	4.270130	3.433525	0.521068
H	4.156350	2.094933	-0.644014
C	2.384554	4.131824	-1.344164
H	1.395344	4.432467	-1.703364

H	2.947794	3.732482	-2.194437
H	2.904184	5.022017	-0.968726
N	-0.270717	0.455467	-0.099867
N	1.492375	1.922024	-0.767175
O	-1.919856	2.016677	-0.088195
Cl	-5.254190	-1.783325	0.245220
Cl	-2.814499	-0.425563	2.388227
Cl	-3.339153	-0.396419	-2.356443
Au	-3.213098	-0.452119	0.029096

10Cy

C	-0.734208	-0.147132	0.263684
C	1.137031	1.374042	0.152964
C	0.337954	2.582347	0.627253
H	-0.653614	2.637584	0.184016
H	0.198026	2.499069	1.712824
C	1.262796	3.737968	0.211148
H	1.308337	4.540737	0.954468
H	0.908777	4.178971	-0.728087
C	2.646021	3.056346	-0.014446
C	3.554120	3.203058	1.222387
H	3.040163	2.859930	2.126860
H	3.845715	4.250614	1.367941
H	4.461307	2.601707	1.101503
C	3.368805	3.587938	-1.259384
H	2.754527	3.436407	-2.153256
H	4.318364	3.062398	-1.407748
H	3.577024	4.660414	-1.159267
N	0.650915	0.054737	0.249035
N	2.348319	1.621476	-0.199562
O	-1.523249	0.641671	-0.209487
Cl	-2.736028	-3.449648	2.604259
Cl	-1.120861	-0.402003	3.249281
Cl	-1.949083	-2.869961	-0.745650
Au	-1.579723	-1.723971	1.310002
H	1.950890	-4.384989	-0.142630
C	2.836978	-3.735442	-0.141625
C	2.896032	-2.971965	1.191349
C	2.755426	-2.768618	-1.333973
H	3.712189	-4.391315	-0.243722
C	1.700141	-2.014971	1.345503
C	1.580844	-1.784515	-1.192161
C	1.662252	-1.044948	0.154070
H	3.697155	-2.202954	-1.404422
H	2.655966	-3.329336	-2.272277
H	1.604354	-1.048884	-2.005122
H	0.630460	-2.323949	-1.267120
H	2.606403	-0.497363	0.162205
H	0.784919	-2.614238	1.399307
H	1.763917	-1.453863	2.283298
H	2.910009	-3.675228	2.033094

H	3.835294	-2.399710	1.242099

10’

C	-0.321386	1.016608	-0.107446
C	-0.047343	-1.368568	-0.446618
C	1.998124	0.086967	0.058149
C	2.575639	1.261047	-0.760640
H	2.122532	2.212238	-0.485302
H	2.412658	1.096530	-1.830932
H	3.655420	1.320497	-0.580686
C	2.177129	0.310580	1.570075
H	1.763586	-0.535874	2.125103
H	1.670733	1.223307	1.890530
H	3.244641	0.402106	1.806495
C	2.756313	-1.184039	-0.368004
H	2.482970	-2.049092	0.236364
H	3.827582	-0.996588	-0.241010
H	2.583297	-1.418784	-1.424274
C	-0.642856	-1.829243	-1.766666
H	-1.315261	-1.105313	-2.227693
H	0.184377	-1.979017	-2.476704
C	-1.314295	-3.142127	-1.338178
H	-1.233131	-3.936045	-2.087801
H	-2.378357	-2.964546	-1.152269
C	-0.594433	-3.512053	-0.001399
C	0.519521	-4.552275	-0.219781
H	1.204946	-4.240875	-1.016288
H	0.087087	-5.519848	-0.501220
H	1.102286	-4.687089	0.697857
C	-1.574514	-3.996567	1.074883
H	-2.308133	-3.216378	1.297390
H	-1.042743	-4.239169	2.001382
H	-2.104456	-4.893315	0.730667
N	0.517996	-0.063085	-0.270594
N	0.027594	-2.250980	0.470221
O	0.029385	2.109768	0.286875
Cl	-4.741436	0.781641	-1.104267
Cl	-2.687594	0.065886	1.652385
Cl	-1.738336	1.565595	-2.769232
Au	-2.342065	0.830813	-0.572521

10•••N1H^{+}

C	-0.897179	0.033394	-0.068902
C	-3.125838	0.632819	-0.282619
C	-2.693419	-1.861550	0.048634
C	-1.697618	-2.937320	-0.411949
H	-0.841745	-3.037629	0.259610
H	-1.342605	-2.762704	-1.429952
H	-2.219695	-3.899259	-0.391748
C	-3.026366	-2.048779	1.539583
H	-3.765495	-1.316000	1.868481
H	-2.126187	-1.937522	2.149840

H	-3.428114	-3.056118	1.696762
C	-3.959264	-2.017423	-0.818298
H	-4.755209	-1.334013	-0.519901
H	-4.338297	-3.036112	-0.698809
H	-3.730528	-1.866533	-1.878455
C	-3.222393	1.449171	-1.556531
H	-2.247487	1.788253	-1.911543
H	-3.658134	0.823806	-2.347212
C	-4.157767	2.582000	-1.098038
H	-4.890865	2.869046	-1.857328
H	-3.570347	3.472236	-0.849880
C	-4.835458	2.016615	0.193538
C	-6.233582	1.441895	-0.095593
H	-6.209663	0.732298	-0.929937
H	-6.928713	2.247363	-0.356727
H	-6.623294	0.920362	0.784244
C	-4.911524	3.054158	1.319608
H	-3.911498	3.413891	1.581925
H	-5.364083	2.620510	2.216860
H	-5.516187	3.912640	1.005334
N	-2.161699	-0.445476	-0.166349
N	-3.958523	0.899915	0.637202
O	-0.611395	1.220857	-0.041856
Cl	3.140498	-2.117020	0.042573
Cl	0.795708	-1.025753	-2.395016
Cl	0.658014	-1.127881	2.359801
Au	0.813109	-1.135782	-0.025287
C	3.076671	1.103363	1.400288
C	2.252549	2.278603	1.800018
H	1.197238	2.029017	1.628367
H	2.361814	2.498827	2.865895
C	2.768020	3.405123	0.868289
H	3.496669	4.025040	1.399675
H	1.961028	4.053164	0.522110
C	3.456937	2.690079	-0.324253
C	4.800025	3.304529	-0.721450
H	5.482852	3.359552	0.132048
H	4.626139	4.320308	-1.088905
H	5.277341	2.726990	-1.516539
C	2.530893	2.498537	-1.533145
H	1.559401	2.094540	-1.236264
H	2.978031	1.821887	-2.265215
H	2.373324	3.471009	-2.009844
N	3.696674	1.330881	0.294952
H	3.136616	0.139289	1.894438
O	4.466095	0.461740	-0.394127
H	4.059433	-0.475580	-0.272563

10Xyl

C	-0.068669	-0.790091	-0.923104
C	-2.444138	-0.603237	-0.351363

C	-2.763038	-2.071781	-0.589785
H	-2.296973	-2.460738	-1.493089
H	-2.367871	-2.661205	0.247640
C	-4.300681	-2.037584	-0.648486
H	-4.766823	-2.873988	-0.117417
H	-4.635336	-2.084517	-1.691275
C	-4.681237	-0.656188	-0.028551
C	-5.117093	-0.798017	1.442590
H	-4.367227	-1.348610	2.021126
H	-6.069829	-1.337103	1.514592
H	-5.237300	0.189638	1.899432
C	-5.774575	0.064858	-0.828538
H	-5.455792	0.216652	-1.865250
H	-5.985581	1.046782	-0.391992
H	-6.701671	-0.521676	-0.833996
N	-1.127869	-0.101708	-0.303666
N	-3.442660	0.149236	-0.066104
O	-0.236186	-1.624532	-1.783541
Cl	4.177068	-0.303537	0.531483
Cl	1.400572	-2.252466	1.293187
Cl	2.225896	1.139852	-1.932694
Au	1.867543	-0.485234	-0.242400
C	-0.809723	1.367484	1.662432
C	-0.929763	1.220445	0.269032
C	-0.607310	2.658610	2.168888
C	-0.934644	2.326996	-0.600123
C	-0.556042	3.764588	1.322584
C	-0.733691	3.598333	-0.049911
C	-0.946704	0.199246	2.605542
C	-1.188036	2.164953	-2.078466
H	-0.715500	4.461296	-0.710319
H	-0.387154	4.756634	1.733759
H	-0.490777	2.788729	3.241706
H	-0.390190	1.591931	-2.559183
H	-1.235889	3.144054	-2.564345
H	-2.137680	1.648031	-2.253620
H	-0.730040	0.511565	3.631438
H	-0.273980	-0.622886	2.349866
H	-1.972223	-0.189711	2.582194

11

C	-1.524860	0.939146	-0.160746
C	0.645570	1.594325	0.117401
C	0.324965	-0.902573	-0.451365
C	-0.563505	-2.060148	0.027323
H	-1.458412	-2.189549	-0.583977
H	-0.858096	-1.950040	1.073483
H	0.017253	-2.982220	-0.071447
C	0.542152	-0.959587	-1.971515
H	1.196600	-0.149422	-2.299595
H	-0.407714	-0.885505	-2.506995

H	1.007564	-1.916989	-2.229659
C	1.667527	-1.019389	0.297088
H	2.400075	-0.285848	-0.039243
H	2.079117	-2.011824	0.096657
H	1.529981	-0.928353	1.379505
C	0.718623	2.292829	1.458489
H	-0.264914	2.539909	1.864692
H	1.211209	1.629119	2.181549
C	1.569496	3.520243	1.079944
H	2.301917	3.787365	1.846365
H	0.919066	4.386759	0.924541
C	2.247449	3.117674	-0.271920
C	3.681988	2.601710	-0.067115
H	3.723110	1.828256	0.707576
H	4.336564	3.423720	0.241275
H	4.075161	2.177997	-0.996378
C	2.227499	4.253549	-1.300374
H	1.201017	4.569461	-1.510569
H	2.686579	3.935101	-2.241191
H	2.782225	5.117397	-0.917559
N	-0.272644	0.470854	-0.092219
N	1.423368	1.990713	-0.797402
O	-1.944623	2.054889	-0.063352
Cl	-3.420054	-0.608270	1.926480
Cl	-3.212013	-0.327673	-2.706357
Au	-3.186884	-0.377174	-0.381423

11’

C	-1.137478	-1.136075	-0.288314
C	0.577128	0.489023	0.281597
C	1.161146	-2.009723	-0.212114
C	0.714553	-3.235583	0.599237
H	-0.234522	-3.645372	0.251225
H	0.623317	-2.989695	1.661600
H	1.474024	-4.016376	0.493003
C	1.240498	-2.302208	-1.716529
H	1.538799	-1.405749	-2.266255
H	0.284652	-2.656249	-2.109932
H	1.985899	-3.085148	-1.890905
C	2.526132	-1.538073	0.309415
H	2.912372	-0.687488	-0.252990
H	3.227703	-2.368625	0.190844
H	2.492089	-1.286401	1.373438
C	0.558694	1.083815	1.674059
H	-0.394779	0.944662	2.187601
H	1.326836	0.592658	2.286869
C	0.896933	2.550724	1.346808
H	1.574297	3.006699	2.073863
H	-0.021811	3.145708	1.330725
C	1.519907	2.495437	-0.087644
C	3.058181	2.515971	-0.049806

H	3.453561	1.759995	0.637593
H	3.410955	3.496604	0.286591
H	3.469740	2.323881	-1.045468
C	0.989997	3.602798	-1.005674
H	-0.095595	3.528261	-1.116600
H	1.436708	3.528107	-2.001666
H	1.233825	4.585430	-0.586523
N	0.129220	-0.865030	0.006344
N	1.098185	1.180912	-0.644284
O	-1.724132	-2.105043	-0.654318
Cl	-2.324996	1.272521	-2.234986
Cl	-2.923812	-0.005575	2.181318
Au	-2.506364	0.521557	-0.050789

11•••Cl^-•••$N1H^+$

C	1.990114	-0.938021	0.186569
C	3.451124	0.792817	-0.046678
C	1.019289	1.310910	-0.768233
C	-0.051080	0.645395	-1.640137
H	-0.725418	0.006236	-1.066089
H	0.386446	0.060182	-2.452708
H	-0.668853	1.444111	-2.060768
C	0.408861	1.970528	0.475008
H	1.180534	2.466928	1.067661
H	-0.088529	1.225433	1.102184
H	-0.329442	2.708345	0.145070
C	1.731322	2.358820	-1.642237
H	2.468377	2.939866	-1.086634
H	0.968494	3.052103	-2.004955
H	2.209255	1.897231	-2.512587
C	4.607332	0.329374	-0.904652
H	4.630647	-0.757211	-1.023343
H	4.511977	0.762301	-1.908550
C	5.793524	0.898891	-0.100654
H	6.562737	1.345750	-0.736031
H	6.266101	0.101885	0.481820
C	5.143955	1.950721	0.862454
C	5.301103	3.388709	0.340104
H	4.964185	3.477339	-0.698301
H	6.353057	3.690454	0.381708
H	4.716893	4.085239	0.949118
C	5.675467	1.840107	2.295745
H	5.497872	0.838857	2.700460
H	5.182748	2.566052	2.949577
H	6.754028	2.032599	2.312446
N	2.092416	0.297216	-0.297341
N	3.689387	1.623766	0.874832
O	2.773677	-1.656145	0.732869
Cl	-2.423516	3.677611	-1.540822
Cl	0.928822	-2.962564	-2.046917
Cl	-0.897057	-1.398424	1.936831

Au	0.162722	-2.066865	-0.039790
C	-3.785456	2.017533	1.002548
C	-3.875101	1.171115	2.228227
H	-2.946159	0.595044	2.336021
H	-3.982180	1.779958	3.131218
C	-5.104015	0.268836	1.947000
H	-5.985253	0.670332	2.456232
H	-4.951454	-0.754704	2.294486
C	-5.321002	0.312448	0.412113
C	-6.782299	0.497515	-0.000047
H	-7.214848	1.389795	0.462675
H	-7.355274	-0.374432	0.329711
H	-6.876814	0.586984	-1.084570
C	-4.666559	-0.865314	-0.324209
H	-3.637128	-1.021330	0.011548
H	-4.667621	-0.695177	-1.403712
H	-5.235275	-1.776266	-0.115384
N	-4.543537	1.560777	0.063909
H	-3.150399	2.877911	0.809869
O	-4.662176	2.020475	-1.183425
H	-3.813340	2.688668	-1.382230

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C	-0.857189	1.866066	-0.459643
C	-0.103208	-0.230201	0.480924
C	0.312199	-1.281727	-0.582809
H	1.356596	-1.584537	-0.459038
H	0.191629	-0.868149	-1.585864
C	-0.681966	-2.443002	-0.342860
H	-1.231307	-2.663245	-1.260371
H	-0.174751	-3.360309	-0.027843
C	-1.659187	-1.938652	0.768515
C	-3.116359	-2.357789	0.536692
H	-3.192400	-3.447616	0.609814
H	-3.472030	-2.069098	-0.454704
H	-3.773833	-1.923206	1.296380
C	-1.225157	-2.475436	2.162101
H	-1.845979	-2.037451	2.947514
H	-0.177216	-2.250925	2.385120
H	-1.341815	-3.564418	2.180627
C	1.494730	1.879459	0.162741
N	0.108668	1.179647	0.103714
N	-1.491935	-0.462882	0.853644
O	-1.067844	2.895521	-0.991573
Cl	-4.806155	1.788007	-1.111779
Cl	-2.445525	-0.245745	-2.354754
Au	-2.854300	0.741629	-0.236606
C	2.443079	1.035559	1.027732
C	1.317989	3.257127	0.820201
C	2.036815	1.994757	-1.269430
H	2.093589	0.954561	2.060567

H	3.409613	1.547098	1.046270
H	2.611103	0.036695	0.618794
H	2.304100	3.715461	0.939674
H	0.859640	3.161850	1.808652
H	0.710746	3.934305	0.216887
H	2.174375	1.008613	-1.721708
H	3.008041	2.498900	-1.246961
H	1.371678	2.583212	-1.906805
H	0.483496	-0.382841	1.391962
Cl	-3.186853	1.892323	1.811641

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Au	-1.081746	-1.216572	-0.364344
Cl	-0.870314	-1.575344	1.978663
Cl	-3.122771	-2.398879	-0.310914
Cl	-1.251110	-1.052676	-2.706881
C	0.652716	-0.063240	-0.533251
N	1.943426	-0.445901	0.376684
O	0.793645	0.864676	-1.253479
C	2.680958	-1.769975	-0.062460
C	1.681618	-2.881584	-0.410703
C	3.495890	-1.376285	-1.301882
C	3.595629	-2.267341	1.065969
C	1.941858	0.031433	1.776211
N	3.002345	0.505175	0.914470
C	2.892874	2.006335	0.796288
C	1.015987	1.187694	2.152284
H	2.163701	-0.723333	2.521837
C	3.938575	2.460620	1.841318
C	3.295860	2.528012	-0.582030
C	1.466572	2.378543	1.274425
H	2.855225	-0.987650	-2.098587
H	3.998824	-2.267688	-1.687575
H	4.254150	-0.629729	-1.056546
H	4.174560	-3.105489	0.668258
H	3.023687	-2.649124	1.916663
H	4.297749	-1.502734	1.400228
H	2.268909	-3.779770	-0.626446
H	1.094632	-2.664285	-1.305276
H	1.012619	-3.113261	0.420083
H	-0.037416	0.928871	2.049508
H	1.184509	1.379451	3.217014
H	1.479319	3.312038	1.843700
H	0.796843	2.527121	0.427478
H	4.934163	2.088523	1.585240
H	3.690591	2.114950	2.850218
H	3.969511	3.554145	1.858312
H	4.307049	2.195003	-0.836265
H	3.300580	3.622694	-0.562027
H	2.607035	2.202964	-1.360027

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C	0.402144	0.046913	-1.766069
C	2.087652	-0.023253	-0.086899
C	0.185107	-1.717792	0.136267
C	-0.868537	-1.147940	1.099882
H	-1.644103	-0.588463	0.572710
H	-0.424013	-0.480696	1.842663
H	-1.352433	-1.976903	1.626318
C	-0.476267	-2.539881	-0.986988
H	0.280317	-2.986835	-1.640020
H	-1.163239	-1.954723	-1.600888
H	-1.054300	-3.348320	-0.530412
C	1.146573	-2.662467	0.883377
H	2.009316	-2.930103	0.264825
H	0.602334	-3.584909	1.102957
H	1.493120	-2.266724	1.838755
C	2.608947	-0.024866	1.336808
H	1.799092	-0.016422	2.065449
H	3.211628	-0.923177	1.501642
C	3.473132	1.251726	1.378499
H	4.316734	1.157772	2.065959
H	2.857679	2.095278	1.702222
C	3.939688	1.478539	-0.082865
C	5.310946	0.845901	-0.373612
H	5.345162	-0.200959	-0.054386
H	6.096945	1.393343	0.155733
H	5.537382	0.882684	-1.444248
C	3.909908	2.955112	-0.493260
H	2.909186	3.375719	-0.362588
H	4.208908	3.081262	-1.539627
H	4.613399	3.523083	0.124047
N	0.974079	-0.603590	-0.552125
N	2.890052	0.731636	-0.824743
O	1.082583	0.122216	-2.755093
Cl	-3.271443	2.495236	-1.298766
Cl	-0.131940	2.458475	0.037054
Cl	-2.423654	-0.249278	-3.108325
Au	-1.343518	1.124228	-1.533180
H	2.741424	0.840479	-1.822744

18•••H_2O

C	0.096468	-0.593333	1.759056
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H	-2.312789	-0.467756	-0.721885
H	-1.861298	1.009002	-1.594121
H	-3.321980	0.984665	-0.612680
C	-2.386797	0.766314	1.830526
H	-1.838003	0.919176	2.763963
H	-2.771281	-0.253350	1.825275
H	-3.247855	1.440807	1.834006

C	-1.313075	2.625076	0.589820
H	-0.849694	2.939785	1.530346
H	-2.284540	3.122355	0.508724
H	-0.697868	2.980649	-0.238365
C	0.760104	1.084438	-1.568663
H	0.288791	0.245621	-2.093132
H	0.157441	1.975388	-1.731346
C	2.226934	1.298424	-1.984173
H	2.472245	2.361520	-1.906133
H	2.414310	0.981528	-3.012538
C	3.066668	0.476987	-0.974508
C	4.358609	1.181843	-0.549698
H	4.151599	2.179124	-0.149861
H	5.022308	1.287456	-1.413311
H	4.894159	0.604328	0.211596
C	3.349901	-0.953338	-1.464670
H	2.428592	-1.471208	-1.745438
H	3.838220	-1.544080	-0.682971
H	4.016890	-0.921195	-2.332253
N	-0.163818	0.438825	0.732030
N	2.126689	0.426381	0.175681
O	1.093811	-0.507164	2.432129
Cl	-2.159540	-4.412338	1.580546
Cl	-0.223982	-2.569077	-0.551474
Cl	-1.649184	-2.012943	3.936023
Au	-1.010792	-2.332034	1.691743
H	0.682052	5.234721	-1.506065
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H	2.385511	0.064153	1.090135
H	0.371387	4.785418	-2.942071

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C	1.063883	-1.724185	-1.447610
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C	-0.575760	-1.798967	0.391462
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H	-1.105930	0.228495	1.001126
H	0.520909	-0.290334	1.496798
H	-0.916735	-0.934947	2.326879
C	-2.018255	-2.256972	0.154675
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H	-2.429758	-2.616733	1.102827
C	0.294978	-2.961663	0.889138
H	0.269286	-3.807806	0.194199
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H	1.328829	-2.636919	1.038152
C	4.439419	-0.322431	0.668771
H	4.480033	-0.436247	1.761775
H	4.860575	-1.246823	0.260034
C	5.168502	0.956668	0.172886

H	5.693298	0.750604	-0.765837
H	5.906913	1.333786	0.885990
C	4.034636	1.982579	-0.071158
C	4.148901	2.726319	-1.406406
H	4.227960	2.022796	-2.240957
H	5.039500	3.363707	-1.408751
H	3.278538	3.368985	-1.580155
C	3.863459	2.971247	1.094523
H	3.805116	2.444371	2.052504
H	2.950256	3.564833	0.975391
H	4.711221	3.663366	1.134067
N	-0.019410	-1.341568	-0.968803
N	2.846543	1.060545	-0.100803
O	1.999444	-2.090032	-2.033442
Cl	-2.339457	1.166428	-3.856312
Cl	-0.346831	1.849023	-1.305065
Cl	-1.772991	-2.073611	-3.488781
Au	-1.115040	-0.115614	-2.376458
H	1.941454	1.430758	-0.396474

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N	-0.495296	1.050264	1.171977
C	-1.587237	1.432018	1.174604
Au	-3.480821	2.079740	1.160732
Cl	-3.528359	1.667220	-1.166048
Cl	-3.312460	2.459604	3.487234
Cl	-5.674497	2.814993	1.137814
C	0.849965	0.530026	1.155338
H	1.368325	0.973635	2.009813
H	1.315047	0.902974	0.238037
C	1.021753	-3.028119	2.510161
C	1.020869	-1.632782	2.449366
C	0.864296	-3.778560	1.342144
C	0.864388	-0.984411	1.218749
C	0.708541	-3.133253	0.111773
C	0.710039	-1.738858	0.048851
H	1.144849	-3.525959	3.466969
H	1.140657	-1.050782	3.359536
H	0.587020	-1.239514	-0.908797
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H	0.864073	-4.863273	1.389681

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Au	-3.437783	1.655300	-0.602716
Cl	-4.167574	-0.367663	0.370024
Cl	-5.472210	2.668951	-0.133890
Cl	-2.612982	3.645937	-1.574885
C	-1.654093	0.812097	-0.933137
N	-0.595088	0.366964	-1.048249
O	0.470446	1.318322	1.671440
C	-1.583047	1.850081	2.624683
C	-0.013294	3.593364	2.396840

N	-0.388416	2.127373	2.183409
H	-1.947805	0.831154	2.580100
C	-2.275765	3.041270	3.204770
C	0.624106	4.141617	1.122177
C	0.966578	3.635554	3.577936
C	-1.389458	4.216407	2.721889
H	-3.310612	3.126807	2.858375
H	-2.314049	2.969279	4.301312
H	-1.304253	5.013083	3.465433
H	-1.820561	4.648650	1.814047
H	1.554037	3.613520	0.897286
H	0.850352	5.203668	1.262374
H	-0.054365	4.047243	0.269205
H	0.496321	3.280933	4.501198
H	1.303569	4.664422	3.738554
H	1.838999	3.010309	3.369814
C	0.755454	-0.142037	-1.073708
H	1.306707	0.501763	-0.382624
H	1.127209	0.004774	-2.091476
C	0.909140	-3.271166	1.087321
C	0.840914	-1.930635	0.703165
C	0.959545	-4.279678	0.119981
C	0.821866	-1.597800	-0.657951
C	0.942466	-3.947645	-1.237128
C	0.873246	-2.607560	-1.625675
H	0.924677	-3.527977	2.142336
H	0.796507	-1.137440	1.444968
H	0.862018	-2.350181	-2.682048
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H	1.014041	-5.321164	0.423042

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C	0.150456	0.270315	-0.120589
C	-0.004640	0.208347	1.407622
C	1.343671	-0.030428	2.103742
C	2.079995	-1.269470	1.551527
C	2.191148	-1.239593	0.012344
C	0.836512	-0.991756	-0.668144
N	1.386255	-2.469903	1.964491
C	0.820785	-3.425633	2.288918
Au	-0.175388	-5.072463	2.839009
Cl	1.743113	-5.776184	4.023428
Cl	-2.037268	-4.269635	1.620124
Cl	-1.333372	-6.974361	3.471545
H	3.075592	-1.348703	2.000752
H	2.885516	-0.423916	-0.225502
H	2.653794	-2.166799	-0.341793
H	0.990583	-0.906417	-1.749385
H	0.182096	-1.860054	-0.516733
H	0.744205	1.155416	-0.391700
H	-0.830879	0.395713	-0.590758

H	-0.705264	-0.594025	1.673042
H	-0.442426	1.138145	1.786991
H	1.223498	-0.125997	3.187987
H	2.012262	0.822005	1.929402

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Au	-2.653697	-2.591715	1.504715
Cl	-2.322389	-1.928409	3.749860
Cl	-4.871681	-1.907794	1.583252
Cl	-2.897414	-3.291551	-0.737807
C	-0.727365	-3.123588	1.420810
N	0.396766	-3.380843	1.360396
O	0.881279	-0.322410	0.324961
C	-1.012952	0.709096	1.195749
C	-0.596869	0.979210	-1.107669
N	-0.194647	0.374776	0.237405
H	-0.810706	0.388401	2.209862
C	-2.137435	1.572879	0.722765
C	-0.495745	-0.089531	-2.192996
C	0.364038	2.146184	-1.376096
C	-2.043838	1.436813	-0.817486
H	-3.104264	1.240886	1.114372
H	-1.997551	2.610296	1.059697
H	-2.283144	2.367768	-1.338173
H	-2.747380	0.671633	-1.158775
H	0.536904	-0.428176	-2.306871
H	-0.832614	0.333099	-3.145322
H	-1.125404	-0.952900	-1.959147
H	0.258869	2.932347	-0.620938
H	0.149095	2.581863	-2.356959
H	1.399064	1.793793	-1.368836
H	4.384472	-1.612087	0.339533
C	4.546204	-2.656584	0.637453
C	3.783272	-3.581318	-0.323663
C	4.074795	-2.847956	2.087274
H	5.623622	-2.844983	0.564388
C	2.261909	-3.392412	-0.209119
C	2.556313	-2.651061	2.222771
C	1.818321	-3.594699	1.252941
H	4.349615	-3.855340	2.432535
H	4.584785	-2.142370	2.752519
H	2.227477	-2.848416	3.248882
H	2.275934	-1.622699	1.969369
H	1.981190	-4.638457	1.551255
H	1.973248	-2.379282	-0.509700
H	1.731903	-4.100747	-0.855170
H	4.087506	-3.393303	-1.359391
H	4.042581	-4.628341	-0.108817

1Me

N	0.347188	0.029425	-0.061635
C	-0.808542	0.071875	-0.049047

Au	-2.809020	0.146136	-0.028107
Cl	-2.826619	-2.125619	0.625828
Cl	-2.670162	2.413337	-0.683685
Cl	-5.119395	0.232558	-0.004300
C	1.770887	-0.022147	-0.077797
H	2.152140	0.858406	-0.599097
H	2.087009	-0.930554	-0.594963
H	2.136666	-0.034377	0.951164

1Me•••N1

Au	-1.887335	2.517335	0.748829
Cl	-1.926268	2.413038	3.109297
Cl	-2.131314	4.822810	0.795926
Cl	-1.821760	2.520619	-1.611484
C	-1.608737	0.536407	0.715686
N	-1.379728	-0.594709	0.707883
O	1.654507	-0.376474	0.725750
C	1.775951	1.741371	1.679280
C	2.899599	1.405521	-0.365258
N	2.018038	0.855119	0.754613
H	1.205357	1.460318	2.555631
C	2.408531	3.064997	1.392216
C	2.311027	0.994530	-1.712930
C	4.301783	0.814900	-0.160011
C	2.831578	2.924914	-0.091818
H	1.716420	3.897549	1.553898
H	3.267240	3.235600	2.057387
H	3.785372	3.414545	-0.304871
H	2.071569	3.380846	-0.733372
H	2.308705	-0.093221	-1.816426
H	2.918336	1.423054	-2.516815
H	1.286169	1.360729	-1.825718
H	4.738325	1.140359	0.790211
H	4.960621	1.142916	-0.970109
H	4.257406	-0.277445	-0.165161
C	-0.983541	-1.963747	0.715131
H	0.101671	-1.977201	0.842132
H	-1.268926	-2.418994	-0.235376
H	-1.484657	-2.472137	1.541451

1•••N1

Au	0.168245	0.205745	2.028032
Cl	1.871687	-0.646606	3.426897
Cl	-0.456547	1.747387	3.649323
Cl	-1.515728	0.988043	0.568362
C	0.758307	-1.066948	0.602264
N	1.140993	-1.757159	-0.240869
C	1.691597	-2.550077	-1.334721
C	1.379949	-1.792313	-2.637752
C	1.007927	-3.927370	-1.291998
C	3.208525	-2.651447	-1.093147
O	3.029322	0.757035	-1.157574

C	3.182736	1.979506	0.814939
C	2.461502	3.124377	-1.113791
N	2.909637	1.823093	-0.450344
H	3.560782	1.142542	1.388447
C	2.960333	3.380429	1.286991
C	1.237343	2.851223	-1.984253
C	3.645658	3.629763	-1.950041
C	2.162656	4.008653	0.117097
H	3.654285	-1.654138	-1.073578
H	3.651846	-3.229336	-1.909447
H	3.420734	-3.163200	-0.150013
H	1.827716	-0.796155	-2.609540
H	0.300342	-1.701831	-2.788813
H	1.802297	-2.355050	-3.475540
H	1.405865	-4.540431	-2.105368
H	-0.073692	-3.835601	-1.425293
H	1.206365	-4.437647	-0.345267
H	2.410451	3.413062	2.232980
H	3.919982	3.888940	1.459435
H	2.431316	5.052828	-0.063487
H	1.093223	3.972261	0.345251
H	1.488631	2.174914	-2.804882
H	0.880063	3.796240	-2.406566
H	0.427076	2.408302	-1.397814
H	4.508110	3.868826	-1.318859
H	3.354405	4.536117	-2.490301
H	3.946922	2.870854	-2.677267

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Au	-0.527979	-1.333722	-2.796161
Cl	-1.505461	-3.112954	-1.591549
Cl	-2.533157	-0.910590	-3.892969
Cl	0.533655	0.430711	-3.959424
C	1.176806	-1.652204	-1.801781
N	2.140476	-1.793336	-1.181531
C	3.315635	-1.877577	-0.321555
C	4.029969	-0.516741	-0.406493
C	4.192782	-3.024094	-0.852123
C	2.804802	-2.156561	1.103759
O	0.973749	0.664446	0.507899
C	-1.320160	0.687323	0.085350
C	-0.062754	2.507290	-0.634103
N	-0.109200	1.171096	0.038914
H	-1.493279	-0.263875	0.572617
C	-2.334004	1.601556	-0.526675
H	0.759938	2.482445	-1.350418
H	0.164718	3.242266	0.144442
C	-1.455814	2.653687	-1.262946
H	2.130831	-1.359662	1.426341
H	3.664603	-2.197555	1.778991
H	2.280725	-3.115549	1.149765

H	3.360868	0.281318	-0.076156
H	4.360990	-0.312176	-1.428805
H	4.908957	-0.544504	0.244275
H	5.080109	-3.107955	-0.218564
H	4.517354	-2.830747	-1.878460
H	3.656080	-3.976561	-0.823668
H	-3.006383	1.072328	-1.209541
H	-2.962190	2.057308	0.252256
H	-1.849922	3.667352	-1.161121
H	-1.409284	2.413446	-2.327846

1•••N3

Au	-1.167910	0.015031	-3.140900
Cl	-2.590883	-1.483619	-1.995925
Cl	-2.973320	1.333564	-3.764183
Cl	0.330582	1.476316	-4.235615
C	0.391235	-1.099838	-2.562741
N	1.289128	-1.718977	-2.183147
C	2.423060	-2.444522	-1.621406
C	3.568534	-1.429167	-1.462098
C	2.781769	-3.568409	-2.608595
C	1.969467	-2.997024	-0.258112
O	1.333672	0.284263	0.394070
C	-0.855928	1.121338	0.443829
C	0.828824	2.693371	0.424457
N	0.438713	1.225990	0.391085
H	-1.403485	0.191944	0.498460
O	-1.525704	2.290245	0.453172
C	1.878909	2.982326	-0.643680
C	1.342411	3.005863	1.836217
C	-0.546536	3.320597	0.121082
H	1.668230	-2.177304	0.398377
H	2.808097	-3.533574	0.195511
H	1.134703	-3.693812	-0.376971
H	3.255944	-0.615169	-0.803994
H	3.866302	-1.020092	-2.431966
H	4.428798	-1.941942	-1.021775
H	3.632898	-4.126699	-2.208963
H	3.062326	-3.161970	-3.584414
H	1.945147	-4.260390	-2.740008
H	-0.774140	4.197973	0.727503
H	-0.667519	3.554732	-0.941612
H	2.806300	2.455380	-0.406972
H	2.087680	4.056993	-0.671010
H	1.543333	2.666436	-1.635402
H	0.560756	2.849595	2.586587
H	1.671307	4.048755	1.890005
H	2.189630	2.358178	2.075582

1•••N4

Au	-0.912814	0.666782	-3.381899
Cl	-2.390784	-1.070848	-2.754950

Cl	-2.691181	2.114543	-3.743483
Cl	0.635983	2.342365	-3.979634
C	0.618373	-0.560477	-2.992819
N	1.494037	-1.258414	-2.710285
C	2.581403	-2.107788	-2.237801
C	3.672805	-1.173235	-1.685827
C	3.080502	-2.927305	-3.439958
C	1.997372	-3.005126	-1.131592
O	1.117774	0.003540	0.273921
C	-1.073239	0.802653	0.404006
C	0.607308	2.183959	1.217905
N	0.212339	0.856323	0.582107
H	-1.546729	-0.046377	-0.070549
C	-1.715093	2.060450	0.886319
C	1.351667	3.020740	0.180151
C	1.411331	1.927301	2.483008
O	-0.650902	2.758234	1.553106
H	1.600342	-2.392991	-0.318485
H	2.796131	-3.644611	-0.744546
H	1.201279	-3.643218	-1.525691
H	3.272699	-0.563201	-0.872686
H	4.062312	-0.519657	-2.471573
H	4.494688	-1.786254	-1.304461
H	3.898105	-3.573289	-3.108241
H	3.455050	-2.275344	-4.234110
H	2.284286	-3.557997	-3.845259
H	-2.120835	2.661816	0.058823
H	-2.521816	1.883285	1.607339
H	2.273289	2.518173	-0.123361
H	1.601098	3.990078	0.619861
H	0.733769	3.187502	-0.706145
H	0.834588	1.316502	3.182257
H	1.641015	2.884287	2.959028
H	2.343427	1.412936	2.239293

1•••N5

Au	-0.683186	-1.554307	-2.655820
Cl	-1.602571	-3.150291	-1.176727
Cl	-2.747911	-1.236304	-3.673871
Cl	0.320931	0.025298	-4.099802
C	1.073194	-1.763284	-1.723959
N	2.066653	-1.826197	-1.138198
C	3.288140	-1.834647	-0.339804
C	3.841362	-0.398129	-0.353910
C	4.257697	-2.831136	-0.998184
C	2.892613	-2.273567	1.081494
O	0.666124	0.424932	0.801682
C	-1.505228	0.671075	-0.026424
O	0.071995	2.261583	-0.399501
N	-0.258517	0.983381	0.191580
H	-1.887549	-0.253257	0.381064

C	-2.221497	1.743437	-0.780754
C	-1.027429	2.574049	-1.291728
H	2.168269	-1.577581	1.509813
H	3.791220	-2.281137	1.705083
H	2.464474	-3.279915	1.076560
H	3.108493	0.297044	0.062393
H	4.095453	-0.087196	-1.371159
H	4.749616	-0.370326	0.255279
H	5.184975	-2.851908	-0.418997
H	4.496206	-2.530662	-2.022225
H	3.836602	-3.840330	-1.013356
H	-2.824041	1.346157	-1.602527
H	-2.885199	2.317179	-0.119171
H	-1.181679	3.652668	-1.235825
H	-0.740829	2.280801	-2.306597

1Ph

N	0.296391	0.089145	-0.160220
C	-0.858899	0.055937	-0.260937
Au	-2.848910	-0.001265	-0.434430
Cl	-2.693839	-2.341591	-0.733427
Cl	-2.881547	2.342581	-0.124759
Cl	-5.152351	-0.067475	-0.635250
C	1.678270	0.128867	-0.039751
C	2.304014	1.360096	0.194913
C	2.404322	-1.063504	-0.156579
C	3.692080	1.388291	0.314200
C	3.791425	-1.011923	-0.033955
C	4.434184	0.208089	0.200479
H	1.708658	2.262637	0.279534
H	4.193119	2.333393	0.496140
H	5.515066	0.239160	0.294696
H	4.369428	-1.926008	-0.121838
H	1.884998	-1.998089	-0.338356

1PhCl

N	0.294857	-0.034764	-0.160386
C	-0.860869	-0.067987	-0.261129
Au	-2.850575	-0.125185	-0.434561
Cl	-2.693608	-2.464949	-0.737820
Cl	-2.882054	2.218187	-0.120365
Cl	-5.153011	-0.191373	-0.635250
C	1.674311	0.004889	-0.040138
C	2.304757	1.233868	0.193611
C	2.404697	-1.184977	-0.155228
C	3.690601	1.269883	0.313887
C	3.790227	-1.141335	-0.033866
C	4.422962	0.083892	0.199526
H	1.714986	2.139974	0.278459
H	4.199929	2.209423	0.494892
Cl	6.161380	0.133858	0.351106
H	4.375900	-2.049402	-0.119388

H	1.891111	-2.122793	-0.336300

1PhCl$_3$

N	0.612593	-0.063115	-0.089423
C	-0.544217	-0.096381	-0.190258
Au	-2.535444	-0.153619	-0.363881
Cl	-2.416675	-2.513332	-0.326419
Cl	-2.546704	2.209184	-0.391961
Cl	-4.836448	-0.219759	-0.564538
C	1.980253	-0.023806	0.029794
C	2.630489	1.187830	0.344044
C	2.743022	-1.194828	-0.161288
C	4.015911	1.228605	0.465422
C	4.128604	-1.155955	-0.041125
C	4.747982	0.055747	0.271050
Cl	1.701632	2.631400	0.581512
H	4.512174	2.160105	0.707302
Cl	6.482614	0.105606	0.422253
H	4.711493	-2.056438	-0.188938
Cl	1.953030	-2.687803	-0.548585

1PhCl$_3$•••N1

Au	-1.643078	3.233170	1.776732
Cl	-0.567185	3.159469	3.879029
Cl	-1.646129	5.549527	1.809921
Cl	-2.700844	3.217542	-0.335546
C	-1.583287	1.235626	1.725433
N	-1.479191	0.083084	1.659219
O	1.023490	-0.040790	0.123175
C	1.769991	2.090303	0.678474
C	1.634915	1.551455	-1.612388
N	1.430988	1.143116	-0.153259
H	1.734015	1.904744	1.744675
C	2.248278	3.325714	-0.014785
C	0.408767	1.142245	-2.424734
C	2.899386	0.831170	-2.101604
C	1.815306	3.079894	-1.481761
H	1.805503	4.234370	0.405613
H	3.338276	3.430049	0.087000
H	2.540778	3.462852	-2.204292
H	0.860324	3.579861	-1.669012
H	0.281911	0.057207	-2.410451
H	0.539633	1.468221	-3.461820
H	-0.499436	1.607583	-2.030619
H	3.784733	1.153134	-1.543140
H	3.062612	1.053462	-3.160854
H	2.788602	-0.250125	-1.983695
C	-1.755859	-3.394927	0.491501
C	-1.935066	-2.017950	0.570616
C	-0.955606	-4.026888	1.444045
C	-1.317103	-1.277375	1.596498
C	-0.337449	-3.318063	2.474559

C	-0.520206	-1.941163	2.549886
H	-2.230888	-3.960181	-0.300272
Cl	-2.928107	-1.212692	-0.601576
Cl	0.232006	-1.045347	3.828222
H	0.278494	-3.824484	3.206854
Cl	-0.724982	-5.753635	1.346166

1PhCl•••N1

Au	1.561693	-1.252273	0.059710
Cl	1.471732	-1.559848	-2.283034
Cl	3.880170	-1.374017	0.029454
Cl	1.563361	-0.967615	2.403469
C	-0.429434	-1.091981	0.074350
N	-1.585183	-1.011455	0.077337
O	-0.468652	1.832021	-0.391633
C	1.557953	2.242335	-1.450921
C	1.038062	3.560033	0.433068
N	0.659894	2.436843	-0.528975
H	1.386487	1.493258	-2.214013
C	2.736624	3.149469	-1.308619
C	0.773319	3.104539	1.866174
C	0.182263	4.779130	0.061441
C	2.537039	3.749712	0.106185
H	3.682880	2.607283	-1.404734
H	2.731874	3.918721	-2.094255
H	2.830800	4.801163	0.162694
H	3.143515	3.194775	0.828117
H	-0.292629	2.925585	2.025337
H	1.105490	3.885585	2.558046
H	1.314851	2.182759	2.097198
H	0.399620	5.125531	-0.954502
H	0.389787	5.599370	0.755793
H	-0.880713	4.530964	0.124393
C	-5.220096	-1.509031	0.220010
C	-3.856357	-1.785189	0.264668
C	-5.646036	-0.205099	-0.048453
C	-2.945285	-0.746931	0.039720
C	-4.731813	0.828436	-0.271865
C	-3.365468	0.563156	-0.228132
H	-5.945420	-2.296031	0.390845
H	-3.500258	-2.788719	0.469855
H	-2.623823	1.338483	-0.394329
H	-5.085628	1.832097	-0.478175
Cl	-7.360898	0.139265	-0.105395

1PhMe

N	0.280459	0.089131	-0.165650
C	-0.875253	0.055455	-0.262084
Au	-2.866010	-0.002743	-0.426482
Cl	-2.712130	-2.343580	-0.722235
Cl	-2.898715	2.341631	-0.120667
Cl	-5.171347	-0.070219	-0.616021

C	1.661100	0.129215	-0.048431
C	2.295370	1.359640	0.163675
C	2.392126	-1.061126	-0.148031
C	3.682091	1.385614	0.277558
C	3.777688	-1.006106	-0.030410
C	4.446101	0.210271	0.186554
H	1.706997	2.268216	0.232801
H	4.179869	2.337404	0.438525
C	5.945942	0.249898	0.344445
H	4.350260	-1.925541	-0.110390
H	1.877630	-2.000939	-0.316903
H	6.358657	1.204418	0.006047
H	6.428878	-0.552730	-0.219923
H	6.226168	0.125630	1.397890

1PhMe•••N1

Au	1.304804	-1.249301	0.116922
Cl	1.169946	-1.701170	-2.199409
Cl	3.618054	-1.440584	0.063464
Cl	1.350117	-0.822580	2.438233
C	-0.683042	-1.034844	0.141944
N	-1.832089	-0.893558	0.131361
O	-0.904217	2.246131	-0.513339
C	1.217272	2.091985	-1.451759
C	0.940218	3.567520	0.364797
N	0.344285	2.537051	-0.592294
H	0.905733	1.391568	-2.216445
C	2.576381	2.682283	-1.254721
C	0.484567	3.251829	1.787490
C	0.439429	4.944173	-0.094582
C	2.453883	3.361919	0.132630
H	3.361110	1.919347	-1.277600
H	2.808037	3.401062	-2.054019
H	3.001020	4.306691	0.188490
H	2.856497	2.695453	0.901146
H	-0.601780	3.333911	1.870690
H	0.946068	3.963637	2.479919
H	0.781358	2.241283	2.082958
H	0.797075	5.183226	-1.101732
H	0.802957	5.715852	0.591293
H	-0.653701	4.967260	-0.099115
C	-5.455593	-1.444087	0.294154
C	-4.088083	-1.695788	0.367827
C	-5.944950	-0.177189	-0.061895
C	-3.198368	-0.655820	0.077017
C	-5.020207	0.841334	-0.347786
C	-3.647255	0.622180	-0.281450
H	-6.153040	-2.247018	0.514454
H	-3.711340	-2.675982	0.639641
H	-2.922663	1.400145	-0.498691
H	-5.379938	1.826883	-0.630075

C	-7.428733	0.093106	-0.118531
H	-7.767335	0.596094	0.796052
H	-8.001539	-0.832680	-0.217425
H	-7.682366	0.744544	-0.960223

1Ph•••N1

Au	-1.022166	3.275204	1.326766
Cl	0.187947	3.293203	3.357296
Cl	-0.905692	5.589248	1.185990
Cl	-2.255940	3.171170	-0.683312
C	-1.079477	1.279349	1.427449
N	-1.100328	0.123595	1.490676
O	1.661683	0.636497	-0.154587
C	2.539096	2.738357	0.306927
C	2.408587	2.092269	-1.955985
N	2.156911	1.775892	-0.483594
H	2.453726	2.614613	1.379245
C	3.094688	3.910466	-0.434968
C	1.168227	1.722472	-2.766294
C	3.629855	1.268873	-2.388643
C	2.687013	3.611462	-1.899997
H	2.681694	4.856935	-0.071456
H	4.185206	3.970623	-0.307727
H	3.456203	3.906414	-2.618692
H	1.773371	4.161635	-2.143942
H	0.975407	0.648626	-2.707756
H	1.328933	1.994810	-3.814692
H	0.284299	2.254184	-2.402171
H	4.526415	1.559951	-1.831070
H	3.821650	1.427591	-3.454517
H	3.447600	0.203829	-2.221446
C	-1.998319	-3.368903	2.159745
C	-2.079259	-1.978299	2.124873
C	-0.891888	-4.022576	1.607033
C	-1.033795	-1.263232	1.527593
C	0.139997	-3.287870	1.014216
C	0.083137	-1.895392	0.965330
H	-2.798711	-3.940220	2.618670
H	-2.926949	-1.450331	2.547896
H	0.864287	-1.295079	0.510589
H	0.996449	-3.798818	0.586047
H	-0.834967	-5.106296	1.638629

1Xyl

N	-0.823548	0.054329	0.070236
C	-1.983381	0.013289	0.077418
Au	-3.981439	-0.056892	0.089580
Cl	-3.837132	-2.371595	0.546706
Cl	-4.005882	2.262059	-0.368009
Cl	-6.294335	-0.138224	0.103347
C	0.563492	0.103417	0.061675
C	1.180766	1.371825	0.095198

C	1.268563	-1.118068	0.019870
C	2.578147	1.388549	0.085117
C	2.663655	-1.035739	0.012466
C	3.311132	0.200880	0.044467
C	0.367489	2.639014	0.145019
H	3.092880	2.344098	0.110080
H	4.396231	0.239355	0.037691
H	3.244431	-1.952430	-0.019379
C	0.546547	-2.439683	-0.020444
H	-0.322137	2.712495	-0.702745
H	1.020740	3.513798	0.129021
H	-0.242135	2.688411	1.054376
H	1.260275	-3.265990	-0.012869
H	-0.069257	-2.532567	-0.922204
H	-0.125580	-2.561462	0.835765

1Xyl•••N1

Au	-3.387846	1.858809	1.517869
Cl	-2.821974	1.951838	3.812482
Cl	-4.046285	4.087991	1.548936
Cl	-3.978268	1.670588	-0.763716
C	-2.774557	-0.039426	1.473716
N	-2.441335	-1.148819	1.440705
O	-0.084120	0.926185	0.908743
C	0.153124	3.152225	1.536184
C	0.859237	2.554981	-0.632113
N	0.241074	2.153957	0.704642
H	-0.238682	2.983487	2.531633
C	0.656214	4.433297	0.954028
C	0.031167	1.954403	-1.765888
C	2.297562	2.018054	-0.642422
C	0.785603	4.096549	-0.553329
H	-0.031474	5.264730	1.139401
H	1.619772	4.713691	1.403686
H	1.658024	4.565312	-1.016426
H	-0.103989	4.448775	-1.083977
H	0.068034	0.863056	-1.733623
H	0.436046	2.292846	-2.725445
H	-1.015417	2.264781	-1.700328
H	2.904469	2.479904	0.143767
H	2.764554	2.235552	-1.608290
H	2.297783	0.935208	-0.490834
C	-2.217693	-4.688407	0.562743
C	-2.696914	-3.376283	0.593133
C	-1.089579	-5.056649	1.299034
C	-1.988170	-2.459081	1.396565
C	-0.414225	-4.119641	2.082722
C	-0.845130	-2.790915	2.153688
H	-2.734743	-5.424647	-0.045175
C	-3.911542	-2.950646	-0.190695
C	-0.133364	-1.760560	2.989552

H	0.463136	-4.416790	2.649310
H	-0.733950	-6.082031	1.260584
H	0.162552	-0.892001	2.390077
H	0.757589	-2.194450	3.449393
H	-0.780885	-1.386911	3.791855
H	-4.301010	-3.784597	-0.778691
H	-3.681087	-2.127015	-0.875172
H	-4.712375	-2.601250	0.471263

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C	-0.659451	0.942102	-0.693381
C	1.567287	0.993384	-0.214438
H	2.402874	0.457533	-0.665527
C	0.393671	-1.341456	-0.185981
C	-0.988223	-1.926765	0.134044
H	-1.679227	-1.843258	-0.706760
H	-1.432837	-1.460526	1.016865
H	-0.859681	-2.993358	0.340814
C	0.912781	-1.899142	-1.525618
H	1.910429	-1.518312	-1.768142
H	0.230684	-1.638463	-2.339069
H	0.980278	-2.989635	-1.463676
C	1.354328	-1.696937	0.963119
H	2.364913	-1.307632	0.810149
H	1.433220	-2.785651	1.019385
H	0.978847	-1.337789	1.925240
C	1.871827	1.508128	1.225958
H	1.262429	0.992000	1.969295
H	2.921749	1.319812	1.469902
C	1.557915	3.017126	1.164342
H	2.220856	3.608818	1.801656
H	0.528743	3.206459	1.485034
C	1.714772	3.382648	-0.330803
C	3.198211	3.525333	-0.728500
H	3.799218	2.658117	-0.436532
H	3.620643	4.403233	-0.230487
H	3.292197	3.657291	-1.809549
C	0.939374	4.628759	-0.760949
H	-0.115458	4.562903	-0.488489
H	1.011592	4.777638	-1.842433
H	1.368578	5.504687	-0.264800
N	0.338282	0.164389	-0.326116
N	1.237707	2.164865	-1.060863
O	-0.267372	2.154809	-0.990346
Cl	-5.005055	0.426617	-0.951668
Cl	-2.779507	1.345609	1.447927
Cl	-2.384475	0.009273	-3.067480
Au	-2.679146	0.676203	-0.820320

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Au	-2.012708	2.749149	0.823718
Cl	-0.628394	2.174435	2.712844

Cl	-4.110903	2.715762	2.111960
Cl	-3.076359	3.258786	-1.269079
C	1.004546	2.552746	-0.546162
N	1.481823	1.282873	-0.579889
O	-0.037614	3.126535	-0.278449
C	0.684653	-0.044387	-0.695340
C	-0.751291	0.262813	-1.133134
C	1.331770	-0.899312	-1.804281
C	0.694103	-0.765895	0.659208
C	2.896845	1.265165	-0.496269
N	3.576015	0.214618	-0.224236
C	5.012769	0.559977	-0.136884
C	3.703728	2.547602	-0.664259
C	5.410928	0.565514	1.351545
C	5.834799	-0.488837	-0.896992
C	5.130848	1.979993	-0.768370
H	1.354459	-0.350038	-2.752461
H	0.709171	-1.788973	-1.948227
H	2.340442	-1.217731	-1.547983
H	0.082456	-1.672921	0.578393
H	0.263569	-0.130291	1.437787
H	1.708292	-1.052450	0.943623
H	-1.231332	-0.683086	-1.403772
H	-0.795935	0.925241	-2.001778
H	-1.345563	0.710099	-0.337380
H	3.383735	3.125899	-1.534409
H	3.565340	3.195804	0.208036
H	5.877367	2.602366	-0.264940
H	5.425283	1.894804	-1.821053
H	5.177213	-0.400652	1.809957
H	4.862500	1.337866	1.901002
H	6.484970	0.756085	1.464619
H	5.702142	-1.480321	-0.451115
H	6.902084	-0.237271	-0.870560
H	5.519290	-0.542267	-1.944590

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Au	-1.304624	1.539942	-1.551725
Cl	-2.479552	2.034190	0.490666
Cl	-3.030767	-0.032780	-2.355658
Cl	0.056640	1.285004	-3.502583
C	1.322705	2.944723	-0.329730
N	2.059515	1.917303	0.114571
O	0.212473	3.035308	-0.850174
C	3.489870	2.217979	0.522064
C	3.561893	3.638462	1.107522
C	3.928106	1.219915	1.607987
C	4.397783	2.107749	-0.716040
C	1.632847	0.535480	0.018392
N	2.224763	-0.293577	-0.742315
C	1.608571	-1.637709	-0.568200

C	0.550782	-0.014683	0.923221
C	1.304805	-2.220731	-1.953452
C	2.621990	-2.525546	0.178032
C	0.317195	-1.391972	0.277625
H	3.266114	1.271033	2.479207
H	4.940232	1.476544	1.936919
H	3.947146	0.193716	1.236572
H	5.438446	2.315881	-0.438991
H	4.087121	2.833257	-1.474535
H	4.332383	1.108798	-1.152183
H	4.586850	3.822611	1.450249
H	2.883518	3.749367	1.959475
H	3.298885	4.395241	0.366117
H	0.959710	-0.079804	1.943205
H	-0.342872	0.611412	0.978890
H	-0.558516	-1.344987	-0.376897
H	0.145940	-2.186612	1.010775
H	2.230455	-2.369375	-2.520720
H	0.659143	-1.546461	-2.522286
H	0.798487	-3.188259	-1.850848
H	3.575028	-2.556569	-0.361305
H	2.237713	-3.548818	0.262053
H	2.813111	-2.151624	1.190978

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C	0.258183	1.961842	-0.991246
C	0.074391	-0.281522	-0.151892
C	0.893337	-1.560236	-0.051126
H	0.935889	-1.897930	0.988493
H	1.916778	-1.426154	-0.402840
C	0.057813	-2.519336	-0.910643
H	0.354277	-2.434533	-1.962040
H	0.161507	-3.564666	-0.609307
C	-1.387609	-2.001945	-0.725631
C	-2.263811	-2.237314	-1.956093
H	-3.279351	-1.866878	-1.795429
H	-2.321725	-3.312517	-2.157117
H	-1.842077	-1.745999	-2.838708
C	-2.030537	-2.595142	0.540200
H	-2.990685	-2.121263	0.746097
H	-1.386126	-2.466660	1.416535
H	-2.192353	-3.667939	0.391473
C	1.856945	1.359381	0.766003
N	0.617813	1.000691	-0.054068
N	-1.145017	-0.520667	-0.530790
O	-0.844704	2.056585	-1.524675
Cl	-3.854882	2.887460	-1.238147
Cl	-4.478218	-0.087790	0.267956
Au	-2.584929	0.990775	-0.740668
C	1.938356	0.486110	2.028755
C	1.672187	2.822481	1.217094

C	3.123530	1.234269	-0.095563
H	0.971343	0.430866	2.538901
H	2.648367	0.949862	2.719003
H	2.299943	-0.524107	1.834447
H	2.536916	3.120830	1.817544
H	0.772215	2.932421	1.830065
H	1.596877	3.500382	0.363979
H	3.299934	0.206161	-0.424408
H	3.996161	1.551358	0.484316
H	3.045704	1.872886	-0.979630

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Au	-2.240261	-0.352286	1.184098
Cl	-1.556841	0.344731	-0.881739
Cl	-4.398101	0.194633	0.903368
C	0.692337	-1.180077	1.194558
N	1.695270	-1.396107	0.647677
O	-0.340355	-0.976585	1.833699
C	3.784793	-2.577767	0.941344
C	2.640050	-2.436277	-1.327865
C	2.975017	-1.691565	-0.024481
C	3.675861	-0.350622	-0.290828
H	3.076916	0.286580	-0.947049
H	4.630636	-0.548023	-0.785276
H	3.877821	0.184248	0.640964
H	4.741847	-2.814157	0.468543
H	3.264186	-3.515804	1.150879
H	3.985805	-2.059238	1.882401
H	3.575689	-2.674099	-1.840807
H	2.033213	-1.816814	-1.993723
H	2.112446	-3.372449	-1.126933

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Au	-0.820625	0.580761	-0.494119
Cl	-3.041694	0.441957	-1.273018
N	1.414008	-3.031692	-1.202639
C	0.426606	-2.416565	-0.957170
O	-0.630113	-1.869020	-0.809486
C	2.802444	-3.361529	-0.862172
C	2.969323	-3.299723	0.665568
C	3.077726	-4.777993	-1.390832
C	3.711587	-2.332411	-1.557044
H	2.417705	-5.508131	-0.912801
H	4.114448	-5.056377	-1.178336
H	2.920059	-4.825479	-2.472301
H	4.759491	-2.564531	-1.340581
H	3.494006	-1.322285	-1.199931
H	3.567975	-2.359819	-2.641237
H	4.000548	-3.551751	0.933527
H	2.302393	-4.014103	1.158320
H	2.748372	-2.295243	1.037553
C	-0.506301	3.430384	-1.209020

N	-0.893793	2.687603	-0.311004
C	-1.453001	3.325876	0.982528
C	-0.649457	4.880619	-0.767071
C	-2.980975	3.285008	0.923067
C	-0.908962	2.633635	2.224576
C	-0.881395	4.760407	0.767860
H	0.225842	5.474463	-1.038493
H	-1.506609	5.302096	-1.305155
H	-1.552725	5.525537	1.169251
H	0.077073	4.849720	1.289600
H	-3.351411	2.258318	0.887102
H	-3.363608	3.809958	0.043015
H	-3.380714	3.771826	1.819461
H	-1.315445	1.623339	2.330350
H	-1.208684	3.209676	3.107131
H	0.181127	2.565508	2.200362
Cl	1.416677	0.510481	0.331987

2Bz

C	-3.906263	-0.295893	-0.617760
C	-1.883700	0.057573	0.405651
H	-0.986449	-0.560431	0.333631
C	-1.922947	0.954027	1.673689
H	-2.610263	0.556984	2.425154
H	-0.928184	0.993750	2.126974
C	-2.362210	2.328710	1.136658
H	-1.972380	3.156532	1.735252
H	-3.454586	2.406799	1.128490
C	-1.824809	2.354951	-0.313661
C	-0.303710	2.608969	-0.355202
H	0.260949	1.897769	0.255649
H	-0.094982	3.613973	0.024155
H	0.063596	2.537829	-1.382049
C	-2.540237	3.346929	-1.231797
H	-3.623358	3.215375	-1.207841
H	-2.198356	3.236879	-2.265172
H	-2.310311	4.364691	-0.901824
N	-3.070289	-0.806267	0.256148
N	-1.983906	0.939926	-0.795790
O	-3.424871	0.756534	-1.216652
Cl	-7.995572	-1.571254	-1.516593
Cl	-6.488318	0.457001	0.760660
Cl	-4.923093	-2.251308	-2.772957
Au	-5.801108	-0.902274	-1.050390
C	-3.281961	-2.005429	1.084529
H	-4.262704	-2.400598	0.810932
H	-3.333482	-1.693760	2.132417
C	-1.029993	-4.625665	-0.533501
C	-2.021934	-3.659337	-0.361800
C	-0.204523	-4.987038	0.536828
C	-2.193216	-3.041139	0.886271

C	-0.374832	-4.379287	1.782306
C	-1.365593	-3.407574	1.954453
H	-0.907420	-5.102672	-1.501235
H	-2.668913	-3.390742	-1.193372
H	-1.500417	-2.941203	2.927768
H	0.258329	-4.659408	2.618934
H	0.563188	-5.742980	0.400744

2Bz•••N1

C	0.561300	0.029538	0.715185
C	-0.776707	1.883170	0.938231
C	-0.080204	3.258512	1.121319
H	0.580123	3.487589	0.284423
H	-0.841010	4.043671	1.161832
C	0.666638	3.123385	2.459618
H	0.785134	4.081467	2.973666
H	1.666881	2.703985	2.304083
C	-0.196472	2.130016	3.271094
C	-1.463479	2.806981	3.834152
H	-2.062791	3.292001	3.057776
H	-1.172304	3.572617	4.560124
H	-2.094472	2.069232	4.336627
C	0.553167	1.419217	4.399134
H	1.474848	0.954673	4.044343
H	-0.072152	0.646949	4.857206
H	0.811254	2.151828	5.170143
N	-0.067935	0.951812	0.031695
N	-0.711261	1.157861	2.248433
O	0.364832	0.124843	2.002299
Cl	3.087910	-3.245894	-0.740776
Cl	3.604710	-0.097546	0.398911
Cl	-0.237036	-2.743388	-0.322332
Au	1.735244	-1.490685	0.032491
C	-4.032767	-0.908444	-2.154417
C	-4.756033	-2.211208	-2.047279
H	-5.751894	-2.142694	-2.508236
H	-4.226681	-3.019816	-2.562305
C	-4.827833	-2.436355	-0.516002
H	-4.026538	-3.114116	-0.208310
H	-5.777546	-2.876217	-0.200971
C	-4.605658	-1.047936	0.126839
C	-3.672353	-1.080884	1.334186
H	-2.718287	-1.553545	1.083955
H	-4.143347	-1.662375	2.133742
H	-3.474932	-0.073769	1.707098
C	-5.914034	-0.309891	0.443792
H	-6.599410	-0.322727	-0.410466
H	-5.708226	0.731003	0.707339
H	-6.411697	-0.793142	1.290388
N	-3.932682	-0.287183	-1.014798
H	-3.640083	-0.442488	-3.049565

O	-3.403896	0.864240	-0.792353
H	-1.815406	1.942817	0.604473
C	-0.221690	1.006802	-1.437459
H	-1.299341	0.960377	-1.624352
H	0.234838	0.093037	-1.823487
C	0.097900	4.305390	-3.324185
C	-0.447236	3.182235	-2.693898
C	1.482027	4.489028	-3.348603
C	0.385943	2.234664	-2.086047
C	2.319749	3.544234	-2.745316
C	1.776471	2.421029	-2.119649
H	-0.558024	5.032561	-3.794078
H	-1.524826	3.039295	-2.673883
H	2.434897	1.693168	-1.652190
H	3.397289	3.677960	-2.767222
H	1.907800	5.359829	-3.838647

2Cy

C	-2.717893	-0.306024	0.087279
C	-0.450903	0.008197	0.210123
H	0.293313	-0.335001	-0.512901
C	0.139065	0.276884	1.620954
H	-0.095203	-0.537385	2.311738
H	1.228755	0.352120	1.558060
C	-0.500355	1.614922	2.033453
H	0.129735	2.186349	2.720502
H	-1.464654	1.446562	2.524612
C	-0.717862	2.354755	0.692047
C	0.598676	2.941246	0.143405
H	1.387744	2.189080	0.044508
H	0.961310	3.717721	0.824089
H	0.432746	3.386656	-0.840791
C	-1.788078	3.446215	0.745314
H	-2.726257	3.076454	1.162449
H	-1.984172	3.848414	-0.253019
H	-1.428556	4.263269	1.378440
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O	-2.550053	0.974122	-0.118940
Cl	-6.891886	-1.603257	0.414666
Cl	-4.548819	-0.313759	2.506167
Cl	-4.602776	-1.473852	-2.072687
Au	-4.657714	-0.923790	0.220453
H	-2.693289	-5.371823	-0.465467
C	-1.700250	-5.308861	-0.000460
C	-1.828350	-4.631781	1.373109
C	-0.756062	-4.525098	-0.925209
H	-1.342154	-6.338078	0.117845
C	-2.276118	-3.165735	1.240840
C	-1.179746	-3.051767	-1.055581
C	-1.297767	-2.404876	0.336938

H	0.268750	-4.577024	-0.528593
H	-0.727155	-4.982250	-1.920541
H	-0.455210	-2.499661	-1.666917
H	-2.149060	-2.975201	-1.561296
H	-0.312611	-2.439546	0.819426
H	-3.281190	-3.144167	0.805320
H	-2.343213	-2.682598	2.220887
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H	-0.862167	-4.675594	1.897437

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C	1.154230	1.498879	1.957131
H	0.555438	0.943470	2.680408
H	2.202089	1.427283	2.259557
C	0.687669	2.962591	1.822592
H	1.241016	3.641089	2.478200
H	-0.375208	3.052270	2.069391
C	0.906573	3.300389	0.328790
C	2.393061	3.581997	0.024683
H	3.049243	2.765516	0.341108
H	2.698943	4.490542	0.553216
H	2.534903	3.738248	-1.048429
C	0.038351	4.447120	-0.191211
H	-1.019250	4.283659	0.024567
H	0.158583	4.567117	-1.272165
H	0.348354	5.378092	0.293833
N	-0.125528	-0.026813	0.351853
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Cl	-5.288517	-0.818437	-0.522589
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Cl	-2.513166	-0.796375	-2.478041
Au	-3.078772	-0.051327	-0.311730
C	6.185383	-0.529393	1.123119
C	7.510629	-0.869306	0.520688
H	8.246844	-0.079125	0.726956
H	7.927743	-1.797054	0.926731
C	7.178302	-0.981564	-0.988684
H	7.020318	-2.031993	-1.252566
H	7.979518	-0.597156	-1.624943
C	5.864736	-0.192024	-1.187783
C	4.864984	-0.883201	-2.111798
H	4.645707	-1.898184	-1.766055
H	5.288489	-0.947820	-3.119146
H	3.928902	-0.322756	-2.162345
C	6.094675	1.267954	-1.601251
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H	5.160239	1.831387	-1.539797
H	6.455975	1.304356	-2.633576

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H	1.927924	0.455238	0.161596
H	-0.607138	-3.698811	2.244931
C	0.423021	-3.318480	2.281073
C	0.409001	-1.797258	2.048595
C	1.274458	-4.047965	1.230986
H	0.795321	-3.527130	3.290589
C	-0.063888	-1.482114	0.621405
C	0.812351	-3.708020	-0.194147
C	0.796421	-2.189829	-0.440660
H	2.327749	-3.755768	1.351796
H	1.227964	-5.130945	1.395327
H	1.461197	-4.190220	-0.934466
H	-0.196650	-4.110724	-0.357703
H	1.822227	-1.800601	-0.396362
H	0.395711	-1.964630	-1.434446
H	-1.097525	-1.826752	0.514927
H	-0.251193	-1.309223	2.773704
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C	-1.197898	-0.555142	-0.957629
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C	-1.962038	-3.213891	0.211032
H	-1.906789	-3.433259	-0.857350
H	-2.895626	-2.684888	0.419207
H	-1.988146	-4.174649	0.733446
C	0.568896	-3.103952	0.241433
H	1.450369	-2.573030	0.613057
H	0.604622	-3.141418	-0.850703
H	0.601460	-4.130249	0.621781
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H	0.059901	-1.843740	2.683272
H	-0.730496	-3.413384	2.625113
H	-1.719262	-1.950178	2.616141
C	-0.859452	0.842458	1.939056
H	-1.783234	0.310290	2.170403
H	-0.288510	0.934704	2.867460
C	-1.130710	2.215986	1.292893
H	-1.167508	3.025397	2.027101
H	-2.085937	2.206075	0.758550
C	0.026320	2.406046	0.286093
C	1.334775	2.822550	0.988831
H	1.629122	2.128144	1.780878
H	1.196932	3.811506	1.436421
H	2.156535	2.877596	0.269965
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N	-0.736816	-1.016706	0.180786
N	0.286662	1.019471	-0.226511
O	-0.802295	0.673963	-1.207798
Cl	-3.740322	-2.161687	-4.148090
Cl	-4.243126	-0.466472	-1.250281
Cl	-0.408255	-2.089249	-3.486675
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O	3.031491	-0.780294	1.238358
H	0.939211	-0.306365	1.274261
H	3.893393	-0.824653	1.686121
H	3.203164	-0.527919	0.309967
O	5.617524	-0.959380	2.538467
H	6.105601	-1.788668	2.458737
H	6.268808	-0.252437	2.447634
O	2.824499	0.204511	-1.402683
H	1.942878	0.558612	-1.160763
H	2.688830	-0.328073	-2.197184

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C	-0.656385	0.870598	-0.728642
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C	0.397487	-1.323431	-0.165240
C	-1.040611	-1.806859	0.079784
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H	-1.466810	-1.332765	0.968439
H	-1.028986	-2.891419	0.231141
C	0.947580	-1.960602	-1.458817
H	1.973336	-1.637594	-1.666016
H	0.322351	-1.684284	-2.312773
H	0.954312	-3.052255	-1.370470
C	1.275753	-1.728513	1.032959
H	2.313602	-1.400371	0.918416
H	1.284604	-2.819400	1.117562
H	0.883750	-1.321421	1.969792
C	2.023600	1.477861	1.155096
H	1.515290	0.899491	1.927916
H	3.101427	1.367006	1.317623
C	1.605524	2.958356	1.153160
H	2.226375	3.577087	1.808704
H	0.565343	3.063239	1.480101
C	1.721062	3.369319	-0.334065
C	3.188950	3.653809	-0.724004
H	3.855726	2.820877	-0.478638
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H	3.262472	3.837970	-1.799407
C	0.857304	4.574128	-0.717288
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N	0.395378	0.157457	-0.332388
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O	-0.302236	2.064631	-1.059577

2Me

C	0.074635	1.478036	-0.269005
C	2.172989	1.258691	-1.172131
H	2.425663	0.953835	-2.191542
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H	3.151157	0.174247	0.475703
H	4.266946	0.876228	-0.694634
C	3.359336	2.362846	0.642054
H	4.358491	2.602302	1.015999
H	2.685273	2.304216	1.503143
C	2.842531	3.424583	-0.356885
C	3.922038	3.813293	-1.388215
H	4.331784	2.948903	-1.920409
H	4.750000	4.310953	-0.874051
H	3.506152	4.499464	-2.130237
C	2.278008	4.684305	0.301572
H	1.532179	4.446265	1.061932
H	1.819109	5.340860	-0.443490
H	3.095813	5.230618	0.781360
N	0.912137	0.604529	-0.778509
N	1.795738	2.703334	-1.160676
O	0.514754	2.700898	-0.359243
Cl	-3.727900	0.716626	1.753883
Cl	-0.460446	0.991413	2.667621
Cl	-2.743029	1.201169	-1.455763
Au	-1.701550	1.121794	0.656037
C	0.723677	-0.838824	-0.875893
H	1.437780	-1.360037	-0.232662
H	0.865516	-1.150371	-1.914535
H	-0.290049	-1.085906	-0.563772

2Me•••N1

C	-0.481959	0.215823	0.127226
C	0.784381	1.508742	1.544218
C	0.046430	2.284235	2.665126
H	-0.482246	1.606340	3.340169
H	0.772820	2.839226	3.265789
C	-0.898688	3.224491	1.898451
H	-1.138016	4.131653	2.460334
H	-1.841546	2.717603	1.664845
C	-0.133655	3.533266	0.590329
C	1.002287	4.551192	0.821551
H	1.705055	4.229442	1.596053
H	0.574813	5.509498	1.133097
H	1.566596	4.702229	-0.102273
C	-1.025112	4.006148	-0.559002
H	-1.864158	3.329157	-0.728498

H	-0.452768	4.091167	-1.487616
H	-1.424886	4.994687	-0.312491
N	0.179664	0.192715	1.254350
N	0.575966	2.247810	0.256729
O	-0.388875	1.361000	-0.493451
Cl	-2.911831	-2.964859	-1.652970
Cl	-3.459671	-0.296039	0.377592
Cl	0.377005	-2.134277	-1.666236
Au	-1.600512	-1.266071	-0.705567
C	4.150190	-2.393614	0.964891
C	4.854748	-3.026871	-0.190699
H	5.871567	-3.333632	0.093966
H	4.341649	-3.927452	-0.543956
C	4.853993	-1.895213	-1.248745
H	4.020325	-2.043727	-1.941097
H	5.776437	-1.866815	-1.834508
C	4.641957	-0.583422	-0.459519
C	3.679168	0.386229	-1.139297
H	2.721534	-0.094910	-1.357322
H	4.117031	0.718902	-2.086231
H	3.497818	1.263475	-0.514563
C	5.955908	0.106617	-0.066674
H	6.661074	-0.600796	0.382486
H	5.764026	0.908262	0.651583
H	6.423416	0.539035	-0.956805
N	4.012897	-1.105858	0.831903
H	3.797439	-2.874971	1.868486
O	3.485529	-0.282156	1.667397
H	1.851482	1.353431	1.720945
C	0.347435	-0.938983	2.163253
H	1.417811	-1.057441	2.353562
H	-0.053355	-1.833704	1.688516
H	-0.189884	-0.753873	3.097518

2•••N1

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C	-1.097865	-2.266586	1.480088
H	-1.777290	-2.491995	0.655701
H	-1.612929	-1.636208	2.209500
H	-0.852287	-3.216854	1.963596
C	0.823617	-2.453412	-0.149714
H	1.779671	-2.034501	-0.478112
H	0.138437	-2.489145	-1.000963
H	1.005233	-3.476957	0.193738
C	1.191530	-1.557125	2.189238
H	2.152362	-1.110656	1.919075
H	1.387371	-2.577727	2.530070
H	0.760002	-1.002678	3.027539
C	1.278488	1.647731	1.637439

H	0.690834	1.274683	2.477976
H	2.330758	1.645213	1.933230
C	0.807177	3.041206	1.174953
H	1.376558	3.852142	1.638217
H	-0.249151	3.191701	1.419636
C	0.988375	3.016456	-0.361767
C	2.465896	3.213834	-0.760179
H	3.132447	2.502491	-0.263010
H	2.779107	4.225311	-0.482436
H	2.583720	3.097047	-1.841128
C	0.103752	4.009320	-1.116995
H	-0.949203	3.895521	-0.852463
H	0.207196	3.878000	-2.198434
H	0.413257	5.028297	-0.863911
N	-0.010993	-0.232249	0.472244
N	0.677610	1.605087	-0.750022
O	-0.823365	1.436733	-0.679868
Cl	-5.320145	-0.810537	-0.267713
Cl	-3.328555	0.937269	1.862250
Cl	-2.573930	-1.407299	-2.171216
Au	-3.042675	-0.246965	-0.166494
C	6.250179	-0.502129	1.433328
C	7.607794	-0.958995	1.005987
H	8.327288	-0.128286	1.039027
H	8.007673	-1.743339	1.657465
C	7.357343	-1.460800	-0.438412
H	7.218255	-2.546454	-0.430940
H	8.189262	-1.237826	-1.111244
C	6.052625	-0.772786	-0.899765
C	5.108829	-1.695326	-1.667408
H	4.869872	-2.589579	-1.083461
H	5.590614	-2.011562	-2.598094
H	4.177391	-1.181301	-1.914733
C	6.297458	0.537973	-1.659513
H	7.001081	1.184390	-1.124539
H	5.358597	1.081183	-1.793991
H	6.716196	0.317747	-2.646322
N	5.413720	-0.404220	0.439228
H	5.927763	-0.215824	2.426597
O	4.198294	0.004280	0.473209
H	2.028539	0.228992	0.106132

2N2

C	1.134302	-0.620480	-1.079990
C	2.524752	-0.191761	0.682509
H	3.383147	-0.763004	1.039019
C	1.291968	-2.498461	0.654036
C	-0.062123	-3.063215	0.202562
H	-0.072019	-3.322028	-0.857589
H	-0.882277	-2.372236	0.413645
H	-0.242749	-3.986769	0.760517

C	2.441812	-3.401817	0.167645
H	3.418101	-3.032575	0.499183
H	2.443394	-3.466570	-0.923572
H	2.311185	-4.408668	0.575998
C	1.290609	-2.398047	2.189680
H	2.221180	-1.988628	2.592624
H	1.179987	-3.406579	2.596118
H	0.451909	-1.798166	2.553416
C	1.936444	0.767339	1.759924
H	0.990433	0.397383	2.156451
H	2.643008	0.846906	2.593381
C	1.784979	2.117631	1.030079
H	1.908856	2.971687	1.700707
H	0.800724	2.196491	0.558786
C	2.883965	2.045754	-0.037956
H	3.873041	2.267901	0.380836
H	2.736853	2.681973	-0.912034
N	1.537785	-1.121021	0.070409
N	2.950618	0.636698	-0.475950
O	1.793134	0.457842	-1.420163
Cl	-2.068894	-1.619484	-3.900906
Cl	-1.769800	0.265175	-1.089500
Cl	1.194956	-2.467655	-3.554979
Au	-0.352720	-1.116285	-2.389245

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C	0.459854	-0.276200	1.260572
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H	-1.198122	-3.573847	-1.060640
H	-2.137660	-3.239050	0.413379
H	-1.040225	-4.628334	0.335440
C	1.315543	-3.142452	-0.101752
H	2.160723	-2.592658	0.323941
H	1.248190	-2.933285	-1.172670
H	1.502049	-4.213348	0.029681
C	0.100467	-3.063151	2.110312
H	0.901132	-2.500019	2.596539
H	0.333284	-4.124063	2.232723
H	-0.843106	-2.868452	2.627623
C	-0.322777	0.108772	2.549809
H	-1.048643	-0.654571	2.830652
H	0.389583	0.214271	3.375205
C	-0.986128	1.459716	2.215459
H	-1.108165	2.096381	3.095563
H	-1.972876	1.311030	1.765757
C	-0.016538	2.057862	1.189195
H	0.869473	2.484825	1.674622
H	-0.437715	2.812459	0.522744
N	-0.221875	-1.284933	0.397661

N	0.486938	0.928355	0.381128
O	-0.603148	0.622130	-0.608282
Cl	-3.520776	-1.919030	-3.823944
Cl	-3.877948	-0.879003	-0.609602
Cl	-0.164508	-1.608345	-3.441440
Au	-2.078680	-1.275158	-2.090096
C	4.882409	-1.310574	-0.859294
C	5.291614	-0.672078	-2.149650
H	6.353271	-0.386429	-2.122863
H	5.168969	-1.346176	-3.003959
C	4.355123	0.566489	-2.232813
H	3.497411	0.339905	-2.871972
H	4.858563	1.443358	-2.645854
C	3.885931	0.789264	-0.788761
H	2.826304	1.024207	-0.673333
H	4.477980	1.525512	-0.234897
N	4.129795	-0.534420	-0.130752
H	5.166679	-2.282721	-0.477250
O	3.640395	-0.765192	1.034894
H	1.492953	-0.584798	1.437299

2N3

C	2.892477	-0.899857	-0.443889
C	1.635894	-0.132485	1.301216
H	1.401489	-0.595296	2.259976
C	0.885018	-2.372275	0.192843
C	0.873926	-2.982422	-1.215177
H	1.817974	-3.469442	-1.466535
H	0.635828	-2.237747	-1.978968
H	0.098640	-3.753696	-1.238947
C	1.401449	-3.394325	1.222481
H	1.395346	-2.985185	2.238503
H	2.418455	-3.711229	0.976877
H	0.750795	-4.274108	1.216058
C	-0.541071	-1.909841	0.541867
H	-0.620215	-1.494943	1.549850
H	-1.198566	-2.781923	0.494074
H	-0.903671	-1.160593	-0.165368
O	0.627318	0.799157	0.989488
C	1.263504	1.983881	0.464494
H	0.609773	2.827554	0.691811
H	1.396358	1.897129	-0.620547
C	2.610667	2.022723	1.210178
C	2.438595	2.513979	2.658439
H	1.642024	1.977165	3.181793
H	2.179333	3.577026	2.651909
H	3.370629	2.384593	3.214067
C	3.707040	2.809013	0.494102
H	3.829350	2.493636	-0.543243
H	4.664110	2.691722	1.010111
H	3.443826	3.871198	0.504219

N	1.813457	-1.172789	0.258712
N	2.936305	0.556541	1.320038
O	3.556334	0.123396	0.036731
Cl	4.689035	-2.521721	-4.096716
Cl	2.481315	-0.054782	-3.334527
Cl	4.878901	-3.232436	-0.788299
Au	3.721108	-1.679316	-2.139381

2N3•••N3

C	-0.708252	0.484113	0.040230
C	1.083720	1.725384	0.738696
C	0.128008	-0.052142	2.405124
C	-1.262690	-0.573509	2.791083
H	-1.594253	-1.394540	2.151650
H	-2.014907	0.219282	2.775107
H	-1.202030	-0.966875	3.809991
C	1.128670	-1.211585	2.251703
H	2.120779	-0.837731	1.979918
H	0.786649	-1.916591	1.488970
H	1.205763	-1.743650	3.205601
C	0.605161	0.933941	3.486626
H	1.610609	1.315184	3.294005
H	0.633461	0.396972	4.438717
H	-0.074427	1.783138	3.585702
O	0.796658	2.965677	1.345000
C	0.128768	3.793294	0.374328
H	0.341179	4.832038	0.633592
H	-0.954606	3.619817	0.397232
C	0.753876	3.346042	-0.959903
C	2.172502	3.917113	-1.133468
H	2.804770	3.711814	-0.265484
H	2.112635	5.002173	-1.263805
H	2.646350	3.485194	-2.018627
C	-0.104868	3.634650	-2.189597
H	-1.126061	3.267829	-2.074516
H	0.332064	3.175368	-3.081041
H	-0.141287	4.716814	-2.349443
N	0.079335	0.677282	1.072744
N	0.942717	1.871602	-0.724644
O	-0.351335	1.187153	-1.009055
Cl	-4.280998	-1.943745	-0.727966
Cl	-3.656371	1.222567	0.320583
Cl	-0.932669	-2.440861	-0.904821
Au	-2.366504	-0.659976	-0.296685
C	5.226537	-1.613446	1.111213
O	5.771275	-2.608990	0.384760
C	5.202319	-2.494500	-0.956974
H	4.434981	-3.269176	-1.051747
H	6.007038	-2.677085	-1.670087
C	4.605185	-1.072998	-1.043884
C	3.205557	-1.042932	-1.650957

H	2.529627	-1.734447	-1.139669
H	3.257297	-1.333061	-2.705519
H	2.782886	-0.037586	-1.588875
C	5.544691	-0.058046	-1.706754
H	6.555299	-0.121290	-1.290565
H	5.166950	0.955351	-1.551067
H	5.598877	-0.250774	-2.782959
N	4.541383	-0.740871	0.437770
H	5.403122	-1.569539	2.175395
O	3.938146	0.321492	0.877036
H	2.084581	1.393142	1.015346

2N4

C	2.084328	-0.493368	-1.059337
C	2.102635	-0.451041	1.221658
H	2.360726	-1.244670	1.923588
C	0.576448	-2.227479	0.082986
C	-0.252992	-2.375890	-1.199354
H	0.350866	-2.702374	-2.048147
H	-0.770507	-1.449226	-1.459582
H	-1.005592	-3.150079	-1.023470
C	1.444337	-3.479839	0.310286
H	2.019296	-3.417109	1.240133
H	2.137332	-3.622537	-0.522894
H	0.797921	-4.360027	0.380462
C	-0.384360	-2.004716	1.264743
H	0.134740	-1.879449	2.219927
H	-1.020396	-2.888191	1.361266
H	-1.035131	-1.142180	1.096104
C	1.259900	0.692116	1.873973
H	0.248161	0.753303	1.471847
H	1.210601	0.555297	2.963030
O	1.942457	1.885507	1.526516
C	3.327550	1.567030	1.325247
C	4.068055	1.443531	2.666363
H	3.646429	0.660600	3.304174
H	3.987892	2.394862	3.198327
H	5.121994	1.211829	2.497015
C	3.943604	2.628057	0.427780
H	3.352302	2.758444	-0.478612
H	4.966056	2.352655	0.157570
H	3.966329	3.574643	0.973119
N	1.516695	-1.041531	-0.003706
N	3.332609	0.205033	0.725066
O	3.052409	0.327174	-0.740314
Cl	1.433875	-0.801286	-5.383163
Cl	0.197863	1.103200	-2.867706
Cl	3.336711	-2.420296	-3.090757
Au	1.765467	-0.652342	-3.071459

2N4•••N4

C	-1.059106	0.301849	-0.055840

C	1.128317	0.727930	0.433463
C	0.117506	-1.484445	1.359415
C	-1.232344	-1.996767	1.878270
H	-1.892323	-2.323407	1.072395
H	-1.747309	-1.245327	2.482079
H	-1.039746	-2.869504	2.509348
C	0.731406	-2.486083	0.362684
H	1.715726	-2.155453	0.016876
H	0.075462	-2.618415	-0.501751
H	0.858166	-3.454952	0.855975
C	1.058547	-1.268137	2.558839
H	2.042479	-0.893216	2.262577
H	1.213680	-2.233238	3.048667
H	0.618988	-0.589073	3.295203
C	1.340945	1.781622	1.565685
H	0.729625	1.585225	2.447585
H	2.400167	1.814325	1.847197
O	0.907389	3.013148	1.000796
C	1.057987	2.924972	-0.422026
C	2.521687	3.146239	-0.838968
H	3.191188	2.393819	-0.411632
H	2.836180	4.132095	-0.485898
H	2.612085	3.109119	-1.927541
C	0.117975	3.927133	-1.073292
H	-0.898211	3.805916	-0.697899
H	0.119921	3.802158	-2.159034
H	0.463527	4.935969	-0.834367
N	-0.037472	-0.167704	0.628354
N	0.747723	1.511534	-0.764733
O	-0.743948	1.343169	-0.783849
Cl	-5.280237	-0.833487	-0.433984
Cl	-3.476913	1.197553	1.594575
Cl	-2.387739	-1.674658	-1.994566
Au	-3.020145	-0.247671	-0.216669
C	6.395207	-0.257781	1.283517
C	7.670211	-0.761629	0.693858
H	8.410133	0.041626	0.551767
H	8.139406	-1.552086	1.292040
O	7.273047	-1.314420	-0.568371
C	5.948058	-0.911637	-0.900317
C	5.125098	-2.126437	-1.297523
H	5.135627	-2.871479	-0.498023
H	5.561979	-2.570941	-2.195476
H	4.094332	-1.835744	-1.510710
C	5.941845	0.199624	-1.946919
H	6.564958	1.038353	-1.623367
H	4.923374	0.556536	-2.117775
H	6.344484	-0.192281	-2.884391
N	5.432524	-0.340725	0.416332
H	6.229246	0.155827	2.268682

O	4.206807	0.009861	0.525847
H	2.025556	0.145670	0.231762

2N5

C	2.072273	-0.895979	-0.994472
C	2.098042	-0.177246	1.177229
H	2.418437	-0.683042	2.087598
C	0.786665	-2.364761	0.682815
C	-0.059525	-2.962575	-0.449294
H	0.550851	-3.449598	-1.211416
H	-0.698848	-2.212206	-0.921178
H	-0.703412	-3.732133	-0.013320
C	1.804639	-3.400111	1.197436
H	2.404996	-3.008119	2.025532
H	2.477025	-3.708972	0.392591
H	1.272549	-4.283375	1.563759
C	-0.159088	-1.916061	1.811661
H	0.367316	-1.481172	2.666390
H	-0.692748	-2.795784	2.179798
H	-0.904374	-1.201671	1.450879
C	1.174512	1.041346	1.438637
H	0.163722	0.861463	1.072903
H	1.132353	1.256403	2.509309
C	1.876314	2.160907	0.672617
H	1.884361	3.127288	1.175931
H	1.520606	2.267023	-0.355789
O	3.273953	1.720355	0.638779
N	1.581207	-1.161602	0.206758
N	3.327641	0.376578	0.526467
O	2.965184	0.044523	-0.996492
Cl	1.078766	-2.312245	-5.024608
Cl	-0.041058	0.113199	-2.908244
Cl	3.269415	-3.248432	-2.606029
Au	1.606838	-1.590870	-2.859477

2N5•••N5

C	-1.421544	-0.243475	-0.829333
C	-0.017585	-0.886007	0.861868
C	-0.077369	-2.394698	-1.251898
C	-1.102920	-2.859099	-2.294419
H	-1.218732	-2.145073	-3.112039
H	-2.080245	-3.056977	-1.846799
H	-0.733749	-3.791048	-2.732745
C	1.228273	-1.948104	-1.936954
H	1.990997	-1.661511	-1.206505
H	1.038614	-1.107939	-2.610565
H	1.627402	-2.780025	-2.525897
C	0.192061	-3.555620	-0.276752
H	0.925591	-3.304806	0.494420
H	0.604376	-4.390190	-0.849659
H	-0.729888	-3.903056	0.198747
C	-0.749373	-1.516046	2.074111

H	-1.423328	-2.314340	1.763781
H	-0.013447	-1.917330	2.774237
C	-1.501796	-0.330213	2.671656
H	-1.494736	-0.284215	3.760564
H	-2.521904	-0.228443	2.290841
O	-0.722970	0.829177	2.224132
N	-0.595510	-1.206813	-0.460321
N	-0.210774	0.593689	0.997152
O	-1.426637	0.779224	-0.028874
Cl	-4.345587	0.136871	-4.081603
Cl	-4.319520	-1.147696	-0.925855
Cl	-1.069686	0.929416	-3.660091
Au	-2.763414	-0.084789	-2.362681
C	4.510168	0.475315	1.643865
C	4.372846	1.651347	2.556068
H	5.038216	1.560695	3.425560
H	4.599173	2.599729	2.060570
C	2.882296	1.542608	2.935602
H	2.249453	2.157269	2.286710
H	2.674084	1.763735	3.983152
O	2.537959	0.152840	2.722335
N	3.503987	-0.342178	1.757252
H	5.315356	0.213295	0.973714
O	3.217267	-1.432394	1.239994
H	1.055886	-1.072076	0.863659

2Ph

C	0.598332	1.538761	1.047240
C	1.219981	1.223951	-1.151966
H	0.573556	0.836796	-1.942279
C	2.729963	1.074249	-1.456705
H	3.151222	0.205276	-0.945043
H	2.873996	0.921542	-2.530231
C	3.327050	2.412028	-0.987534
H	4.241315	2.675317	-1.526375
H	3.568196	2.375468	0.080467
C	2.191994	3.434225	-1.234562
C	2.066279	3.798872	-2.727682
H	1.934376	2.920895	-3.367642
H	2.974290	4.316099	-3.052878
H	1.210225	4.460176	-2.883207
C	2.305918	4.709471	-0.397816
H	2.429085	4.490962	0.664331
H	1.420830	5.339973	-0.524175
H	3.179385	5.275422	-0.735962
N	0.817865	0.611461	0.138721
N	0.928353	2.672318	-0.923374
O	0.698418	2.743138	0.564566
Cl	-0.286479	1.032854	5.302174
Cl	2.505206	1.531626	3.423867
Cl	-2.091802	1.087691	2.434520

Au	0.177280	1.302602	3.023974
C	-0.163925	-1.566790	-0.358658
C	0.786477	-0.815024	0.337527
C	-0.193532	-2.951150	-0.188114
C	1.702524	-1.421833	1.200002
C	0.713633	-3.571377	0.676764
C	1.654091	-2.807585	1.371689
H	-0.886760	-1.072465	-0.999985
H	2.422436	-0.817622	1.742449
H	2.352064	-3.284689	2.052186
H	0.680806	-4.647714	0.814613
H	-0.935756	-3.540882	-0.716631

2PhCl

C	0.260637	1.540925	0.691176
C	1.596750	1.227079	-1.164677
H	1.263851	0.842561	-2.130961
C	3.119383	1.077556	-0.928191
H	3.338841	0.214431	-0.294762
H	3.624619	0.916194	-1.884664
C	3.519585	2.420778	-0.293371
H	4.563052	2.682267	-0.488950
H	3.380822	2.392390	0.792943
C	2.536617	3.437482	-0.920702
C	2.924325	3.786931	-2.372074
H	3.017864	2.901903	-3.008982
H	3.888731	4.304110	-2.374704
H	2.171884	4.443595	-2.815826
C	2.359163	4.721390	-0.108727
H	2.120489	4.514493	0.935897
H	1.565233	5.343951	-0.531724
H	3.293357	5.290361	-0.141611
N	0.770830	0.613868	-0.094231
N	1.242835	2.674583	-1.049126
O	0.528879	2.744520	0.278187
Cl	-2.030153	1.018128	4.380471
Cl	1.241533	1.494190	3.574031
Cl	-2.743690	1.098554	1.070532
Au	-0.812546	1.296506	2.402696
C	0.016504	-1.562230	-0.903156
C	0.668573	-0.810496	0.077954
C	-0.072683	-2.946164	-0.766443
C	1.227610	-1.426054	1.200376
C	0.485684	-3.559039	0.358394
C	1.127728	-2.810419	1.345689
H	-0.442068	-1.070829	-1.755201
H	1.715644	-0.829856	1.964599
H	1.544462	-3.299513	2.218682
Cl	0.371715	-5.297496	0.532841
H	-0.583821	-3.541271	-1.514495

2PhCl$_3$

C	0.464284	1.199181	0.278056
C	2.501290	0.868997	-0.786310
H	2.612947	0.454277	-1.789163
C	3.779772	0.761774	0.075947
H	3.741370	-0.097439	0.748549
H	4.644935	0.626651	-0.580087
C	3.833391	2.110158	0.812693
H	4.851650	2.396480	1.089530
H	3.235167	2.074590	1.729738
C	3.201427	3.106730	-0.187490
C	4.180698	3.482416	-1.317868
H	4.570953	2.608163	-1.848290
H	5.031906	4.024869	-0.894829
H	3.683430	4.124368	-2.049271
C	2.646261	4.375025	0.463004
H	1.968491	4.147516	1.287648
H	2.112681	4.988330	-0.269128
H	3.482510	4.962327	0.854624
N	1.292984	0.261736	-0.158488
N	2.118203	2.309940	-0.875496
O	0.876145	2.389587	-0.031525
Cl	-3.215846	0.862012	2.637073
Cl	-0.157189	2.163092	3.129348
Cl	-2.289844	-0.047405	-0.455898
Au	-1.260622	1.036585	1.367241
C	0.743625	-1.870235	-1.243193
C	1.097879	-1.151137	-0.086033
C	0.553500	-3.248808	-1.211495
C	1.267958	-1.866944	1.112817
C	0.714016	-3.920581	-0.000728
C	1.069290	-3.246003	1.165027
Cl	0.521879	-1.043040	-2.761124
Cl	1.728847	-1.048099	2.580093
H	1.191125	-3.777048	2.100583
Cl	0.469057	-5.647904	0.054267
H	0.269951	-3.780652	-2.110834

2PhCl$_3$•••N1

C	0.947079	-0.930984	-0.159123
C	-1.210635	-0.921183	0.702754
C	-1.368119	-1.183143	2.218278
H	-0.852360	-0.429070	2.816007
H	-2.431848	-1.135099	2.463834
C	-0.797524	-2.598333	2.406604
H	-1.239870	-3.119077	3.260481
H	0.287114	-2.566047	2.559364
C	-1.116488	-3.306571	1.069197
C	-2.604749	-3.700830	0.973681
H	-3.277229	-2.844549	1.078438
H	-2.835592	-4.420054	1.766358
H	-2.804108	-4.172481	0.007255

C	-0.233342	-4.521173	0.778087
H	0.828498	-4.289063	0.878246
H	-0.414299	-4.901991	-0.231698
H	-0.481595	-5.314062	1.490609
N	0.009986	-0.139908	0.340426
N	-0.946071	-2.230178	0.026614
O	0.525877	-2.148105	-0.306037
Cl	5.126772	-0.093733	-1.199329
Cl	3.548909	-2.000746	1.073702
Cl	2.142484	0.887615	-2.385991
Au	2.890665	-0.529879	-0.655744
C	-5.969081	1.138152	0.548777
C	-7.173577	1.436311	-0.285132
H	-8.097163	1.222714	0.271942
H	-7.224903	2.489620	-0.581009
C	-6.988079	0.490665	-1.498470
H	-6.528255	1.040742	-2.325352
H	-7.933847	0.078231	-1.858987
C	-6.028057	-0.620812	-1.018588
C	-4.968382	-1.006118	-2.048375
H	-4.403486	-0.129368	-2.379402
H	-5.457324	-1.449084	-2.921958
H	-4.265863	-1.732304	-1.633940
C	-6.759460	-1.856011	-0.474708
H	-7.542754	-1.575969	0.237452
H	-6.055845	-2.523755	0.028910
H	-7.225873	-2.400949	-1.301342
N	-5.347457	0.057317	0.170167
H	-5.610705	1.678059	1.416195
O	-4.316147	-0.485075	0.704929
H	-2.090817	-0.450094	0.264672
C	0.886880	3.226538	1.758708
C	0.825573	1.843868	1.586101
C	0.196190	4.047342	0.871254
C	0.094723	1.271732	0.529240
C	-0.547282	3.518972	-0.182223
C	-0.589164	2.137107	-0.345459
H	1.465570	3.646853	2.571439
Cl	1.694181	0.840817	2.715224
Cl	-1.501645	1.494325	-1.683111
H	-1.069998	4.165832	-0.875236
Cl	0.261531	5.780729	1.083404

2PhCl•••N1

C	-1.021054	-0.889135	0.055850
C	1.172617	-0.880913	-0.663668
C	1.386375	-1.014568	-2.191418
H	0.879442	-0.213640	-2.736063
H	2.455498	-0.933334	-2.402489
C	0.835855	-2.413930	-2.518592
H	1.330948	-2.869810	-3.380608

H	-0.237504	-2.370361	-2.734426
C	1.074134	-3.221434	-1.220328
C	2.556306	-3.619769	-1.061660
H	3.227423	-2.756067	-1.077477
H	2.837536	-4.289843	-1.880534
H	2.702557	-4.145172	-0.113914
C	0.181478	-4.454546	-1.074976
H	-0.873667	-4.212554	-1.215561
H	0.305701	-4.911866	-0.088717
H	0.469083	-5.190998	-1.831814
N	-0.035331	-0.092443	-0.302657
N	0.835939	-2.230789	-0.113612
O	-0.659622	-2.137201	0.106309
Cl	-5.174435	0.107546	1.024698
Cl	-3.488607	-0.906765	-1.748132
Cl	-2.228546	0.052134	2.701325
Au	-2.949133	-0.416383	0.508512
C	5.799179	1.404300	-0.308682
C	7.098099	1.728288	0.356393
H	7.934510	1.621602	-0.349209
H	7.131754	2.759196	0.724750
C	7.161551	0.688251	1.504051
H	6.813773	1.146583	2.435002
H	8.174113	0.314975	1.676792
C	6.198428	-0.448500	1.093260
C	5.329934	-0.967140	2.236990
H	4.780855	-0.151422	2.717654
H	5.967292	-1.441456	2.990028
H	4.608324	-1.702152	1.873692
C	6.900812	-1.596957	0.355752
H	7.547646	-1.222233	-0.444471
H	6.163736	-2.274709	-0.082313
H	7.518791	-2.162071	1.060326
N	5.307035	0.260230	0.074087
H	5.282414	1.974660	-1.070381
O	4.239612	-0.315610	-0.343108
H	2.046251	-0.479021	-0.149658
C	-1.041666	3.284006	-1.532228
C	-1.004172	1.897777	-1.373272
C	-0.157732	4.080832	-0.804632
C	-0.096269	1.331458	-0.475065
C	0.756518	3.517718	0.088945
C	0.783673	2.134641	0.255370
H	-1.749554	3.736234	-2.217403
H	-1.684245	1.265307	-1.934560
H	1.473555	1.684866	0.961310
H	1.425937	4.153884	0.656677
Cl	-0.192442	5.821489	-1.013300

2PhMe

C	-0.186036	1.305310	0.080845

C	1.137276	1.385534	-1.806809
H	0.808733	1.125083	-2.815167
C	2.671520	1.321756	-1.617674
H	2.971374	0.382030	-1.147243
H	3.163340	1.369247	-2.593614
C	2.980632	2.563440	-0.764298
H	3.998644	2.933284	-0.914318
H	2.860018	2.340569	0.301563
C	1.915430	3.594135	-1.207696
C	2.257288	4.216401	-2.576590
H	2.407817	3.463991	-3.356910
H	3.180287	4.798286	-2.490801
H	1.452175	4.880656	-2.900714
C	1.654006	4.702186	-0.186110
H	1.444300	4.300485	0.806722
H	0.811041	5.327368	-0.494939
H	2.543253	5.336597	-0.119540
N	0.392207	0.552236	-0.830315
N	0.679879	2.767537	-1.465057
O	-0.033473	2.577102	-0.150949
Cl	-2.348986	0.040995	3.668478
Cl	0.835401	0.994375	2.930771
Cl	-3.119544	0.490069	0.398506
Au	-1.200653	0.718438	1.743393
C	-0.200516	-1.543443	-1.937561
C	0.413912	-0.886920	-0.868803
C	-0.173295	-2.935813	-1.989642
C	1.052343	-1.609380	0.141037
C	0.450122	-3.689611	-0.982414
C	1.059059	-3.003708	0.077970
H	-0.715630	-0.974722	-2.705401
H	1.517995	-1.090231	0.972738
H	1.544949	-3.563942	0.871783
C	0.431733	-5.198812	-1.022293
H	-0.659314	-3.444400	-2.817582
H	1.294894	-5.623377	-0.501747
H	0.433567	-5.572626	-2.050453
H	-0.470311	-5.586668	-0.533174

2PhMe•••N1

C	0.085202	-0.836759	-0.108881
C	-1.545013	-0.692648	1.521756
C	-1.146918	-0.933123	2.994475
H	-0.440176	-0.174358	3.339846
H	-2.035864	-0.861380	3.627765
C	-0.566143	-2.356226	2.986700
H	-0.646872	-2.850776	3.958857
H	0.493701	-2.341032	2.708268
C	-1.385040	-3.083287	1.894305
C	-2.790650	-3.467295	2.399652
H	-3.353965	-2.605770	2.770692

H	-2.699589	-4.188853	3.217857
H	-3.369246	-3.923607	1.592154
C	-0.690759	-4.315279	1.310756
H	0.324712	-4.092230	0.978582
H	-1.254243	-4.717190	0.463312
H	-0.638318	-5.088989	2.083136
N	-0.473059	-0.010797	0.745214
N	-1.634710	-2.027520	0.844130
O	-0.463068	-2.020829	-0.100576
Cl	3.429801	-0.173336	-2.860483
Cl	3.048104	-1.473343	0.258832
Cl	0.089538	0.392945	-2.915217
Au	1.635787	-0.518844	-1.388676
C	-6.334211	1.100217	0.026252
C	-7.309688	0.809220	-1.068543
H	-7.860958	-0.119807	-0.863259
H	-8.060617	1.599153	-1.178077
C	-6.394330	0.685512	-2.312501
H	-6.381485	1.636444	-2.854322
H	-6.731010	-0.087913	-3.007457
C	-4.980642	0.380621	-1.766688
C	-3.871323	1.148712	-2.480931
H	-4.052734	2.227600	-2.442630
H	-3.842776	0.842559	-3.531477
H	-2.893250	0.942550	-2.042697
C	-4.673381	-1.121699	-1.696635
H	-5.497711	-1.675852	-1.234229
H	-3.763756	-1.305443	-1.119481
H	-4.523729	-1.510356	-2.708659
N	-5.099376	0.884526	-0.327447
H	-6.546563	1.413543	1.040845
O	-4.047679	0.999843	0.398736
H	-2.480437	-0.147389	1.382060
C	1.555858	2.988217	1.636334
C	1.213134	1.659039	1.386090
C	0.609449	4.017110	1.530385
C	-0.095771	1.354529	1.004415
C	-0.702051	3.675144	1.166357
C	-1.064836	2.355542	0.897598
H	2.577296	3.223013	1.922819
H	1.954099	0.871924	1.480208
H	-2.080719	2.109042	0.601942
H	-1.454543	4.454569	1.080828
C	0.998047	5.455923	1.774472
H	0.151200	6.042433	2.143224
H	1.345111	5.927143	0.846446
H	1.810641	5.532592	2.503071

2Ph•••N1

C	-0.534757	0.634931	-0.268468
C	0.856858	2.250577	0.621351

C	0.371631	3.515146	1.344687
H	-0.040448	3.274777	2.328006
H	1.220891	4.186412	1.502240
C	-0.652296	4.112542	0.368736
H	-0.806445	5.184208	0.522779
H	-1.624213	3.618123	0.478342
C	-0.056341	3.806715	-1.026130
C	1.039887	4.821921	-1.403731
H	1.835626	4.871893	-0.654194
H	0.601322	5.820370	-1.501335
H	1.497156	4.543345	-2.356754
C	-1.102807	3.734098	-2.139888
H	-1.915825	3.045990	-1.899948
H	-0.651118	3.421702	-3.086000
H	-1.529213	4.732383	-2.280480
N	-0.035491	1.074721	0.861810
N	0.687667	2.493270	-0.842741
O	-0.175861	1.359828	-1.296329
Cl	-3.085499	-2.842619	-1.043888
Cl	-3.574715	0.481414	-0.554093
Cl	0.236006	-2.308136	-0.665485
Au	-1.718308	-0.984730	-0.620224
C	3.795825	-1.906336	0.938249
C	4.272301	-2.957522	-0.009571
H	5.251189	-3.348842	0.303088
H	3.589434	-3.812530	-0.050340
C	4.341668	-2.195867	-1.357414
H	3.440626	-2.406662	-1.939896
H	5.207101	-2.486071	-1.958874
C	4.382306	-0.693729	-0.993470
C	3.479500	0.167765	-1.872997
H	2.456210	-0.217682	-1.882981
H	3.860684	0.152866	-2.899509
H	3.460605	1.201754	-1.522208
C	5.805898	-0.124465	-0.918336
H	6.461410	-0.764990	-0.318668
H	5.792233	0.873427	-0.471855
H	6.225870	-0.051746	-1.926459
N	3.833902	-0.708957	0.431915
H	3.463441	-2.042289	1.959394
O	3.525728	0.400102	1.009519
H	1.882178	1.944194	0.842296
C	-1.750154	-0.103171	3.952816
C	-1.556279	0.415205	2.670254
C	-0.654209	-0.476325	4.734353
C	-0.253889	0.529487	2.176025
C	0.642837	-0.340911	4.229498
C	0.854823	0.159125	2.943362
H	-2.759602	-0.208320	4.337666
H	-2.401511	0.717090	2.060504

H	1.856000	0.242351	2.526328
H	1.495910	-0.634050	4.834080
H	-0.809939	-0.873033	5.733047

2Xyl

C	-3.672538	-0.179168	0.532270
C	-1.418533	-0.255412	0.032189
H	-1.037136	-0.679287	-0.898037
C	-0.353643	-0.181372	1.147070
H	-0.400754	-1.053936	1.802081
H	0.641928	-0.172427	0.693485
C	-0.661154	1.148982	1.851928
H	0.214815	1.571051	2.352257
H	-1.444078	1.020081	2.607877
C	-1.177859	2.061235	0.713877
C	-0.020730	2.605001	-0.147757
H	0.608803	1.808897	-0.557330
H	0.614487	3.255666	0.461479
H	-0.416104	3.184189	-0.986078
C	-2.055527	3.217861	1.195505
H	-2.869136	2.874053	1.836859
H	-2.484874	3.762138	0.349268
H	-1.434472	3.913534	1.768286
N	-2.649261	-1.001127	0.416863
N	-1.930527	1.126916	-0.206773
O	-3.358592	1.053556	0.248330
Cl	-7.813545	-0.965313	1.736141
Cl	-5.113890	0.471240	3.161654
Cl	-6.002654	-1.450259	-1.057369
Au	-5.604203	-0.547812	1.082572
C	-2.622329	-3.210534	-0.634717
C	-2.654603	-2.444416	0.551620
C	-2.594241	-4.602694	-0.507096
C	-2.658440	-3.030987	1.831907
C	-2.595202	-5.211249	0.747694
C	-2.627393	-4.432052	1.899580
C	-2.624122	-2.586658	-2.010822
C	-2.723608	-2.245956	3.120322
H	-2.635075	-4.907306	2.876362
H	-2.577545	-6.294265	0.825402
H	-2.585057	-5.212146	-1.405926
H	-2.393827	-1.212565	3.014558
H	-2.109455	-2.727919	3.886736
H	-3.750157	-2.202393	3.498540
H	-2.974127	-3.311990	-2.749020
H	-1.616337	-2.278211	-2.317887
H	-3.283744	-1.718098	-2.067111

2Xyl•••N1

C	-1.026766	0.564153	-0.141743
C	1.159830	0.690350	0.594208
C	1.424510	1.184620	2.034844

H	0.975304	0.521514	2.776926
H	2.503917	1.181950	2.204988
C	0.848236	2.609442	2.044103
H	1.336084	3.256950	2.778261
H	-0.224543	2.600259	2.269399
C	1.071172	3.105119	0.595130
C	2.545118	3.486453	0.345430
H	3.230874	2.655450	0.534588
H	2.819598	4.318637	1.002029
H	2.676823	3.802334	-0.693240
C	0.155010	4.257732	0.181270
H	-0.895049	4.038022	0.382742
H	0.266062	4.480954	-0.884154
H	0.435320	5.151410	0.747811
N	-0.076104	-0.131401	0.446794
N	0.852995	1.882162	-0.257700
O	-0.628138	1.748686	-0.508111
Cl	-5.207928	-0.464356	-0.989094
Cl	-3.613977	1.581341	1.166418
Cl	-2.222072	-1.322226	-2.285952
Au	-2.969125	0.077818	-0.543004
C	5.947375	-1.399531	0.708604
C	7.287338	-1.743194	0.141741
H	8.091699	-1.422342	0.819339
H	7.414243	-2.821409	-0.003028
C	7.301120	-0.961527	-1.196596
H	7.016757	-1.629925	-2.015283
H	8.285538	-0.549193	-1.432077
C	6.239872	0.151340	-1.041975
C	5.367553	0.350033	-2.279315
H	4.901319	-0.590604	-2.588463
H	5.986949	0.713652	-3.105485
H	4.577767	1.078882	-2.084667
C	6.828274	1.481066	-0.549926
H	7.477332	1.334142	0.319757
H	6.027848	2.171786	-0.272731
H	7.421898	1.937891	-1.347830
N	5.377383	-0.404211	0.090340
H	5.453678	-1.844079	1.563652
O	4.256066	0.154232	0.363448
H	2.009884	0.149035	0.182154
C	-0.801811	-3.179594	2.485132
C	-0.810949	-1.834113	2.085843
C	-0.151263	-4.152419	1.733699
C	-0.134977	-1.507032	0.895082
C	0.509944	-3.799036	0.557196
C	0.535012	-2.473764	0.112915
H	-1.321661	-3.456296	3.398098
C	-1.561641	-0.834351	2.933326
C	1.250229	-2.123752	-1.170280

H	1.003529	-4.561783	-0.038099
H	-0.164018	-5.188548	2.059160
H	0.649366	-1.461054	-1.798153
H	1.451204	-3.031899	-1.744014
H	2.212969	-1.634941	-0.977752
H	-2.636740	-0.882269	2.730943
H	-1.261739	0.197560	2.753242
H	-1.416175	-1.055822	3.995040

3

C	-1.721796	-0.099966	1.265372
C	0.090016	0.770245	0.051739
C	1.513146	0.956536	-0.427469
H	1.614673	0.564351	-1.443980
H	2.234269	0.434094	0.203102
C	1.671119	2.486266	-0.377557
H	2.129406	2.777873	0.572842
H	2.302056	2.866714	-1.184333
C	0.228623	3.057413	-0.456359
C	0.048552	4.261732	0.471779
H	-0.970681	4.648831	0.422544
H	0.740296	5.054512	0.166312
H	0.276038	3.991703	1.508418
C	-0.188162	3.391574	-1.897467
H	-1.247742	3.653418	-1.935670
H	-0.010269	2.544278	-2.569590
H	0.395081	4.244331	-2.260484
C	0.073639	-1.785449	0.533968
N	-0.507339	-0.369495	0.533098
N	-0.579046	1.888537	0.025625
O	-2.139373	-0.834723	2.112263
Cl	-4.666585	1.100258	1.410293
Cl	-3.406255	3.789146	-0.200954
Au	-2.550367	1.691933	0.645666
C	1.012389	-1.996676	-0.670327
C	-1.083356	-2.795552	0.360149
C	0.820128	-2.022005	1.856687
H	0.541997	-1.685475	-1.608342
H	1.216880	-3.067582	-0.747450
H	1.977048	-1.501905	-0.567107
H	-0.648638	-3.791969	0.241673
H	-1.662406	-2.571083	-0.541498
H	-1.758391	-2.818827	1.212420
H	1.654015	-1.321472	1.972703
H	1.229237	-3.037584	1.873196
H	0.146414	-1.909200	2.708669

33

Au	-1.280706	-1.027171	-0.375419
Cl	-1.407281	-0.267653	-2.647105
Cl	-1.081206	-1.692505	1.923186
Cl	-3.679152	-1.035284	-0.208448

C	1.348812	-2.221322	-0.863383
N	0.793906	-1.129016	-0.528529
C	1.685759	0.078776	-0.257988
C	2.859996	-1.978258	-0.848215
C	1.678460	1.001491	-1.486863
C	1.249360	0.841829	0.992685
C	3.047915	-0.640488	-0.088839
H	3.392100	-2.818733	-0.391467
H	3.196671	-1.924129	-1.893122
H	3.879374	-0.030419	-0.460064
H	3.227132	-0.839665	0.974384
H	0.670071	1.360127	-1.704143
H	2.037265	0.476670	-2.377782
H	2.331657	1.863523	-1.300770
H	0.271908	1.313499	0.849147
H	1.979054	1.632308	1.208620
H	1.174443	0.175746	1.855186

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Au	0.500740	0.142808	-1.395841
Cl	1.224568	-0.144546	-3.602550
Cl	-0.654606	0.363193	0.628686
C	3.217034	-0.030768	-0.051450
N	2.430361	0.732538	-0.565762
C	2.850323	2.231785	-0.653432
C	4.466496	0.679782	0.439784
C	3.326255	2.498624	-2.079004
C	1.706592	3.140313	-0.234942
C	4.019040	2.175087	0.385474
H	4.770274	0.340347	1.431511
H	5.277726	0.437462	-0.255412
H	4.829885	2.858577	0.116526
H	3.642559	2.475668	1.368322
H	2.531805	2.311267	-2.805319
H	4.182349	1.871806	-2.344992
H	3.629173	3.548720	-2.154778
H	0.909823	3.151870	-0.983696
H	2.092527	4.161203	-0.135652
H	1.277645	2.832211	0.721728

3PhCl$_3$

Au	-1.658832	0.759018	-0.825529
Cl	-2.115047	-0.333050	1.213628
Cl	-3.911921	0.587355	-1.503118
Cl	-1.090515	1.926856	-2.811788
C	0.301570	0.872001	-0.234569
N	1.216973	0.056831	0.025645
O	0.612283	2.272197	-0.077484
C	2.680700	2.119073	1.031312
N	1.935591	2.588305	0.094041
H	2.275083	1.489796	1.814079
C	4.091344	2.567239	0.847472

C	2.633858	3.391622	-0.983613
C	3.979033	3.655700	-0.253136
H	4.522508	2.927822	1.786101
H	4.690088	1.700305	0.537404
H	3.959462	4.645859	0.211196
H	4.817339	3.627187	-0.951164
C	2.778404	2.501474	-2.225906
C	1.820948	4.651519	-1.281019
H	0.852679	4.394927	-1.718006
H	2.372670	5.264104	-2.000409
H	1.658549	5.244948	-0.376095
H	3.362629	1.601166	-2.014039
H	3.293304	3.073678	-3.003329
H	1.799665	2.204757	-2.611620
C	1.032191	-3.496025	-1.154857
C	1.028156	-2.101369	-1.178904
C	1.163616	-4.152409	0.065393
C	1.142192	-1.339891	0.000119
C	1.310605	-3.441757	1.255293
C	1.313845	-2.052171	1.202663
H	0.931691	-4.052832	-2.078142
Cl	0.908069	-1.304119	-2.728135
Cl	1.536155	-1.167913	2.701613
H	1.419931	-3.954403	2.202648
Cl	1.161683	-5.903511	0.106331

4

C	0.062313	0.136336	-0.087413
C	-0.026357	0.061804	1.460916
N	1.445051	-0.087869	1.780381
C	2.204187	-0.427863	0.797331
C	1.420519	-0.510109	-0.470291
C	-0.557765	1.336484	2.116227
C	-0.757504	-1.187999	1.970144
O	1.844261	-0.052574	3.079030
C	2.397538	-1.327262	3.621132
N	2.672180	-2.217140	2.806629
C	3.169410	-3.594799	3.034662
C	4.117639	-3.902711	1.861362
Au	2.441582	-1.002291	5.641144
Cl	0.267945	-1.954550	5.731369
Cl	4.572037	-0.029715	5.334843
Cl	2.500268	-0.661469	7.983962
C	1.940770	-4.522715	2.984557
C	3.920435	-3.771938	4.365234
H	3.263335	-0.590083	0.941760
H	3.601919	-3.782908	0.902301
H	4.480249	-4.933141	1.927875
H	4.985829	-3.235419	1.877505
H	1.412224	-4.420072	2.030595
H	1.246843	-4.287258	3.796340

H	2.259938	-5.564867	3.088204
H	4.340747	-4.782142	4.407426
H	3.255916	-3.655570	5.225507
H	4.739958	-3.054441	4.460402
H	1.932671	-0.002792	-1.293350
H	1.326594	-1.565294	-0.758172
H	-0.784496	-0.369313	-0.554604
H	0.051044	1.181763	-0.408959
H	-0.528227	1.256974	3.205421
H	-1.597795	1.484688	1.810446
H	0.020794	2.213433	1.810566
H	-0.393032	-2.095189	1.478982
H	-1.824564	-1.081452	1.753157
H	-0.636239	-1.306520	3.050337

4Bz

Au	-3.488117	-1.557538	1.956009
Cl	-2.310456	-1.564017	4.003291
Cl	-5.505781	-2.242509	2.985841
Cl	-4.488036	-1.468081	-0.189243
C	-1.740380	-1.000909	1.054355
N	-0.760544	-1.602487	0.576395
O	-1.740893	0.457926	1.005542
C	0.495300	0.786519	0.379162
N	-0.762222	1.015970	0.230424
H	0.866762	0.216146	1.219941
C	1.276555	1.414422	-0.725108
C	-1.161478	1.763014	-1.022341
C	0.230754	2.318055	-1.430985
H	2.145857	1.958531	-0.344093
H	1.662119	0.615189	-1.371748
H	0.337304	3.347604	-1.077261
H	0.349210	2.320664	-2.515871
C	-1.732776	0.748692	-2.023117
C	-2.181989	2.843671	-0.664899
H	-3.115818	2.398307	-0.313731
H	-2.399208	3.434466	-1.559803
H	-1.797706	3.516093	0.108034
H	-0.992138	-0.009520	-2.294314
H	-2.029938	1.283918	-2.929792
H	-2.613787	0.244300	-1.616518
C	-0.649273	-3.065979	0.575008
H	-0.750817	-3.397530	-0.463556
H	-1.463705	-3.521168	1.151068
C	2.933840	-4.389770	0.787416
C	1.691896	-3.998755	0.276492
C	3.191363	-4.280078	2.155862
C	0.696722	-3.496893	1.124057
C	2.201105	-3.782406	3.009892
C	0.961281	-3.393648	2.498373
H	3.693501	-4.784933	0.118778

H	1.492658	-4.094395	-0.788498
H	0.190379	-3.015885	3.165637
H	2.390285	-3.706243	4.076895
H	4.152703	-4.588693	2.556535

4Cy

Au	-1.822253	0.436239	0.145333
Cl	-2.246431	0.095757	2.446778
Cl	-4.088365	0.071276	-0.440164
Cl	-1.212240	0.858944	-2.108522
C	0.141005	0.718711	0.647656
N	1.158329	0.042510	0.847346
O	0.259620	2.193658	0.820832
C	2.378847	2.267550	1.804579
N	1.530994	2.666766	0.921209
H	2.074397	1.622082	2.616705
C	3.729063	2.844431	1.540426
C	2.086353	3.527566	-0.191254
H	-0.216144	-4.233235	1.835399
C	0.784856	-4.263932	1.383704
C	1.757354	-3.450073	2.251435
C	0.709776	-3.703671	-0.045067
H	1.088947	-5.317418	1.363478
C	1.414589	-1.951456	2.237536
C	0.339278	-2.210503	-0.046918
C	1.348048	-1.411705	0.794651
H	1.680314	-3.842544	-0.544512
H	-0.026006	-4.260474	-0.636138
H	0.305966	-1.817532	-1.068437
H	-0.665481	-2.094058	0.377181
H	2.341999	-1.546913	0.343916
H	0.442411	-1.778511	2.716208
H	2.161899	-1.385498	2.808349
H	1.749605	-3.818286	3.284161
H	2.782193	-3.590829	1.876920
C	3.451611	3.908682	0.444812
H	4.175693	3.256091	2.450534
H	4.392826	2.039896	1.197794
H	3.384415	4.899257	0.903586
H	4.239475	3.940284	-0.309661
C	2.220683	2.659507	-1.450083
C	1.152849	4.716482	-0.420551
H	0.181753	4.382610	-0.793864
H	1.599472	5.379092	-1.167924
H	1.000292	5.287410	0.500425
H	2.901953	1.818755	-1.288114
H	2.619623	3.278255	-2.259453
H	1.250117	2.265301	-1.763783

4Me

Au	-1.568071	0.996944	0.394121
Cl	-1.431900	0.667475	2.726157

Cl	-3.924537	0.778275	0.387861
Cl	-1.494043	1.361060	-1.947124
C	0.470099	1.150073	0.393633
N	1.416210	0.341593	0.357782
O	0.781365	2.576720	0.456315
C	3.086508	2.439269	0.856838
N	2.082701	2.903545	0.199907
H	2.942766	1.836556	1.743400
C	4.369519	2.868361	0.228489
C	2.410201	3.678044	-1.058721
C	3.918463	3.941310	-0.798049
H	5.078600	3.240469	0.973924
H	4.834619	1.992227	-0.242359
H	4.052219	4.938389	-0.368485
H	4.491265	3.894317	-1.725740
C	2.150580	2.763555	-2.264180
C	1.554686	4.943487	-1.111754
H	0.496225	4.694157	-1.217494
H	1.855751	5.536863	-1.980250
H	1.687351	5.553905	-0.213413
H	2.776298	1.866598	-2.231145
H	2.386090	3.317695	-3.177631
H	1.102346	2.455405	-2.308888
C	1.206475	-1.099507	0.275760
H	1.750987	-1.579647	1.093863
H	1.624057	-1.462145	-0.668446
H	0.151107	-1.383191	0.333670

4N2

C	0.951940	3.144516	0.033658
C	1.597755	2.292897	-1.076104
N	0.406140	1.700248	-1.726286
C	-0.683224	1.757911	-1.032991
C	-0.471652	2.541518	0.220519
H	2.163082	2.855724	-1.820006
H	2.215402	1.462637	-0.718072
O	0.581796	0.861843	-2.777115
C	0.479265	-0.585670	-2.387410
N	-0.160189	-0.831262	-1.357683
C	-0.412589	-2.114602	-0.661374
C	-1.873970	-2.056411	-0.180587
Au	1.613947	-1.560867	-3.777893
Cl	3.447712	-1.138907	-2.320564
Cl	-0.321949	-1.824302	-5.098876
Cl	2.967540	-2.717871	-5.333494
C	0.545784	-2.155144	0.544203
C	-0.206540	-3.352795	-1.549436
H	-1.597306	1.313259	-1.400266
H	-2.040861	-1.180723	0.456239
H	-2.115542	-2.951792	0.400316
H	-2.561408	-2.005572	-1.031038

H	0.389283	-1.290378	1.198456
H	1.587061	-2.158182	0.209687
H	0.364941	-3.062263	1.129708
H	-0.502875	-4.246738	-0.991037
H	0.841384	-3.474789	-1.836653
H	-0.810934	-3.298326	-2.458674
H	-1.252404	3.293507	0.369150
H	-0.528173	1.850760	1.071797
H	1.535090	3.118212	0.955133
H	0.874474	4.186393	-0.287267

4N3

C	0.592414	3.146029	-2.041583
C	1.759219	2.148199	-1.809534
N	1.082657	0.923317	-2.357255
C	-0.203576	1.081682	-2.473784
O	-0.609061	2.315210	-2.278353
C	3.004149	2.471055	-2.636974
C	2.085415	1.945388	-0.325760
O	1.697812	-0.298740	-2.327042
C	1.174383	-1.240312	-1.313191
N	0.089801	-0.952065	-0.786059
C	-0.676928	-1.657534	0.267941
C	-2.157045	-1.553888	-0.144514
Au	2.589542	-2.719403	-1.246140
Cl	3.627242	-1.507418	0.513689
Cl	1.444458	-3.754693	-3.033306
Cl	4.214830	-4.438233	-1.150708
C	-0.435667	-0.885882	1.579338
C	-0.289058	-3.135340	0.440895
H	-0.906774	0.319807	-2.774136
H	-2.455271	-0.507276	-0.270539
H	-2.795239	-1.999464	0.624829
H	-2.336965	-2.086113	-1.084429
H	-0.734096	0.163140	1.477282
H	0.620371	-0.926849	1.861362
H	-1.027962	-1.330656	2.385545
H	-0.962448	-3.598947	1.169198
H	0.731074	-3.244463	0.818578
H	-0.373363	-3.683513	-0.501318
H	0.376600	3.776353	-1.179885
H	0.721961	3.753134	-2.940240
H	3.752442	1.684671	-2.511472
H	3.440059	3.413349	-2.291501
H	2.765409	2.562421	-3.700496
H	1.182291	1.755016	0.260028
H	2.567530	2.850984	0.055747
H	2.769446	1.104357	-0.184083

4N4

O	-0.101137	3.300159	-0.878262
C	1.100292	2.573856	-1.149280

N	0.522156	1.387047	-1.899674
C	-0.751586	1.276764	-1.768124
C	-1.241332	2.445249	-0.975051
C	2.000651	3.387657	-2.061499
C	1.784840	2.079421	0.120137
O	1.349904	0.456302	-2.418379
C	1.257161	-0.913945	-1.784020
N	0.277402	-1.121920	-1.062187
C	-0.079401	-2.313637	-0.253405
C	-1.613046	-2.426482	-0.316006
Au	2.942228	-1.861349	-2.451694
Cl	4.025680	-1.088320	-0.486031
Cl	1.710975	-2.492755	-4.364516
Cl	4.881243	-2.986909	-3.196881
C	0.377151	-2.022690	1.188685
C	0.559492	-3.614659	-0.766978
H	-1.320192	0.473289	-2.212138
H	-2.087308	-1.508493	0.048358
H	-1.956336	-3.257216	0.307970
H	-1.948602	-2.611224	-1.341860
H	-0.090569	-1.109288	1.571763
H	1.463528	-1.906452	1.233695
H	0.087749	-2.852618	1.841365
H	0.169382	-4.458266	-0.188385
H	1.646022	-3.606350	-0.647113
H	0.328050	-3.783939	-1.822115
H	-2.052825	2.983391	-1.476173
H	-1.599137	2.115871	0.012556
H	2.883933	2.806678	-2.337498
H	2.322983	4.283376	-1.524915
H	1.464654	3.690285	-2.964006
H	1.082462	1.538579	0.759479
H	2.160527	2.948017	0.666729
H	2.622948	1.417950	-0.116657

4Ph

Au	-0.312525	1.031178	2.512441
Cl	1.790286	0.866801	3.564645
Cl	-1.474708	0.813014	4.558915
Cl	-2.332226	1.283807	1.285148
C	0.701146	1.190391	0.743773
N	1.195492	0.398692	-0.086014
O	0.861011	2.618251	0.493976
C	2.375332	2.524393	-1.292529
N	1.284568	2.954273	-0.761288
H	3.094992	1.962643	-0.712914
C	2.458776	2.935042	-2.723908
C	0.331278	3.678456	-1.687116
C	1.304636	3.963170	-2.863744
H	3.444425	3.340126	-2.971338
H	2.316075	2.042583	-3.347760

H	1.705092	4.977251	-2.775654
H	0.793254	3.884600	-3.824538
C	-0.805559	2.714535	-2.055240
C	-0.192915	4.934862	-0.992157
H	-0.809716	4.674630	-0.128643
H	-0.811261	5.497032	-1.698336
H	0.626346	5.580013	-0.660779
H	-0.430119	1.822057	-2.564780
H	-1.496217	3.232579	-2.727219
H	-1.361459	2.401514	-1.167137
C	-0.228464	-3.044326	0.098452
C	-0.161651	-1.649917	0.128680
C	0.920693	-3.807593	-0.122502
C	1.072823	-1.012268	-0.063832
C	2.147024	-3.167145	-0.325409
C	2.223093	-1.774572	-0.310175
H	-1.185943	-3.532229	0.254726
H	-1.056875	-1.059644	0.292882
H	3.172435	-1.270741	-0.464439
H	3.046352	-3.751429	-0.496659
H	0.861740	-4.891610	-0.138377

4PhCl

Au	-0.305571	1.031098	2.357881
Cl	1.313799	0.865981	4.062282
Cl	-2.092877	0.823772	3.887799
Cl	-1.783827	1.269371	0.512563
C	1.249887	1.188663	1.039504
N	1.999717	0.395084	0.430433
O	1.480959	2.612934	0.854312
C	3.518377	2.539244	-0.305066
N	2.306107	2.952489	-0.182166
H	4.000371	1.980167	0.485502
C	4.085762	2.961047	-1.618289
C	1.721723	3.675243	-1.376897
C	3.037198	3.976335	-2.146293
H	5.090406	3.379779	-1.507768
H	4.180932	2.071459	-2.255233
H	3.370424	4.994613	-1.926311
H	2.887992	3.895269	-3.224229
C	0.791533	2.704377	-2.117826
C	0.977709	4.922155	-0.899285
H	0.106523	4.650501	-0.298450
H	0.630504	5.481972	-1.772780
H	1.627441	5.573863	-0.307365
H	1.329968	1.819494	-2.470098
H	0.370579	3.221539	-2.985109
H	-0.034230	2.380576	-1.478308
C	0.575869	-3.042103	0.122091
C	0.642556	-1.649439	0.175725
C	1.734566	-3.795508	0.309097

C	1.869575	-1.013402	0.415463
C	2.963702	-3.175685	0.541295
C	3.028299	-1.784181	0.580426
H	-0.372707	-3.535140	-0.059452
H	-0.255301	-1.059978	0.023017
H	3.977750	-1.290281	0.761263
H	3.856808	-3.773027	0.687399
Cl	1.650483	-5.549261	0.241323

4PhMe

Au	-0.321415	1.040347	2.519497
Cl	1.779049	0.861506	3.574436
Cl	-1.489122	0.823144	4.564848
Cl	-2.336181	1.302157	1.285449
C	0.699155	1.203588	0.755849
N	1.210191	0.417764	-0.068537
O	0.840246	2.634954	0.502506
C	2.381988	2.554300	-1.258742
N	1.276394	2.970803	-0.747809
H	3.102176	2.010074	-0.663284
C	2.482380	2.956541	-2.691412
C	0.325201	3.668538	-1.695751
C	1.313582	3.964490	-2.857008
H	3.465027	3.376963	-2.924978
H	2.364980	2.058218	-3.311927
H	1.695518	4.985580	-2.767320
H	0.820394	3.872173	-3.826116
C	-0.784973	2.679202	-2.077577
C	-0.237264	4.918631	-1.019709
H	-0.861051	4.651040	-0.163498
H	-0.857481	5.460745	-1.739760
H	0.562485	5.584485	-0.681721
H	-0.382485	1.791997	-2.575506
H	-1.474394	3.179402	-2.764219
H	-1.349684	2.359866	-1.197293
C	-0.151156	-3.051119	0.135013
C	-0.107672	-1.657026	0.171674
C	0.995935	-3.816980	-0.116307
C	1.107330	-0.994141	-0.050893
C	2.198873	-3.135087	-0.354817
C	2.256392	-1.742711	-0.336404
H	-1.100741	-3.549916	0.311057
H	-1.012150	-1.087124	0.356823
H	3.194644	-1.228849	-0.523172
H	3.104489	-3.700407	-0.560268
C	0.944406	-5.326758	-0.107198
H	1.674321	-5.757525	-0.799896
H	-0.047478	-5.694621	-0.386481
H	1.169604	-5.720194	0.892139

4Xyl

Au	-1.794292	0.758535	-0.060260

Cl	-2.083763	0.568804	2.272281
Cl	-4.129500	0.677556	-0.423614
Cl	-1.386632	1.145786	-2.364498
C	0.238431	0.788672	0.246096
N	1.161140	-0.038894	0.363945
O	0.579970	2.210240	0.348394
C	2.818865	2.016182	1.042901
N	1.906486	2.528771	0.292667
H	2.566488	1.360236	1.864047
C	4.171153	2.478792	0.614129
C	2.388146	3.408705	-0.840893
C	3.854203	3.629913	-0.377193
H	4.779696	2.787724	1.469196
H	4.693472	1.636341	0.141646
H	3.937966	4.590671	0.138731
H	4.536802	3.644070	-1.228535
C	2.272249	2.615663	-2.148920
C	1.549814	4.687112	-0.877537
H	0.513054	4.467708	-1.142712
H	1.963844	5.357645	-1.636513
H	1.567390	5.204333	0.086521
H	2.899261	1.719228	-2.133266
H	2.602783	3.253188	-2.974221
H	1.237599	2.316566	-2.338033
C	1.149949	-3.535077	-0.897975
C	1.182722	-2.134751	-0.911428
C	1.040256	-4.246933	0.295304
C	1.078645	-1.461103	0.322574
C	0.987264	-3.557984	1.506269
C	1.020156	-2.159246	1.547005
H	1.214223	-4.067422	-1.843076
C	1.358051	-1.388367	-2.210816
C	1.004308	-1.429670	2.867632
H	0.921661	-4.107229	2.441515
H	1.009289	-5.332322	0.282601
H	1.885379	-0.782037	2.972878
H	1.018745	-2.140223	3.698165
H	0.116518	-0.798681	2.973414
H	1.482242	-2.090821	-3.039129
H	2.249058	-0.748608	-2.178608
H	0.504580	-0.743715	-2.439195

6

Au	-2.128035	-0.279880	1.105928
Cl	-3.273941	-0.774318	3.074258
Cl	-0.858476	0.151435	-0.831543
Cl	-3.944871	0.825858	0.268798
C	0.654527	-1.490203	1.363833
N	1.709906	-1.686808	0.898438
O	-0.403972	-1.351319	1.948103
C	3.974764	-2.530782	0.824857

C	2.516288	-2.455534	-1.252198
C	2.901727	-1.742377	0.055539
C	3.355123	-0.296181	-0.209613
H	2.571215	0.268587	-0.720902
H	4.247412	-0.309405	-0.842609
H	3.602874	0.213072	0.726165
H	4.882278	-2.590528	0.217288
H	3.634800	-3.547850	1.039586
H	4.222424	-2.036689	1.768626
H	3.393084	-2.508984	-1.904438
H	1.724982	-1.910031	-1.772924
H	2.170280	-3.474059	-1.054104

6•••Im

Au	1.405168	-2.216387	-2.370575
Cl	3.529306	-2.682945	-3.207996
Cl	-0.690971	-1.762799	-1.394430
Cl	0.594942	-1.899056	-4.485107
N	1.142057	-2.066806	1.703694
C	1.630699	-2.291450	0.665703
O	2.234609	-2.527445	-0.365136
C	0.313342	-1.954020	2.900494
C	-0.741836	-3.072471	2.850576
C	1.238967	-2.111633	4.118735
C	-0.344664	-0.563667	2.878747
H	1.730289	-3.088780	4.114441
H	0.645043	-2.027276	5.033323
H	2.005328	-1.331698	4.131014
H	-0.970319	-0.448970	3.768943
H	-0.973620	-0.446880	1.992562
H	0.409515	0.228009	2.880022
H	-1.381343	-3.003903	3.735574
H	-0.267039	-4.058007	2.843448
H	-1.367814	-2.976658	1.959457
C	-0.578569	2.996924	-0.737788
N	0.547417	3.533773	-0.472532
C	1.463430	3.359936	-1.634541
C	-0.720941	2.337699	-2.090656
C	2.096970	4.715710	-1.971421
C	2.554567	2.356842	-1.220332
C	0.568548	2.811959	-2.794645
H	-0.768775	1.247678	-1.967460
H	-1.641558	2.636049	-2.605008
H	0.339195	3.615825	-3.502384
H	1.061831	2.014221	-3.356938
H	2.681025	5.091004	-1.125032
H	1.325394	5.456304	-2.206625
H	2.760816	4.623768	-2.838613
H	3.069152	2.707692	-0.320072
H	3.293675	2.238655	-2.020214
H	2.126556	1.371548	-1.003998

H	-1.378813	3.001025	0.004582

7

Au	-1.330448	-1.020135	-0.379430
Cl	-1.458017	-0.341850	-2.630685
Cl	-1.128453	-1.821208	1.828982
Cl	-3.635454	-0.962931	-0.193380
C	1.394352	-2.143843	-0.838740
N	0.756966	-1.081633	-0.522797
C	1.686662	0.086182	-0.261773
C	2.884430	-1.986110	-0.832196
C	1.666428	1.007485	-1.492353
C	1.258723	0.841378	0.997170
C	3.053802	-0.638166	-0.099634
H	3.377193	-2.829022	-0.337728
H	3.248851	-1.967657	-1.868557
H	3.873295	-0.036393	-0.498559
H	3.251312	-0.818893	0.961554
H	0.662647	1.390273	-1.686749
H	2.003777	0.484910	-2.392765
H	2.335806	1.854338	-1.310646
H	0.293117	1.335797	0.854486
H	2.002437	1.614019	1.217564
H	1.178112	0.172786	1.857307
H	0.865449	-3.058727	-1.092762

9

Au	-1.114283	-0.951868	-0.792046
Cl	-3.435369	-0.819146	-1.138530
Cl	-1.391110	-0.861841	2.049434
Cl	1.225937	-1.149110	-0.658388
N	-1.052628	-4.420864	1.247626
C	-1.174157	-3.741395	0.299722
O	-1.277209	-3.156231	-0.762718
C	-1.084321	-4.829712	2.655558
C	-2.426361	-4.368153	3.248049
C	-0.947760	-6.359729	2.689587
C	0.100109	-4.143484	3.357709
H	-1.776794	-6.840092	2.160956
H	-0.959024	-6.698746	3.729618
H	-0.007361	-6.680280	2.231424
H	0.099413	-4.428063	4.414864
H	0.010400	-3.056868	3.280212
H	1.049473	-4.458114	2.913829
H	-2.467077	-4.649756	4.305222
H	-3.264193	-4.846009	2.730715
H	-2.523694	-3.282376	3.165074
C	-1.073430	1.823969	0.022663
N	-0.980321	1.097143	-1.026604
C	-0.761464	1.885318	-2.299648
C	-0.988304	3.287793	-0.280918
C	0.719925	1.776870	-2.690749

C	-1.666766	1.371591	-3.418141
C	-1.140020	3.318219	-1.818537
H	-1.759278	3.849251	0.255643
H	-0.018818	3.665639	0.071241
H	-0.510770	4.073708	-2.294562
H	-2.180804	3.529604	-2.081792
H	1.004769	0.738919	-2.874907
H	1.373550	2.167950	-1.905216
H	0.888681	2.354647	-3.605028
H	-1.389399	0.356274	-3.716922
H	-1.555927	2.023128	-4.291106
H	-2.715439	1.363066	-3.112957
H	-1.190917	1.348439	1.002281

$AuCl_3$

Au	-1.421866	0.249886	-1.680537
Cl	-1.063913	2.089856	-3.011880
Cl	-1.225892	-1.622931	-0.361900
Cl	-3.705289	0.395039	-1.632813

CN^tBu

N	2.206318	-1.402851	0.486042
C	2.042952	-0.239596	0.433991
C	2.407030	-2.833073	0.550058
C	1.589463	-3.482809	-0.582177
C	3.910969	-3.113688	0.368839
C	1.921169	-3.323271	1.927066
H	4.260701	-2.738584	-0.597146
H	4.091129	-4.192330	0.410581
H	4.492788	-2.631834	1.159719
H	2.061182	-4.406095	2.002243
H	0.859863	-3.098158	2.065552
H	2.485435	-2.841931	2.730908
H	1.724923	-4.568562	-0.556574
H	1.917490	-3.113363	-1.557978
H	0.524547	-3.261180	-0.467827

CN^tBu•••**N1**

C	-1.325797	-0.110396	2.292921
N	-2.074335	-0.161846	1.389373
C	-2.983047	-0.220769	0.261970
C	-2.940299	1.141141	-0.456134
C	-4.391379	-0.519742	0.807985
C	-2.501030	-1.340402	-0.679497
O	0.447393	0.708491	-1.293881
C	1.157913	1.972796	0.521766
C	2.377105	0.024200	0.015358
N	1.206948	0.956862	-0.293598
H	0.400179	2.731926	0.377497
C	2.230294	1.939414	1.561676
C	3.449178	0.282919	-1.052373
C	1.886885	-1.421226	-0.025652
C	2.790660	0.501198	1.424869

H	-1.496124	-1.117106	-1.047091
H	-3.180419	-1.410523	-1.535033
H	-2.492916	-2.305123	-0.162861
H	-1.932681	1.336114	-0.834178
H	-3.239500	1.945787	0.222846
H	-3.635698	1.125682	-1.301661
H	-5.100952	-0.572185	-0.023557
H	-4.717491	0.267116	1.494623
H	-4.408134	-1.474920	1.341088
H	2.994828	2.705842	1.366728
H	1.835514	2.134021	2.564634
H	2.327689	-0.140829	2.179945
H	3.874487	0.456793	1.563317
H	3.034733	0.119143	-2.050832
H	4.290525	-0.401820	-0.904767
H	3.827232	1.309300	-0.996829
H	1.075847	-1.579660	0.690955
H	2.713752	-2.091012	0.233050
H	1.525910	-1.675981	-1.024900

H_2O

O	-0.067495	-0.107891	0.000000
H	0.867925	0.130380	0.000000
H	-0.550430	0.727511	0.000000

$(H_2O)_3$

O	3.745684	-1.800898	0.817264
H	4.558954	-1.305349	1.006378
H	3.451462	-1.529044	-0.067192
O	6.201048	-0.512811	1.762382
H	5.987607	-0.070491	2.593919
H	6.816762	-1.221490	1.988975
O	2.530541	-1.252692	-1.791310
H	1.619680	-0.980864	-1.620681
H	2.472875	-2.095162	-2.259900

Im

C	2.441665	1.907628	-0.227209
N	1.486906	2.668801	-0.591906
C	1.309306	3.757801	0.407121
C	3.133209	2.256608	1.073055
H	2.743634	1.063575	-0.849276
C	1.794838	5.065550	-0.243495
C	-0.177511	3.863651	0.766967
C	2.195510	3.349542	1.630120
H	4.150383	2.620963	0.872813
H	3.238021	1.387322	1.732470
H	2.737511	4.202576	2.048554
H	1.568115	2.937235	2.427672
H	1.251017	5.253256	-1.174455
H	2.863205	5.014273	-0.480970
H	1.633334	5.913278	0.431875
H	-0.546833	2.915745	1.172306

H	-0.772205	4.108493	-0.118661
H	-0.336568	4.644981	1.519184

Im-H$^-$

C	2.454025	1.816763	-0.295199
N	1.479592	2.636005	-0.573849
C	1.308403	3.749091	0.427054
C	3.127099	2.273149	1.042823
C	1.805610	5.057806	-0.219826
C	-0.180532	3.889512	0.777426
C	2.181479	3.344431	1.644457
H	4.125075	2.679753	0.807858
H	3.297508	1.420182	1.714409
H	2.702527	4.202255	2.092884
H	1.551218	2.903178	2.429549
H	1.301119	5.208507	-1.182082
H	2.882836	5.001444	-0.415944
H	1.613394	5.934510	0.418513
H	-0.555310	2.955655	1.213087
H	-0.763972	4.090046	-0.130128
H	-0.360167	4.705414	1.494409

N1

C	-0.822741	-1.695206	-0.439070
C	-1.727078	-0.543831	-0.743976
H	-2.272650	-0.676264	-1.685036
H	-2.486694	-0.417390	0.041673
C	-0.744578	0.653759	-0.799680
H	-1.175954	1.571318	-0.390057
H	-0.467504	0.852726	-1.839964
C	0.502456	0.205646	-0.007230
C	0.462210	0.618594	1.470420
H	-0.501059	0.369807	1.928313
H	0.615327	1.699127	1.557457
H	1.252499	0.105876	2.025160
C	1.826696	0.596354	-0.658983
H	1.873660	0.244199	-1.694286
H	2.665403	0.161730	-0.110526
H	1.926522	1.686883	-0.659107
N	0.365775	-1.317332	-0.048222
H	-1.059808	-2.751140	-0.457921
O	1.341797	-2.041935	0.330065

N1H$^+$

C	1.740511	0.502027	-1.780211
C	0.346083	0.294248	-2.254881
H	0.136071	0.890492	-3.148112
H	0.230298	-0.758164	-2.550219
C	-0.512675	0.684919	-1.022515
H	-1.384097	0.039149	-0.904654
H	-0.868343	1.712679	-1.134407
C	0.424451	0.582267	0.211607
C	0.374795	-0.781882	0.912658

H	0.450815	-1.607451	0.199086
H	-0.581314	-0.869821	1.435847
H	1.174075	-0.884752	1.651250
C	0.281160	1.745795	1.193650
H	0.436858	2.714107	0.707910
H	0.954152	1.651121	2.053465
H	-0.735454	1.736659	1.596671
N	1.769595	0.684390	-0.509443
H	2.662583	0.483406	-2.354479
O	2.958705	0.739386	0.159865
H	2.855141	1.398615	0.871604

N2

C	-0.699292	-1.082237	-0.088786
C	-1.435001	0.221216	-0.047555
H	-2.306527	0.234026	-0.711464
H	-1.809598	0.432760	0.965118
C	-0.347639	1.243987	-0.483360
H	-0.421550	2.189853	0.058692
H	-0.452180	1.462035	-1.550357
C	0.979019	0.520885	-0.222167
H	1.434594	0.754514	0.745234
H	1.735188	0.635060	-1.000242
N	0.597205	-0.928707	-0.178342
H	-1.106620	-2.081366	-0.008509
O	1.511522	-1.813456	-0.189762

N3

C	-0.868328	-0.725632	-0.504286
O	-1.373156	0.533062	-0.471046
C	-0.228135	1.430092	-0.559924
H	-0.412730	2.267637	0.114472
H	-0.170679	1.789596	-1.593281
C	1.001665	0.582928	-0.176711
C	1.396278	0.707469	1.299987
H	0.523722	0.600757	1.952464
H	1.851114	1.686214	1.485014
H	2.119008	-0.071290	1.556123
C	2.196153	0.774028	-1.106199
H	1.905359	0.652183	-2.154015
H	2.963027	0.031194	-0.875094
H	2.618745	1.775396	-0.973142
N	0.422815	-0.809652	-0.381292
H	-1.536252	-1.568076	-0.594141
O	1.174881	-1.854296	-0.351340

N4

C	-0.565538	-0.888470	-1.053526
C	-1.250807	0.430797	-0.930000
H	-1.606208	0.825930	-1.890476
H	-2.108763	0.399197	-0.239748
O	-0.234714	1.308314	-0.420364
C	0.908325	0.566495	-0.003125

C	0.998119	0.482846	1.518230
H	0.063657	0.098537	1.937229
H	1.178151	1.482121	1.923566
H	1.817085	-0.179056	1.810353
C	2.163911	1.125758	-0.654275
H	2.045391	1.157982	-1.740426
H	3.023711	0.499585	-0.405795
H	2.336279	2.141666	-0.288728
N	0.633055	-0.829221	-0.547188
H	-0.951508	-1.809793	-1.466202
O	1.520125	-1.731509	-0.437157

N5

C	-0.049745	-1.126470	0.021749
C	-0.661289	0.234745	0.090501
H	-1.401814	0.413417	-0.694907
H	-1.153541	0.406658	1.058384
C	0.593388	1.111303	-0.093457
H	0.597243	2.011968	0.523207
H	0.739950	1.379177	-1.147172
O	1.699722	0.297433	0.336181
N	1.245898	-1.089540	0.182748
H	-0.526627	-2.090589	-0.069046
O	2.121845	-1.945822	0.258162

OCN^{t}Bu

N	2.374071	-1.345977	0.459674
C	1.545444	-0.471598	0.515942
O	0.832629	0.473206	0.550605
C	2.461334	-2.810830	0.541528
C	1.616366	-3.426596	-0.588032
C	3.941650	-3.183772	0.369156
C	1.947716	-3.267674	1.918688
H	4.316113	-2.836768	-0.598400
H	4.065524	-4.269932	0.421624
H	4.548173	-2.725437	1.155829
H	2.036160	-4.355137	2.012115
H	0.895136	-2.997363	2.052802
H	2.529192	-2.803905	2.721036
H	1.696919	-4.518531	-0.566547
H	1.961958	-3.074369	-1.564521
H	0.560203	-3.159436	-0.477599

TS10’-3

C	1.211354	-0.916687	1.835451
C	1.427487	0.436999	-0.126103
C	1.249131	1.717233	-0.931604
H	2.211928	2.208726	-1.098396
H	0.592369	2.430867	-0.427444
C	0.650021	1.178001	-2.242764
H	-0.440197	1.268621	-2.215601
H	1.014145	1.717586	-3.123321
C	1.034617	-0.329883	-2.271523

C	-0.111430	-1.197596	-2.802195
H	0.170224	-2.253226	-2.811666
H	-0.355799	-0.878897	-3.824239
H	-0.993932	-1.097247	-2.165160
C	2.325349	-0.597226	-3.067651
H	2.636323	-1.636317	-2.927003
H	3.142489	0.056540	-2.738542
H	2.152785	-0.425471	-4.136573
C	2.025149	1.447627	2.195533
N	1.598180	0.332776	1.253332
N	1.314396	-0.624157	-0.844858
O	0.979755	-1.036481	3.007651
Cl	2.612920	-3.749285	1.958092
Cl	1.082410	-4.232200	-1.195644
Au	1.158956	-2.457481	0.504679
C	2.787753	2.566337	1.456785
C	3.026883	0.878891	3.230456
C	0.781725	2.032663	2.889370
H	3.590832	2.163431	0.831477
H	3.250248	3.206068	2.214187
H	2.145367	3.205533	0.852114
H	3.395926	1.706625	3.845409
H	3.881740	0.420897	2.722048
H	2.577781	0.135026	3.883945
H	0.093635	2.462700	2.154028
H	1.081916	2.825438	3.585180
H	0.250505	1.258019	3.444733
Cl	-1.453958	-1.595289	0.580356

TS10’-3,N1H$^+$

C	-1.104211	-1.326785	-0.194688
C	-2.916820	0.221489	-0.320881
C	-4.233813	0.701744	-0.918906
H	-5.043953	0.611585	-0.190564
H	-4.520784	0.134552	-1.807914
C	-3.906419	2.177543	-1.215760
H	-3.579509	2.284787	-2.255267
H	-4.766592	2.835915	-1.064390
C	-2.723324	2.511680	-0.261951
C	-1.675078	3.416661	-0.916939
H	-0.834208	3.591563	-0.240088
H	-2.128470	4.381398	-1.172091
H	-1.281212	2.961840	-1.830308
C	-3.195041	3.113625	1.073919
H	-2.356665	3.182237	1.772755
H	-3.974828	2.498646	1.537086
H	-3.598053	4.119400	0.914277
C	-3.389052	-2.357800	-0.220643
N	-2.485341	-1.116855	-0.224956
N	-2.135263	1.178917	0.020295
O	-0.553325	-2.365854	-0.459418

Cl	0.192793	-0.902028	2.534801
Cl	1.520206	2.107377	1.099992
Au	0.049088	0.265825	0.391186
C	-4.826778	-1.998195	0.199996
C	-2.866822	-3.351425	0.842241
C	-3.386075	-2.986983	-1.623448
H	-4.845168	-1.410781	1.123200
H	-5.355201	-2.934479	0.397958
H	-5.388089	-1.477712	-0.574667
H	-3.584963	-4.172522	0.925115
H	-2.784881	-2.865037	1.818984
H	-1.897862	-3.773780	0.585166
H	-3.780906	-2.289556	-2.369485
H	-4.019184	-3.880927	-1.626813
H	-2.376567	-3.278904	-1.919221
Cl	0.637650	0.479521	-2.087068
C	2.981849	-1.340798	0.407554
C	3.724245	-0.799201	1.572068
H	3.085985	-0.032202	2.031835
H	3.895754	-1.571138	2.328250
C	5.019876	-0.215800	0.946052
H	5.874166	-0.860931	1.169966
H	5.236149	0.778733	1.339670
C	4.787142	-0.159388	-0.592810
C	5.890402	-0.845897	-1.403150
H	6.062912	-1.870355	-1.057735
H	6.819838	-0.281289	-1.282060
H	5.638080	-0.871396	-2.466165
C	4.487207	1.249962	-1.117074
H	3.677543	1.720327	-0.552197
H	4.209201	1.220975	-2.174109
H	5.391564	1.858288	-1.016675
N	3.527529	-0.986050	-0.701283
H	2.069895	-1.929527	0.417649
O	3.026400	-1.283041	-1.932257
H	2.180238	-0.726192	-2.035640

TS10-11

C	-1.600581	1.218229	-0.027280
C	0.638981	1.679119	0.138822
C	0.055386	-0.797430	-0.309687
C	-0.890290	-1.793579	0.371171
H	-1.824595	-1.956333	-0.173183
H	-1.097780	-1.514001	1.407618
H	-0.418586	-2.779017	0.352029
C	0.113734	-1.017328	-1.826899
H	0.839818	-0.341421	-2.288193
H	-0.863281	-0.864591	-2.287883
H	0.396058	-2.056320	-2.021930
C	1.453697	-0.987677	0.311633
H	2.215410	-0.364730	-0.159816

H	1.736792	-2.032361	0.161781
H	1.442527	-0.799136	1.391407
C	0.835852	2.382036	1.468550
H	-0.106324	2.714142	1.909306
H	1.301314	1.681929	2.175089
C	1.773059	3.526998	1.046027
H	2.554061	3.740616	1.782398
H	1.194037	4.444749	0.898265
C	2.361677	3.047155	-0.321582
C	3.749694	2.403330	-0.154199
H	3.738741	1.627944	0.619442
H	4.487872	3.161293	0.132110
H	4.072377	1.941181	-1.092526
C	2.419810	4.170993	-1.362802
H	1.421729	4.583190	-1.541129
H	2.807492	3.795727	-2.315168
H	3.072629	4.979960	-1.013675
N	-0.376243	0.656405	-0.018392
N	1.421685	2.002410	-0.805986
O	-1.891950	2.373380	0.146419
Cl	-2.442634	-4.183904	-1.599340
Cl	-3.796861	-0.258282	1.893636
Cl	-3.317400	0.461350	-2.688523
Au	-3.329742	0.047102	-0.390330

TS10-11,N1H^{+}

C	1.817115	0.598267	-0.649533
C	3.862506	-0.230444	-0.071591
C	2.050300	-0.416428	1.765307
C	1.011446	0.520061	2.394651
H	0.008591	0.409905	1.977825
H	1.317391	1.567368	2.341710
H	0.909839	0.243058	3.447654
C	1.509272	-1.846215	1.622126
H	2.270532	-2.510606	1.206623
H	0.627843	-1.870308	0.977632
H	1.213058	-2.212775	2.610149
C	3.298058	-0.397142	2.669878
H	4.073646	-1.087119	2.335827
H	2.987838	-0.709560	3.669938
H	3.715784	0.611557	2.752367
C	4.877298	0.871777	-0.285370
H	4.480015	1.700271	-0.876825
H	5.176385	1.281308	0.688127
C	5.999552	0.081599	-0.986272
H	6.998242	0.360725	-0.639754
H	5.961084	0.258465	-2.065754
C	5.667477	-1.417904	-0.680031
C	6.502061	-1.965772	0.489972
H	6.442073	-1.309750	1.365100
H	7.554422	-2.044045	0.196878

H	6.149599	-2.959745	0.782099
C	5.817593	-2.316486	-1.912522
H	5.165792	-1.976352	-2.723272
H	5.553887	-3.351124	-1.673003
H	6.852982	-2.295144	-2.270654
N	2.501350	0.079561	0.372827
N	4.235356	-1.423224	-0.265510
O	2.156948	0.884579	-1.760344
Cl	-2.580769	-0.375243	3.023162
Cl	0.227968	3.273968	0.160760
Cl	-1.029916	-0.996218	-1.208410
Au	-0.254591	1.077120	-0.437293
C	-3.955021	-1.890653	0.421714
C	-4.283378	-2.808553	-0.707695
H	-3.419639	-2.860055	-1.382056
H	-4.474837	-3.826740	-0.354696
C	-5.523676	-2.146733	-1.361871
H	-6.433271	-2.663363	-1.041866
H	-5.485722	-2.182063	-2.452585
C	-5.547318	-0.681983	-0.850276
C	-6.928926	-0.217738	-0.386195
H	-7.337298	-0.889306	0.375191
H	-7.607999	-0.214669	-1.244447
H	-6.885709	0.791773	0.028355
C	-4.912571	0.313168	-1.832894
H	-3.923017	-0.023210	-2.156111
H	-4.812348	1.298666	-1.371234
H	-5.556180	0.405772	-2.712919
N	-4.630626	-0.795199	0.342656
H	-3.229660	-2.019576	1.220978
O	-4.556531	0.271327	1.142075
H	-3.791062	0.073358	1.911143

TS10-20

C	-0.539278	0.853065	-0.253896
C	1.669141	0.367659	0.275861
C	0.734865	-0.928443	-1.705490
C	-0.577130	-1.634484	-2.090431
H	-1.317500	-0.952599	-2.504685
H	-1.006489	-2.164023	-1.236936
H	-0.335000	-2.371534	-2.864561
C	1.338005	-0.208509	-2.927345
H	2.285825	0.264821	-2.662395
H	0.650974	0.553853	-3.300260
H	1.515035	-0.939268	-3.726138
C	1.695734	-2.032137	-1.210945
H	2.704329	-1.657737	-1.031587
H	1.759120	-2.804345	-1.983913
H	1.309099	-2.497775	-0.298749
C	1.614330	0.154604	1.778829
H	0.708196	0.552118	2.233455

H	1.611916	-0.925895	1.971854
C	2.912233	0.850131	2.215771
H	3.429703	0.332894	3.030338
H	2.692668	1.868787	2.555038
C	3.766254	0.900997	0.909239
C	4.773149	-0.262173	0.841749
H	4.278247	-1.223885	1.014789
H	5.553211	-0.138112	1.602465
H	5.251149	-0.297940	-0.143050
C	4.495014	2.238928	0.732706
H	3.777689	3.065513	0.711362
H	5.057824	2.253130	-0.206862
H	5.194482	2.407371	1.560797
N	0.546250	0.066767	-0.568529
N	2.792314	0.742661	-0.199737
O	-0.552844	1.726029	0.579267
Cl	-4.956811	0.109886	-0.661308
Cl	-1.637415	-1.609990	1.577466
Cl	-1.587324	1.561761	-2.072130
Au	-2.597483	-0.105736	-0.067201

TS11’-3

C	-1.839255	-0.031066	1.092812
C	0.082120	0.846972	0.057460
C	1.481999	0.895552	-0.532088
H	1.465762	0.491009	-1.549656
H	2.215001	0.323047	0.038929
C	1.761003	2.412545	-0.511291
H	2.347046	2.669356	0.377178
H	2.321906	2.744443	-1.388919
C	0.353658	3.076069	-0.420960
C	0.317666	4.273445	0.534722
H	-0.701012	4.659176	0.629591
H	0.964761	5.073579	0.158958
H	0.667397	3.986283	1.531646
C	-0.193949	3.470502	-1.803908
H	-1.232959	3.802063	-1.723784
H	-0.156852	2.629313	-2.504576
H	0.398139	4.292178	-2.220527
C	-0.027817	-1.711603	0.640037
N	-0.611904	-0.291102	0.515767
N	-0.490094	1.989269	0.128855
O	-2.378725	-0.559630	2.014585
Cl	-3.577513	-0.174667	-1.223967
Cl	-3.658257	3.673289	1.099711
Au	-2.937830	1.553086	0.311288
C	0.714325	-2.070608	-0.663646
C	-1.169774	-2.737604	0.789142
C	0.897622	-1.760358	1.865348
H	0.082978	-1.882402	-1.536804
H	0.941355	-3.139581	-0.639315

H	1.662785	-1.551287	-0.785786
H	-0.730131	-3.734718	0.703438
H	-1.914099	-2.622074	-0.003937
H	-1.672037	-2.676370	1.753504
H	1.734656	-1.061584	1.776669
H	1.312969	-2.767887	1.971228
H	0.343672	-1.523851	2.778227

TS18-19

C	0.120376	0.651107	-0.856353
C	2.318543	0.291333	0.804464
C	-0.527070	-1.334880	0.538656
C	-1.645783	-0.502890	1.179825
H	-2.281417	-0.045986	0.416481
H	-1.228086	0.281676	1.818773
H	-2.271002	-1.151835	1.801422
C	-1.093524	-2.449304	-0.363358
H	-0.290031	-2.965325	-0.895387
H	-1.809051	-2.051750	-1.085079
H	-1.616218	-3.176056	0.266508
C	0.355911	-1.985865	1.616186
H	1.180214	-2.544921	1.165943
H	-0.260654	-2.686333	2.187066
H	0.764026	-1.234419	2.294442
C	3.443426	-0.698927	0.645102
H	3.496719	-1.390768	1.490395
H	3.213377	-1.299288	-0.244693
C	4.723896	0.162031	0.470072
H	5.407205	-0.254940	-0.273493
H	5.262823	0.228251	1.420605
C	4.218827	1.566894	0.049920
C	4.240912	1.783109	-1.470321
H	3.734432	0.970980	-2.000444
H	5.277521	1.832396	-1.819669
H	3.749490	2.723705	-1.740957
C	4.905681	2.716104	0.792102
H	4.834530	2.587256	1.876719
H	4.464076	3.683014	0.525713
H	5.965390	2.752584	0.520021
N	0.372902	-0.443588	-0.287651
N	2.776719	1.466253	0.495587
O	0.270420	1.817836	-1.023007
Cl	-0.985644	-0.832733	-5.215977
Cl	-2.693833	0.231800	-2.456644
Cl	1.796039	-0.944503	-3.254298
Au	-0.479843	-0.397615	-2.945536
H	2.168693	2.277897	0.435189

TS18-2

C	-0.442922	-1.401883	1.279751
C	1.123377	-0.043551	0.258391
C	-1.271428	0.595345	-0.273094

C	-1.537586	0.009304	-1.670084
H	-1.879334	-1.024809	-1.616973
H	-0.649741	0.039490	-2.307764
H	-2.314664	0.606044	-2.158360
C	-2.578441	0.679357	0.530388
H	-2.396041	0.948632	1.573352
H	-3.146044	-0.250937	0.515422
H	-3.208533	1.449496	0.075337
C	-0.709215	2.026966	-0.396480
H	-0.513532	2.463019	0.589255
H	-1.450742	2.655882	-0.896042
H	0.202908	2.074567	-1.001884
C	1.829257	-0.422461	-1.046475
H	1.523376	-1.448649	-1.283254
H	1.542684	0.211199	-1.886415
C	3.306691	-0.297509	-0.649888
H	3.683128	0.704495	-0.888376
H	3.944678	-1.022428	-1.159975
C	3.318499	-0.507480	0.893605
C	4.349863	0.350409	1.633271
H	4.201158	1.415611	1.425695
H	5.358276	0.078621	1.306717
H	4.280751	0.195983	2.713191
C	3.490522	-2.003673	1.264690
H	2.779658	-2.639436	0.733391
H	3.345262	-2.155337	2.335712
H	4.509118	-2.298976	0.993197
N	-0.237244	-0.206526	0.512137
N	1.956443	-0.149136	1.357506
O	0.455365	-1.855626	1.954327
Cl	-3.927358	-4.124842	0.883130
Cl	-1.048583	-3.481455	-0.861184
Cl	-2.962420	-1.727497	3.100586
Au	-2.112196	-2.615772	1.086496
H	1.552328	1.028771	0.689811

TS1-2N5

C	2.680187	-0.547156	1.233304
C	0.226175	0.517209	2.000626
H	0.209495	-0.215737	2.793169
C	1.336277	-2.352765	0.172142
C	2.474471	-3.379266	0.302433
H	2.712821	-3.579633	1.350549
H	3.381797	-3.041466	-0.204028
H	2.161414	-4.317697	-0.166155
C	0.045823	-2.928973	0.780410
H	-0.782757	-2.217215	0.696207
H	0.188643	-3.179067	1.836695
H	-0.241096	-3.842459	0.251543
C	1.117440	-1.971661	-1.303614
H	0.289970	-1.261433	-1.409074

H	0.869749	-2.868068	-1.880977
H	2.021006	-1.521915	-1.723722
C	-0.920516	1.104592	1.245645
H	-1.528382	0.330208	0.772527
H	-1.570523	1.672270	1.924432
C	-0.174472	1.993518	0.228088
H	-0.622490	2.977083	0.087169
H	-0.040588	1.492342	-0.734406
O	1.148133	2.216191	0.806547
N	1.620265	-1.094760	0.907271
N	1.289703	1.254748	1.820447
O	2.528354	0.766647	1.958222
Cl	6.994615	-1.356827	1.001234
Cl	4.641667	-0.040066	-1.070503
Cl	4.547049	-1.753112	3.331647
Au	4.690089	-0.904544	1.130750

TS1-4

Au	-1.430371	-1.260337	1.133764
Cl	-0.612577	-2.401090	3.034056
Cl	-3.653620	-1.577493	1.803029
Cl	-2.116644	-0.176199	-0.858874
C	0.484678	-1.054140	0.540973
N	1.468254	-1.447343	0.003791
C	2.049837	-2.602911	-0.709114
C	2.885270	-2.058934	-1.877324
C	0.914494	-3.506865	-1.218524
C	2.936646	-3.347975	0.302910
O	0.788017	0.733781	1.315722
C	3.062245	0.904683	0.928338
C	1.676389	2.530425	-0.093057
N	1.836286	1.316023	0.814041
H	3.283881	0.041673	1.541846
C	4.014614	1.771291	0.169871
C	0.736583	3.528001	0.581608
C	1.114139	2.045935	-1.435927
C	3.146427	3.007515	-0.182482
H	3.739585	-2.702905	0.672826
H	3.391377	-4.215556	-0.184925
H	2.345880	-3.695065	1.154668
H	3.686671	-1.407304	-1.515508
H	2.260496	-1.494019	-2.575431
H	3.340388	-2.891559	-2.421831
H	1.339880	-4.352986	-1.767415
H	0.247792	-2.957801	-1.889451
H	0.324185	-3.898054	-0.385389
H	4.897653	2.024743	0.765183
H	4.377315	1.245591	-0.723656
H	3.375501	3.410958	-1.171232
H	3.323648	3.799692	0.551434
H	-0.262947	3.102501	0.693772

H	0.665966	4.427913	-0.037271
H	1.107001	3.816045	1.570255
H	1.805395	1.359238	-1.935290
H	0.959323	2.909840	-2.089525
H	0.154421	1.540697	-1.299506

TS1-4Bz

Au	-4.426093	-1.787756	-0.460850
Cl	-4.750165	-2.441212	1.789724
Cl	-6.696857	-2.070407	-0.950790
Cl	-3.949091	-1.207445	-2.705676
C	-2.468178	-1.609255	-0.031193
N	-1.377031	-2.038517	0.131649
O	-2.468044	0.363273	0.359391
C	-0.316558	0.489703	1.200322
N	-1.256932	0.829651	0.370511
H	-0.532340	-0.188620	2.015246
C	0.980401	1.157308	0.876680
C	-0.789136	1.766180	-0.737138
C	0.562221	2.241095	-0.150783
H	1.458084	1.574937	1.768682
H	1.685516	0.428069	0.455703
H	0.426343	3.198331	0.361903
H	1.309094	2.385414	-0.934619
C	-0.637093	0.936205	-2.018807
C	-1.820975	2.879193	-0.909346
H	-2.777495	2.470738	-1.242805
H	-1.461780	3.588257	-1.661745
H	-1.979920	3.420676	0.028312
H	0.125595	0.158657	-1.904256
H	-0.332368	1.594833	-2.837806
H	-1.583404	0.461514	-2.291421
C	-0.520184	-3.206578	0.212071
H	0.264126	-3.091533	-0.540634
H	-1.118338	-4.086256	-0.051973
C	2.050090	-3.648902	3.000115
C	1.481161	-3.472620	1.734655
C	1.232549	-3.702886	4.130857
C	0.093764	-3.357019	1.591232
C	-0.154817	-3.585117	3.992406
C	-0.724484	-3.415760	2.729312
H	3.127518	-3.742737	3.099417
H	2.121482	-3.433099	0.856526
H	-1.803604	-3.326572	2.629059
H	-0.795796	-3.630593	4.867767
H	1.671816	-3.839198	5.114644

TS1-4Cy

Au	-1.303777	0.485071	-1.777458
Cl	-2.589836	-0.523214	-0.070451
Cl	-3.100311	0.411285	-3.282109
Cl	0.121312	1.419775	-3.423564

C	0.247630	0.475032	-0.490040
N	1.159194	-0.071305	0.042512
O	0.061755	2.295384	0.183477
C	1.598342	2.146331	1.904058
N	1.134272	2.676787	0.814009
H	1.034801	1.372203	2.407541
C	2.897606	2.759637	2.313245
C	2.044978	3.736669	0.207792
H	1.013551	-4.582047	-0.294599
C	2.023991	-4.293937	0.026453
C	1.936745	-3.554325	1.370784
C	2.666294	-3.411964	-1.055554
H	2.593103	-5.223377	0.144714
C	1.205073	-2.208288	1.236030
C	1.928346	-2.071356	-1.201458
C	1.870422	-1.341101	0.150981
H	3.719499	-3.225781	-0.799074
H	2.669652	-3.929546	-2.021324
H	2.413882	-1.433266	-1.947459
H	0.902349	-2.246672	-1.548326
H	2.891387	-1.099507	0.472543
H	0.156623	-2.369309	0.957612
H	1.204218	-1.672420	2.192327
H	1.420959	-4.171468	2.115150
H	2.951489	-3.381607	1.758456
C	2.983646	4.015813	1.407165
H	2.918190	2.999244	3.381168
H	3.720700	2.054892	2.132798
H	2.627528	4.890331	1.960242
H	4.003556	4.222499	1.075885
C	2.766333	3.109050	-0.992419
C	1.194763	4.934231	-0.212093
H	0.491892	4.651563	-0.998928
H	1.849913	5.722534	-0.595681
H	0.629303	5.335913	0.634432
H	3.390426	2.262581	-0.687411
H	3.412805	3.862447	-1.452732
H	2.050504	2.763770	-1.742816

TS1-4Me

Au	-1.640716	0.646388	0.605041
Cl	-1.643153	0.423309	2.955497
Cl	-3.921118	1.167902	0.576440
Cl	-1.518358	0.751789	-1.760562
C	0.305590	0.129424	0.627096
N	1.191311	-0.656866	0.593075
O	1.053640	1.974664	0.785434
C	3.278392	1.401739	1.056878
N	2.306039	2.010585	0.447389
H	3.083145	0.861747	1.973947
C	4.585786	1.599321	0.360271

C	2.732278	2.716993	-0.834656
C	4.268488	2.735450	-0.647136
H	5.385108	1.861219	1.060929
H	4.896770	0.670880	-0.137623
H	4.577361	3.695776	-0.223189
H	4.788444	2.607404	-1.599024
C	2.276439	1.856855	-2.020611
C	2.091386	4.103199	-0.867099
H	1.003018	4.025012	-0.913476
H	2.441668	4.639182	-1.754679
H	2.362492	4.686128	0.018539
H	2.769050	0.878708	-2.019919
H	2.536681	2.367667	-2.952686
H	1.194221	1.703789	-2.002603
C	1.563250	-2.045368	0.507166
H	2.167650	-2.307481	1.378774
H	2.162276	-2.198649	-0.393550
H	0.674780	-2.681115	0.470589

TS1-4N2

Au	3.174909	0.359730	-3.325652
Cl	1.998667	-0.755200	-5.037864
Cl	4.713850	1.253521	-4.851312
Cl	4.310527	1.344862	-1.482007
C	1.903126	-0.450923	-1.989619
N	1.585534	-1.320591	-1.240799
C	1.959820	-2.687846	-0.821397
C	2.381237	-2.604942	0.654498
C	3.114398	-3.200903	-1.697688
C	0.710525	-3.567703	-0.988057
O	0.674468	1.037247	-1.830361
C	-0.461549	0.393289	0.085012
C	0.994028	2.214208	0.258527
N	0.333677	1.174479	-0.581078
H	-0.981802	-0.403551	-0.428805
C	-0.537291	0.775345	1.528523
H	0.928235	3.164116	-0.273918
H	2.049478	1.936622	0.336356
C	0.199948	2.147035	1.574198
H	-0.116659	-3.197323	-0.374414
H	0.939495	-4.590408	-0.673582
H	0.387948	-3.591297	-2.032681
H	1.560158	-2.234649	1.276474
H	3.242814	-1.942614	0.777599
H	2.657571	-3.601925	1.010606
H	3.374639	-4.221104	-1.398205
H	4.001678	-2.571770	-1.582861
H	2.829035	-3.210583	-2.753165
H	-1.571986	0.834360	1.881610
H	-0.038427	0.014632	2.143498
H	0.848771	2.235829	2.447245

H	-0.530572	2.959047	1.617406

TS1-4N3

Au	3.463460	-2.258650	-2.713224
Cl	1.678149	-3.024225	-4.057827
Cl	5.051786	-3.183925	-4.162352
Cl	5.158572	-1.527363	-1.223385
C	2.084368	-1.516835	-1.450965
N	1.311015	-1.557390	-0.558937
C	0.627560	-2.346588	0.480077
C	0.649045	-1.533154	1.782937
C	1.373953	-3.681315	0.648996
C	-0.814427	-2.577143	-0.003218
O	2.055973	0.379203	-2.298290
C	0.295384	1.279307	-1.072247
C	2.360696	2.284599	-0.755667
N	1.529643	1.242644	-1.475468
H	-0.484750	0.619125	-1.419743
O	0.014913	2.246027	-0.194809
C	3.158731	3.087856	-1.781622
C	3.270696	1.580938	0.256520
C	1.215240	3.089071	-0.094135
H	-1.347836	-1.629080	-0.122768
H	-1.351145	-3.177640	0.737364
H	-0.825826	-3.109510	-0.958028
H	0.140235	-0.572663	1.657211
H	1.676362	-1.348535	2.110503
H	0.134381	-2.093338	2.569121
H	0.886026	-4.276049	1.427549
H	2.413623	-3.511115	0.942123
H	1.363099	-4.253349	-0.282707
H	1.378441	3.292128	0.964381
H	0.991934	4.018125	-0.625694
H	3.865984	2.434209	-2.297066
H	3.721183	3.877802	-1.274137
H	2.502058	3.547258	-2.526413
H	2.686190	1.040057	1.006990
H	3.885094	2.327329	0.770179
H	3.933148	0.872115	-0.246699

TS1-4N4

Au	4.162437	-1.334333	-2.504750
Cl	2.861825	-2.466715	-4.117748
Cl	6.135504	-1.710838	-3.711256
Cl	5.349114	-0.236959	-0.771206
C	2.466393	-1.075436	-1.441319
N	1.664243	-1.465584	-0.647876
C	1.392295	-2.649817	0.200616
C	1.337228	-2.159186	1.655917
C	2.503791	-3.695556	0.015517
C	0.031223	-3.211793	-0.240582
O	1.986184	0.645780	-2.093434

C	-0.099542	0.824051	-1.083661
C	1.470262	2.457454	-0.519459
N	1.101148	1.228416	-1.339333
H	-0.525045	-0.041968	-1.569643
C	-0.734279	1.755780	-0.103279
C	2.013514	3.543084	-1.431430
C	2.433252	2.044488	0.588671
O	0.191789	2.841547	-0.010839
H	-0.762549	-2.468577	-0.113209
H	-0.218509	-4.083779	0.371348
H	0.058395	-3.522148	-1.288865
H	0.552486	-1.407931	1.789321
H	2.294673	-1.725622	1.958387
H	1.118283	-3.003420	2.316617
H	2.292405	-4.566902	0.643379
H	3.476172	-3.289125	0.307953
H	2.561635	-4.025919	-1.025258
H	-1.699799	2.141056	-0.449736
H	-0.888088	1.271208	0.873466
H	2.954516	3.219252	-1.881904
H	2.194422	4.442819	-0.837991
H	1.294419	3.778911	-2.219550
H	1.975815	1.298985	1.244983
H	2.678120	2.928070	1.183537
H	3.353818	1.629387	0.169635

TS1-4Ph

Au	-1.000280	3.117387	2.221733
Cl	0.352606	3.696415	4.062049
Cl	-2.762281	4.440601	3.005747
Cl	-2.279572	2.376629	0.360386
C	0.474635	1.924088	1.547755
N	0.985305	0.860622	1.415397
O	1.543344	3.315860	0.614642
C	3.348686	2.005692	0.006598
N	2.343102	2.782836	-0.259946
H	3.622107	1.818223	1.036639
C	4.007598	1.497375	-1.233559
C	2.067760	2.940554	-1.750891
C	3.391633	2.394614	-2.338979
H	5.098129	1.574571	-1.178742
H	3.772846	0.433582	-1.375755
H	4.070328	3.225345	-2.555264
H	3.220535	1.851561	-3.270931
C	0.849274	2.075903	-2.100214
C	1.813694	4.416880	-2.049975
H	0.914860	4.766423	-1.537229
H	1.672939	4.545191	-3.127705
H	2.658560	5.036836	-1.734777
H	1.043286	1.013889	-1.917413
H	0.616644	2.201705	-3.161995

H	-0.027167	2.375213	-1.519832
C	-0.341267	-2.575459	1.277608
C	-0.288192	-1.183848	1.205465
C	0.789852	-3.311759	1.644403
C	0.920492	-0.534343	1.497557
C	1.987007	-2.651967	1.936475
C	2.061921	-1.261090	1.854801
H	-1.274105	-3.083574	1.053624
H	-1.158952	-0.598034	0.928723
H	2.983663	-0.737734	2.086060
H	2.865604	-3.218682	2.228818
H	0.737616	-4.394353	1.704876

TS1-4PhCl

Au	-1.191507	2.765988	2.308861
Cl	0.006812	3.078559	4.312713
Cl	-3.009262	3.986326	3.125257
Cl	-2.322063	2.289566	0.271601
C	0.330134	1.662579	1.589407
N	0.849254	0.629961	1.322547
O	1.493651	3.189934	0.991692
C	3.353449	1.983777	0.335582
N	2.365844	2.797951	0.113923
H	3.539894	1.632501	1.342088
C	4.118788	1.677222	-0.909823
C	2.217653	3.195758	-1.351134
C	3.589557	2.741699	-1.906059
H	5.200172	1.740023	-0.751969
H	3.907284	0.650923	-1.240198
H	4.277628	3.592163	-1.932347
H	3.499856	2.353261	-2.922872
C	1.039061	2.406395	-1.935892
C	1.981359	4.702785	-1.429678
H	1.039694	4.973501	-0.947144
H	1.934399	5.003498	-2.480915
H	2.792254	5.257144	-0.947334
H	1.224772	1.327641	-1.906805
H	0.896833	2.699565	-2.980379
H	0.114395	2.616662	-1.392595
C	-0.447865	-2.705654	0.439108
C	-0.391356	-1.328650	0.641635
C	0.666711	-3.493982	0.736780
C	0.788968	-0.751640	1.133862
C	1.841399	-2.923781	1.231597
C	1.905355	-1.544455	1.421288
H	-1.354112	-3.163781	0.059035
H	-1.246892	-0.698205	0.420853
H	2.808986	-1.087181	1.809590
H	2.695114	-3.550107	1.464290
Cl	0.590660	-5.226266	0.485044

TS1-4PhCl$_3$

Au	-1.625348	1.765184	-0.441820
Cl	-2.662538	1.104671	1.573392
Cl	-3.512740	2.981534	-1.090922
Cl	-0.511819	2.331711	-2.454910
C	-0.028793	0.660921	0.121135
N	0.510084	-0.390704	0.240373
O	1.050815	2.103634	0.856052
C	2.806042	0.902772	1.777962
N	2.313674	1.801486	0.981868
H	2.154009	0.361701	2.451908
C	4.285483	0.772104	1.620271
C	3.350427	2.457811	0.075296
C	4.653742	2.030914	0.793319
H	4.795414	0.728653	2.587764
H	4.527051	-0.162541	1.095549
H	4.983008	2.827518	1.467524
H	5.458191	1.842183	0.079333
C	3.205290	1.847123	-1.324399
C	3.107536	3.965553	0.059101
H	2.138054	4.196010	-0.388009
H	3.889879	4.446137	-0.536442
H	3.136462	4.383929	1.069875
H	3.406348	0.770844	-1.317457
H	3.925662	2.323782	-1.996154
H	2.201369	2.015013	-1.722557
C	1.167343	-3.724386	-1.225211
C	0.947082	-2.352738	-1.121018
C	1.142975	-4.506598	-0.071792
C	0.707496	-1.747903	0.130907
C	0.904446	-3.943817	1.181348
C	0.696003	-2.570644	1.274759
H	1.345483	-4.170083	-2.195917
Cl	0.959923	-1.376533	-2.559810
Cl	0.394106	-1.865063	2.841229
H	0.877422	-4.558530	2.072363
Cl	1.415179	-6.228790	-0.198471

TS1-4PhMe

Au	-2.310949	3.039276	0.314451
Cl	-1.875891	3.636399	2.552130
Cl	-4.276628	4.307937	0.285270
Cl	-2.671645	2.284943	-1.909725
C	-0.662523	1.883805	0.327210
N	-0.116367	0.834163	0.422684
O	0.673429	3.317328	-0.058014
C	2.597461	2.056003	0.163836
N	1.780584	2.809612	-0.508059
H	2.413337	1.871514	1.214143
C	3.730740	1.568371	-0.678095
C	2.158987	2.965984	-1.976484
C	3.620970	2.457257	-1.944612

H	4.693850	1.668130	-0.167524
H	3.600519	0.500832	-0.903099
H	4.306027	3.306047	-1.856133
H	3.875100	1.915910	-2.858437
C	1.226813	2.069485	-2.802192
C	2.017686	4.435830	-2.367126
H	0.978843	4.761177	-2.278052
H	2.335320	4.563063	-3.406713
H	2.639388	5.076773	-1.734423
H	1.345892	1.013865	-2.537039
H	1.470627	2.184230	-3.862775
H	0.179801	2.348429	-2.659010
C	-1.318139	-2.615270	-0.085105
C	-1.256742	-1.226129	-0.144272
C	-0.344339	-3.366350	0.594743
C	-0.190873	-0.561488	0.481494
C	0.711494	-2.677183	1.207633
C	0.800224	-1.286124	1.148733
H	-2.144471	-3.125530	-0.572871
H	-2.011705	-0.652360	-0.672317
H	1.619591	-0.763034	1.630530
H	1.477829	-3.234234	1.739523
C	-0.450166	-4.870381	0.677246
H	0.485980	-5.319775	1.019885
H	-0.701183	-5.306510	-0.295185
H	-1.238089	-5.168507	1.379621

TS1-4Xyl

Au	-6.556648	-2.408031	1.521685
Cl	-6.360971	-3.161315	3.751359
Cl	-8.833035	-2.969890	1.454960
Cl	-6.606851	-1.649576	-0.724065
C	-4.577083	-1.984157	1.564871
N	-3.458731	-2.360306	1.392723
O	-4.662530	-0.232716	2.182220
C	-2.390090	0.202436	2.369032
N	-3.584270	0.473859	1.944097
H	-2.227686	-0.629825	3.039827
C	-1.381002	1.166011	1.837030
C	-3.657715	1.672495	1.007233
C	-2.263320	2.301412	1.254454
H	-0.697171	1.510739	2.618897
H	-0.763581	0.675075	1.072772
H	-2.346444	3.111534	1.985160
H	-1.848909	2.721117	0.335567
C	-3.842164	1.150003	-0.422227
C	-4.825008	2.560138	1.437055
H	-5.776144	2.037404	1.314686
H	-4.838333	3.458390	0.812077
H	-4.726344	2.867979	2.482532
H	-2.981401	0.555775	-0.744739

H	-3.941256	2.001460	-1.102217
H	-4.742130	0.535182	-0.505063
C	-1.264740	-4.600309	-0.544686
C	-2.190570	-3.586642	-0.271441
C	-0.715336	-5.374124	0.477452
C	-2.545400	-3.381553	1.076214
C	-1.089292	-5.144979	1.801706
C	-2.008505	-4.143509	2.133917
H	-0.981742	-4.784429	-1.577225
C	-2.791407	-2.756027	-1.377024
C	-2.427673	-3.907532	3.563647
H	-0.670336	-5.754309	2.597509
H	-0.001837	-6.158011	0.242238
H	-2.159612	-2.899684	3.905049
H	-1.936624	-4.621674	4.228999
H	-3.510609	-4.005435	3.693384
H	-2.449426	-3.111527	-2.351977
H	-2.503250	-1.701906	-1.285854
H	-3.885814	-2.785761	-1.366137

TS1-6L

C	0.993023	-1.401821	0.589265
N	2.202020	-1.443072	0.275208
C	2.882375	-2.564007	-0.397276
C	3.477921	-2.024066	-1.711022
C	1.931654	-3.737896	-0.698438
C	4.016146	-3.035263	0.533270
O	0.674472	-0.003415	1.307028
C	2.892855	0.676136	1.240431
C	1.353058	2.031261	0.051309
N	1.620861	0.940296	1.056644
H	3.204572	0.010285	2.030445
C	3.758887	1.665048	0.523877
C	0.771899	3.230861	0.815281
C	0.385743	1.543590	-1.027617
C	2.783515	2.305555	-0.493924
H	4.703759	-2.212212	0.756089
H	4.588726	-3.842801	0.063763
H	3.606581	-3.406438	1.478160
H	4.157560	-1.188074	-1.513945
H	2.683804	-1.672200	-2.377641
H	4.039680	-2.808791	-2.229719
H	2.481312	-4.546415	-1.194229
H	1.112818	-3.419133	-1.349564
H	1.489448	-4.126431	0.222953
H	4.166318	2.397440	1.235514
H	4.616587	1.182251	0.045727
H	2.901124	1.821580	-1.467734
H	2.963001	3.375443	-0.628268
H	-0.158818	2.949692	1.316826
H	0.557535	4.049614	0.120386

H	1.473098	3.596793	1.572897
H	0.763233	0.643134	-1.518252
H	0.267928	2.330448	-1.779988
H	-0.593966	1.313168	-0.602989

TS1-6N5

Au	-3.229272	0.142144	1.193755
Cl	-3.158750	-0.523795	3.453181
Cl	-5.588771	0.243480	1.202071
Cl	-3.106818	0.836794	-1.065856
C	-1.136030	-0.141894	1.104532
N	-0.349072	-1.068569	0.867201
O	-0.796627	1.132699	1.329783
C	1.292077	2.089030	0.241515
N	0.804400	1.368327	1.173717
H	0.702583	2.298588	-0.643058
C	2.669792	2.555459	0.612768
O	1.574517	1.224773	2.287168
C	2.896977	1.777881	1.929577
H	3.407715	2.314116	-0.157018
H	2.665799	3.644602	0.743435
H	3.571666	0.927942	1.806021
H	3.207640	2.395286	2.771995
C	-0.567057	-2.510751	0.647537
C	-1.982321	-2.847920	0.147194
C	0.472411	-2.937720	-0.406074
C	-0.286914	-3.214006	1.989688
H	0.285582	-2.434647	-1.360443
H	0.419793	-4.018352	-0.571452
H	1.484761	-2.686865	-0.073262
H	-0.364732	-4.299121	1.864874
H	-1.008201	-2.896464	2.747905
H	0.720308	-2.978210	2.347902
H	-2.037644	-3.915974	-0.087495
H	-2.228283	-2.284525	-0.757461
H	-2.738210	-2.637547	0.908950

TS22’-26

C	2.122488	2.270680	-0.049149
C	0.593292	0.364930	0.059717
C	0.359220	-1.028180	-0.524554
H	0.437971	-1.786549	0.259887
H	1.077431	-1.280172	-1.307518
C	-1.085678	-0.902484	-1.019958
H	-1.101696	-0.519840	-2.046464
H	-1.632261	-1.850540	-0.995782
C	-1.698644	0.154357	-0.069647
C	-2.815355	0.955662	-0.735480
H	-3.255012	1.671635	-0.038493
H	-3.594793	0.256937	-1.067562
H	-2.440773	1.528658	-1.586338
C	-2.195442	-0.486747	1.241484

H	-2.468508	0.292089	1.956873
H	-1.429791	-1.126562	1.697200
H	-3.079380	-1.101633	1.035748
C	3.154382	0.114018	0.358002
N	1.876232	0.925120	0.225629
N	-0.504479	1.009579	0.250048
O	1.344363	3.203427	0.113522
Cl	0.419928	4.690882	2.723486
Cl	-2.575986	2.916113	2.421640
Au	-0.530095	3.088809	1.151356
C	2.912157	-1.205106	1.116793
C	4.134271	0.946259	1.215708
C	3.776223	-0.141347	-1.026362
H	2.274786	-1.045948	1.992477
H	3.877814	-1.577348	1.472123
H	2.476891	-1.989119	0.496930
H	5.060711	0.376773	1.350704
H	3.704687	1.154707	2.200591
H	4.372667	1.898798	0.739547
H	3.122248	-0.743677	-1.663770
H	4.727224	-0.675481	-0.917956
H	3.964664	0.811349	-1.529185
Cl	-1.468366	4.070102	-1.325599

TS2-10Bz,N1

C	0.731424	0.075234	0.961398
C	-1.374303	1.116332	1.023307
C	-1.404117	2.653008	1.219994
H	-0.526368	3.125976	0.777084
H	-2.284404	3.080963	0.731788
C	-1.452503	2.794912	2.758036
H	-2.146603	3.571641	3.091023
H	-0.461123	3.045746	3.147602
C	-1.864329	1.388177	3.271859
C	-3.406558	1.243579	3.412361
H	-3.924478	1.555653	2.501021
H	-3.740273	1.876563	4.240354
H	-3.680394	0.208231	3.632367
C	-1.189936	0.983633	4.591753
H	-0.103178	1.018934	4.493258
H	-1.477997	-0.030625	4.882660
H	-1.501193	1.675916	5.380954
N	-0.321030	0.514412	0.210705
N	-1.471583	0.452404	2.216000
O	0.669679	0.067063	2.188385
Cl	4.369950	-1.689619	-0.880167
Cl	3.495658	1.366981	0.371066
Cl	1.158697	-2.700593	-0.227624
Au	2.427978	-0.710250	0.069669
C	-2.582392	-2.044082	0.343727
C	-2.688012	-3.465292	-0.094586

H	-1.695115	-3.895800	-0.255953
H	-3.170234	-4.063013	0.690771
C	-3.531989	-3.375471	-1.391017
H	-4.262865	-4.183346	-1.471059
H	-2.873082	-3.434628	-2.261953
C	-4.226891	-1.991714	-1.352854
C	-5.651136	-2.043488	-0.781230
H	-5.684002	-2.606154	0.157397
H	-6.312573	-2.537018	-1.499464
H	-6.028937	-1.034489	-0.596837
C	-4.186499	-1.247644	-2.686428
H	-3.160996	-1.143868	-3.053252
H	-4.630411	-0.253775	-2.595520
H	-4.755542	-1.817198	-3.427636
N	-3.361714	-1.263810	-0.334468
H	-1.962115	-1.649326	1.141082
O	-3.525577	0.039971	-0.200442
H	-2.410105	0.668990	0.490448
C	-0.359460	0.569663	-1.264420
H	-1.229298	-0.005230	-1.592137
H	0.527680	0.041868	-1.616453
C	0.664640	4.050818	-2.467773
C	0.726877	2.775584	-1.903020
C	-0.538500	4.531810	-2.995321
C	-0.419010	1.966811	-1.855813
C	-1.681068	3.729580	-2.957773
C	-1.619223	2.452962	-2.390720
H	1.559269	4.665675	-2.501601
H	1.666378	2.412339	-1.495127
H	-2.510247	1.830853	-2.359993
H	-2.617852	4.093184	-3.370612
H	-0.581976	5.522859	-3.437830

TS2-10Cy,N1

C	-0.524029	0.817656	-0.202515
C	1.481001	0.975017	0.996347
C	1.480332	1.781031	2.320995
H	0.524549	1.704165	2.842560
H	2.257562	1.407667	2.996646
C	1.775972	3.212314	1.827084
H	2.424677	3.774137	2.505482
H	0.841627	3.771605	1.719054
C	2.419070	3.012447	0.426466
C	3.964117	2.921034	0.507752
H	4.278321	2.209696	1.278231
H	4.371369	3.904090	0.763412
H	4.381004	2.612510	-0.455310
C	2.028481	4.100280	-0.587503
H	0.944106	4.143455	-0.702919
H	2.470204	3.896657	-1.567391
H	2.392076	5.071126	-0.233665

N	0.309649	0.169343	0.677682
N	1.920181	1.712007	-0.056299
O	-0.157932	1.825530	-0.797503
Cl	-4.668302	-0.432199	-1.238851
Cl	-3.234202	1.783982	0.934970
Cl	-1.514258	-1.246722	-2.270789
Au	-2.454713	0.209238	-0.653210
C	5.373843	-0.421414	0.251004
C	6.252962	-0.586227	-0.941686
H	6.779865	0.339936	-1.193180
H	7.026855	-1.336521	-0.727191
C	5.259996	-1.041447	-2.040705
H	5.685447	-1.804722	-2.695668
H	4.981587	-0.186123	-2.662827
C	4.005292	-1.571472	-1.301042
C	4.033171	-3.089531	-1.073897
H	4.992443	-3.420480	-0.661564
H	3.875368	-3.597068	-2.029864
H	3.236360	-3.390847	-0.389835
C	2.697306	-1.114287	-1.941967
H	2.620036	-0.024564	-1.968961
H	1.824018	-1.504011	-1.417781
H	2.663547	-1.492471	-2.968518
N	4.192647	-0.917601	0.068351
H	5.633340	-0.001876	1.215847
O	3.255078	-0.988587	0.990348
H	2.415878	0.082861	0.968987
H	-2.311195	-3.369707	2.244646
C	-1.387567	-3.283696	2.832891
C	-1.351177	-1.907965	3.514792
C	-0.176277	-3.474769	1.907908
H	-1.417986	-4.080653	3.585734
C	-1.249766	-0.772585	2.481893
C	-0.048274	-2.333802	0.882697
C	-0.006729	-0.973629	1.597311
H	0.740039	-3.521743	2.515674
H	-0.248627	-4.431628	1.377581
H	0.863435	-2.462513	0.292431
H	-0.887975	-2.361580	0.182549
H	0.859844	-0.992911	2.267935
H	-2.154164	-0.771151	1.867718
H	-1.216343	0.202627	2.977719
H	-2.248534	-1.759185	4.125860
H	-0.492327	-1.862111	4.201696

TS2-10,H_2O

C	-0.314053	-0.713255	-0.822470
C	1.176888	0.062757	0.794651
C	-0.068189	-2.188931	1.303188
C	-1.592414	-2.376374	1.408070
H	-2.026832	-2.813837	0.508414

H	-2.106826	-1.433189	1.606236
H	-1.797529	-3.066472	2.232302
C	0.594299	-3.478146	0.786607
H	1.683980	-3.404692	0.818867
H	0.287857	-3.708108	-0.234409
H	0.293035	-4.313151	1.427850
C	0.452732	-1.894839	2.724492
H	1.531143	-1.728231	2.755548
H	0.248282	-2.777855	3.335593
H	-0.063278	-1.051761	3.189267
C	0.692450	1.104097	1.832613
H	-0.365994	0.967907	2.065565
H	1.251796	1.006249	2.768130
C	0.971057	2.447510	1.124162
H	1.364927	3.211323	1.800422
H	0.050266	2.837987	0.680482
C	1.974742	2.093891	-0.005965
C	3.449205	2.240276	0.449296
H	3.635636	1.727683	1.398042
H	3.675112	3.302523	0.583030
H	4.129046	1.836441	-0.306696
C	1.755283	2.892910	-1.299659
H	0.737461	2.756296	-1.669560
H	2.452224	2.573461	-2.080081
H	1.923755	3.955995	-1.098087
N	0.283240	-1.022217	0.377526
N	1.751511	0.663753	-0.278754
O	0.018461	0.288996	-1.459809
Cl	-3.201890	-3.108113	-3.204331
Cl	-3.426733	-0.529271	-0.994120
Cl	0.185014	-3.011691	-2.814922
Au	-1.687457	-1.852214	-1.883380
O	3.319959	-1.488383	1.023095
H	2.300872	-0.603314	1.070607
H	4.201456	-1.122200	1.266443
H	3.316025	-1.689948	0.033890
O	5.808556	-0.548743	1.761986
H	6.266996	-1.069372	2.434854
H	6.464304	-0.349091	1.080475
O	3.032729	-1.592059	-1.589217
H	2.590399	-0.720175	-1.573879
H	2.384189	-2.188831	-2.007813

TS2-10Me,N1

C	-0.544870	2.844623	0.630850
C	1.274454	1.526245	1.299244
C	1.059861	0.698021	2.591117
H	0.014893	0.398621	2.704901
H	1.666009	-0.212952	2.565984
C	1.518381	1.678689	3.694511
H	2.101619	1.191113	4.480506

H	0.650251	2.148499	4.166956
C	2.342737	2.760211	2.942419
C	3.851400	2.391582	2.857135
H	3.996862	1.375006	2.480280
H	4.283715	2.458681	3.860284
H	4.382761	3.085321	2.200326
C	2.191399	4.173046	3.526185
H	1.141911	4.473998	3.531796
H	2.757740	4.901191	2.938675
H	2.571633	4.180663	4.552899
N	0.149312	1.695922	0.387939
N	1.851089	2.743808	1.561845
O	-0.079981	3.721322	1.352849
Cl	-4.512019	3.473785	-1.250341
Cl	-3.315094	2.100308	1.668492
Cl	-1.222856	3.915293	-2.159122
Au	-2.390544	3.106283	-0.255379
C	2.612694	2.576227	-1.650325
C	2.537659	3.085770	-3.048673
H	1.616686	3.657912	-3.201822
H	3.375692	3.768076	-3.245393
C	2.593627	1.792476	-3.901778
H	3.225194	1.903695	-4.786164
H	1.586359	1.536214	-4.242004
C	3.130451	0.681974	-2.964290
C	4.645361	0.462199	-3.087008
H	5.191009	1.410016	-3.035983
H	4.866896	-0.009332	-4.049090
H	5.005513	-0.191314	-2.288102
C	2.366064	-0.636162	-3.071246
H	1.291364	-0.483391	-2.936878
H	2.717602	-1.354185	-2.326779
H	2.525182	-1.059696	-4.067563
N	2.880567	1.310454	-1.601130
H	2.471409	3.141231	-0.734729
O	3.014966	0.561032	-0.523945
H	2.132708	1.054830	0.552160
C	-0.425696	0.524831	-0.282477
H	-1.130981	-0.002238	0.367653
H	0.392301	-0.142681	-0.555780
H	-0.944457	0.842817	-1.187887

TS2-10,N1

C	-0.591904	0.468630	-0.186740
C	1.402699	1.277696	0.707227
C	-0.064160	-0.232983	2.263260
C	-1.500693	0.075777	2.724950
H	-2.253216	-0.493337	2.176563
H	-1.742779	1.136327	2.628440
H	-1.589865	-0.209225	3.778104
C	0.149829	-1.753944	2.169323

H	1.204783	-1.983819	1.998437
H	-0.448005	-2.194427	1.369357
H	-0.149679	-2.217599	3.115302
C	0.882883	0.334094	3.341087
H	1.938839	0.195282	3.104041
H	0.689726	-0.218417	4.264666
H	0.692041	1.388752	3.549618
C	1.367602	2.686614	1.354519
H	0.422951	2.870441	1.869482
H	2.172747	2.792960	2.089250
C	1.563200	3.613239	0.139210
H	2.159338	4.501616	0.368147
H	0.591389	3.948712	-0.235574
C	2.236320	2.705905	-0.922711
C	3.780588	2.755824	-0.819812
H	4.117530	2.591251	0.208824
H	4.131656	3.742101	-1.138500
H	4.232646	2.002453	-1.471493
C	1.816018	3.027830	-2.365185
H	0.732020	2.966362	-2.472589
H	2.271065	2.325480	-3.070205
H	2.145237	4.040946	-2.620273
N	0.247309	0.399838	0.905558
N	1.797093	1.332526	-0.591214
O	-0.235592	1.014966	-1.228954
Cl	-4.760275	-1.024659	-0.648046
Cl	-3.280489	1.921579	0.251804
Cl	-1.634592	-2.344966	-0.996964
Au	-2.535387	-0.250815	-0.340058
C	5.277956	-0.248765	0.164410
C	6.019332	-0.942984	-0.926853
H	6.429443	-0.236871	-1.656204
H	6.876143	-1.484298	-0.501821
C	4.945489	-1.885065	-1.525483
H	5.354790	-2.856480	-1.810604
H	4.512967	-1.428656	-2.420255
C	3.847057	-2.034101	-0.442830
C	4.062411	-3.249862	0.470251
H	5.092398	-3.304614	0.838953
H	3.849479	-4.161959	-0.094621
H	3.386338	-3.213313	1.327747
C	2.434285	-1.995525	-1.017036
H	2.240599	-1.060315	-1.546473
H	1.675007	-2.113553	-0.244062
H	2.323847	-2.827671	-1.719342
N	4.130044	-0.792714	0.406211
H	5.614095	0.583968	0.770469
O	3.319962	-0.430977	1.385049
H	2.433528	0.485302	1.035518

TS2-10N2,N2

C	2.319324	-1.372931	-1.868025
C	0.649368	-1.855499	-0.324307
C	2.996847	-1.227929	0.645260
C	4.349654	-1.903353	0.359232
H	4.954999	-1.348156	-0.359117
H	4.227591	-2.921651	-0.016277
H	4.917497	-1.940720	1.294173
C	3.201257	0.270037	0.933138
H	2.275247	0.725977	1.293534
H	3.543283	0.803900	0.044613
H	3.958265	0.384971	1.715974
C	2.409661	-1.900278	1.902852
H	1.433819	-1.498862	2.185215
H	3.090369	-1.695475	2.733490
H	2.340310	-2.985415	1.798076
C	0.392684	-3.351837	-0.006860
H	1.314564	-3.934035	-0.070869
H	-0.004644	-3.466226	1.006487
C	-0.639462	-3.765734	-1.081712
H	-1.437378	-4.396575	-0.681138
H	-0.150100	-4.316504	-1.889617
C	-1.164688	-2.418852	-1.616954
H	-2.100716	-2.101070	-1.131614
H	-1.353642	-2.399021	-2.694556
N	2.025356	-1.392564	-0.521553
N	-0.154349	-1.405722	-1.323239
O	1.439295	-1.569179	-2.708481
Cl	6.141916	-0.315205	-3.872472
Cl	4.592497	-3.214468	-2.951416
Cl	3.469592	1.374691	-2.564944
Au	4.133774	-0.904482	-2.754359
C	-2.067468	1.165816	0.229096
C	-2.267993	2.288258	-0.734564
H	-3.031711	2.049157	-1.481677
H	-2.622658	3.178256	-0.195673
C	-0.851140	2.479083	-1.346000
H	-0.601383	3.529773	-1.500159
H	-0.787842	1.970906	-2.310757
C	0.100941	1.801401	-0.349025
H	0.559236	2.483526	0.373721
H	0.879360	1.198859	-0.814799
N	-0.815463	0.907891	0.424011
H	-2.818154	0.606693	0.775665
O	-0.343238	0.011898	1.272190
H	0.143561	-0.990880	0.544724

TS2-10N3,N3

C	-0.564208	0.506600	-0.165112
C	1.473316	1.246963	0.673055
C	-0.044761	-0.087675	2.320649
C	-1.487896	0.249850	2.733754

H	-2.231511	-0.347777	2.203064
H	-1.718432	1.305545	2.576458
H	-1.598141	0.023464	3.798753
C	0.177223	-1.609348	2.334680
H	1.229849	-1.845424	2.156165
H	-0.436919	-2.112043	1.584923
H	-0.094737	-2.001922	3.320220
C	0.889375	0.574496	3.353163
H	1.945792	0.375995	3.160441
H	0.655744	0.140194	4.329184
H	0.735452	1.652881	3.408432
O	1.442274	2.525767	1.285358
C	1.529548	3.489466	0.219944
H	2.116853	4.339587	0.575891
H	0.523026	3.826019	-0.056578
C	2.202139	2.705409	-0.930230
C	3.743987	2.807739	-0.855993
H	4.100916	2.598788	0.157295
H	4.053016	3.823311	-1.122739
H	4.208931	2.112491	-1.560993
C	1.716263	3.108960	-2.327004
H	0.630982	3.026885	-2.399423
H	2.162190	2.465561	-3.091092
H	2.013999	4.143203	-2.530389
N	0.272463	0.451785	0.922923
N	1.819480	1.305574	-0.633918
O	-0.196024	1.022187	-1.221499
Cl	-4.677667	-1.111220	-0.656606
Cl	-3.318980	1.906977	0.118226
Cl	-1.523801	-2.361088	-0.868115
Au	-2.490559	-0.260414	-0.335761
C	5.176605	-0.303984	-0.011513
O	5.753768	-0.888419	-1.046817
C	4.816531	-1.920855	-1.530629
H	5.403175	-2.820028	-1.717505
H	4.391013	-1.541396	-2.462384
C	3.751368	-2.088951	-0.418066
C	4.017127	-3.293437	0.493627
H	5.054502	-3.314189	0.843424
H	3.816357	-4.216453	-0.058568
H	3.355801	-3.264459	1.362491
C	2.329763	-2.080054	-0.973590
H	2.116509	-1.157339	-1.517097
H	1.590606	-2.189181	-0.179736
H	2.207995	-2.929819	-1.652849
N	4.057413	-0.831702	0.374529
H	5.653806	0.539396	0.468046
O	3.355539	-0.438197	1.434386
H	2.466739	0.468684	1.083495

TS2-10N4,N4

C	-0.692426	0.466350	-0.201166
C	1.376655	1.115755	0.671367
C	-0.041063	-0.517140	2.125833
C	-1.503676	-0.444710	2.602244
H	-2.178904	-1.045830	1.991080
H	-1.878105	0.580555	2.630801
H	-1.545456	-0.857533	3.615033
C	0.349850	-1.982351	1.860442
H	1.418207	-2.067948	1.648000
H	-0.221520	-2.390167	1.023459
H	0.131647	-2.582131	2.750614
C	0.815496	0.055226	3.272438
H	1.885847	0.064481	3.059512
H	0.672794	-0.589502	4.143618
H	0.488900	1.059978	3.555912
C	1.491898	2.478231	1.407573
H	0.508542	2.970773	1.437409
H	1.904245	2.421649	2.413916
O	2.423561	3.165105	0.586542
C	2.261555	2.662477	-0.757974
C	3.627511	2.676244	-1.444938
H	4.348366	2.084463	-0.876671
H	3.993017	3.704600	-1.502296
H	3.545337	2.271003	-2.456428
C	1.254462	3.526141	-1.544917
H	0.296170	3.578556	-1.027689
H	1.080009	3.104708	-2.536760
H	1.674986	4.531544	-1.638135
N	0.196771	0.289611	0.849677
N	1.734539	1.304076	-0.621719
O	-0.370611	1.092289	-1.202783
Cl	-4.895292	-0.928299	-0.630397
Cl	-3.332652	1.895566	0.520828
Cl	-1.787271	-2.245883	-1.190650
Au	-2.652379	-0.209526	-0.332332
C	5.358562	-0.038274	0.255804
C	6.163967	-0.642063	-0.844685
H	6.446630	0.086220	-1.613138
H	7.085170	-1.102385	-0.452716
O	5.288471	-1.611497	-1.419272
C	4.194958	-1.898981	-0.546059
C	4.434285	-3.171193	0.263568
H	5.402970	-3.139538	0.770844
H	4.425031	-4.024125	-0.419296
H	3.645773	-3.307721	1.007456
C	2.898661	-1.902681	-1.334348
H	2.716084	-0.933264	-1.800651
H	2.049262	-2.153450	-0.696624
H	2.981035	-2.665155	-2.113175
N	4.268090	-0.707730	0.410926

H	5.607250	0.797052	0.898444
O	3.352767	-0.513895	1.334784
H	2.419842	0.336294	0.968019

TS2-10N5,N5

C	-0.646078	-1.895642	0.040310
C	0.220195	0.070908	-0.948636
C	1.190102	-0.579000	1.333483
C	0.282923	0.102908	2.376542
H	-0.579116	-0.519076	2.626306
H	-0.074608	1.077691	2.030501
H	0.855996	0.272126	3.294150
C	1.840302	-1.836692	1.937892
H	2.331841	-2.439975	1.172467
H	1.130743	-2.467519	2.476156
H	2.592085	-1.515760	2.665824
C	2.343197	0.372225	0.958819
H	3.067819	-0.101505	0.295603
H	2.861310	0.640938	1.883413
H	2.009293	1.308571	0.504425
C	-0.497107	1.410799	-0.679206
H	-1.342955	1.227671	-0.009283
H	0.150591	2.165512	-0.233685
C	-0.942264	1.785844	-2.083794
H	-0.257674	2.468815	-2.594432
H	-1.969885	2.135546	-2.181270
O	-0.868917	0.502410	-2.829801
N	0.376899	-0.927130	0.081827
N	-0.252262	-0.431668	-2.126764
O	-1.488686	-1.878177	-0.839258
Cl	-0.944764	-5.618922	2.469589
Cl	-2.326909	-2.492844	2.611634
Cl	0.835512	-4.564381	-0.267392
Au	-0.748833	-3.584822	1.239497
C	2.153751	-1.912635	-3.313542
C	2.570063	-3.328532	-3.128175
H	1.733080	-3.896823	-2.698739
H	2.871357	-3.804080	-4.065612
C	3.733994	-3.179001	-2.122406
H	4.716651	-3.282269	-2.589847
H	3.636131	-3.836660	-1.259113
O	3.640337	-1.806186	-1.613517
N	2.739344	-1.146652	-2.454449
H	1.418965	-1.491176	-3.983584
O	2.568212	0.108998	-2.193080
H	1.466076	0.193317	-1.533415

TS2-10PhCl$_3$,N1

C	0.983027	-1.190125	-0.496134
C	-1.247469	-1.301254	0.292479
C	-1.313903	-2.032394	1.661116
H	-0.313348	-2.405134	1.904923

H	-1.629244	-1.373153	2.471158
C	-2.302620	-3.157516	1.335630
H	-3.334454	-2.843207	1.540138
H	-2.118458	-4.069221	1.909698
C	-2.116577	-3.385272	-0.195945
C	-3.431870	-3.660979	-0.947759
H	-4.150171	-2.848626	-0.795044
H	-3.878712	-4.588057	-0.573917
H	-3.250618	-3.766759	-2.020635
C	-1.122918	-4.544318	-0.480964
H	-0.195433	-4.416547	0.078280
H	-0.874342	-4.579635	-1.543453
H	-1.601386	-5.484430	-0.186843
N	-0.092209	-0.459869	0.017436
N	-1.525267	-2.154313	-0.723896
O	0.804726	-2.303503	-0.946543
Cl	5.176226	0.204166	0.061836
Cl	3.013084	-1.889833	1.658037
Cl	2.730505	0.810538	-2.207900
Au	2.925139	-0.490498	-0.253338
C	-5.052530	-0.371278	1.429380
C	-6.516132	-0.455075	1.152077
H	-6.908564	-1.463316	1.319081
H	-7.058271	0.207929	1.840349
C	-6.619075	0.000173	-0.326794
H	-7.485738	0.640654	-0.503164
H	-6.715346	-0.874287	-0.976743
C	-5.296620	0.743810	-0.642736
C	-5.400266	2.266876	-0.478294
H	-5.864900	2.538640	0.475243
H	-6.013037	2.674886	-1.287366
H	-4.410234	2.726440	-0.527068
C	-4.683142	0.363557	-1.987942
H	-4.546277	-0.718335	-2.074671
H	-3.715331	0.846903	-2.133873
H	-5.357873	0.686229	-2.786913
N	-4.406009	0.238227	0.487471
H	-4.525233	-0.699763	2.317434
O	-3.129914	0.543520	0.492343
H	-2.234280	-0.506941	0.282230
C	-0.378087	1.809980	-0.863481
C	-0.065609	0.954002	0.212007
C	-0.342650	3.195862	-0.737891
C	0.247737	1.554859	1.444681
C	-0.002111	3.744212	0.496115
C	0.289329	2.941495	1.594457
Cl	-0.852245	1.141477	-2.401944
Cl	0.596323	0.584341	2.848576
H	0.551811	3.377316	2.549969
Cl	0.048069	5.485270	0.672523

H	-0.565071	3.828248	-1.587784

TS2-10PhCl,N1

C	-0.635927	-1.226649	0.160840
C	1.447047	-0.975036	-0.908954
C	1.439642	-1.401960	-2.400530
H	0.449585	-1.797018	-2.653749
H	1.664537	-0.573495	-3.074230
C	2.527267	-2.482357	-2.388941
H	3.509605	-2.033841	-2.579535
H	2.366452	-3.261303	-3.138703
C	2.475599	-3.051991	-0.938917
C	3.858105	-3.404200	-0.360252
H	4.518933	-2.531144	-0.365926
H	4.321325	-4.188983	-0.967058
H	3.767628	-3.765449	0.667876
C	1.564997	-4.307858	-0.857504
H	0.590959	-4.119505	-1.311223
H	1.402939	-4.595895	0.182844
H	2.062211	-5.125618	-1.389425
N	0.274763	-0.318734	-0.350651
N	1.872872	-2.001345	-0.112789
O	-0.308135	-2.380765	0.376264
Cl	-4.892413	-0.104427	0.740009
Cl	-2.883407	-1.086600	-1.876865
Cl	-2.091661	-0.257594	2.712257
Au	-2.604179	-0.658533	0.436541
C	5.488722	0.181722	-0.344195
C	6.489168	0.160242	0.762574
H	7.001990	-0.804187	0.835127
H	7.266275	0.914190	0.574303
C	5.628653	0.485707	2.009643
H	6.151542	1.129270	2.720338
H	5.367590	-0.441444	2.528172
C	4.342221	1.162748	1.476026
C	4.424729	2.695579	1.451725
H	5.358074	3.043267	0.996499
H	4.380862	3.074086	2.477121
H	3.585231	3.114378	0.891430
C	3.067721	0.676620	2.160568
H	2.941898	-0.405426	2.062337
H	2.187112	1.168272	1.744191
H	3.123321	0.921948	3.225621
N	4.356470	0.696093	0.022202
H	5.629895	-0.115732	-1.376737
O	3.332705	0.923677	-0.759420
H	2.360630	-0.157339	-0.765426
C	-0.237092	1.922144	0.480442
C	-0.036900	1.063598	-0.605365
C	-0.526124	3.269850	0.266583
C	-0.142407	1.554029	-1.910676

C	-0.593558	3.753319	-1.039868
C	-0.409210	2.904601	-2.131808
H	-0.207711	1.527968	1.490303
H	-0.051890	0.886024	-2.757976
H	-0.497841	3.288137	-3.141850
Cl	-0.931289	5.453584	-1.316670
H	-0.703151	3.932520	1.106091

TS2-10PhMe,N1

C	0.632692	-1.057800	-0.204415
C	-1.435200	-0.876168	0.908808
C	-1.444475	-1.396848	2.369770
H	-0.462376	-1.821557	2.605448
H	-1.663771	-0.608618	3.091706
C	-2.543243	-2.461917	2.279948
H	-3.523643	-2.013893	2.481879
H	-2.401874	-3.286030	2.984028
C	-2.476474	-2.944232	0.799560
C	-3.850187	-3.274183	0.189888
H	-4.520239	-2.409842	0.243981
H	-4.310574	-4.100039	0.742010
H	-3.747922	-3.569763	-0.858012
C	-1.553078	-4.185155	0.654006
H	-0.582926	-4.014352	1.122946
H	-1.382262	-4.412809	-0.399748
H	-2.045232	-5.036096	1.136432
N	-0.256446	-0.191404	0.403118
N	-1.872602	-1.841499	0.044225
O	0.293369	-2.185382	-0.520179
Cl	4.864303	0.136486	-0.840874
Cl	2.990825	-1.202746	1.719985
Cl	1.960161	0.229017	-2.670108
Au	2.590119	-0.462790	-0.494572
C	-5.459359	0.294063	0.367207
C	-6.447892	0.296681	-0.750631
H	-6.953817	-0.668433	-0.855658
H	-7.231875	1.040685	-0.551322
C	-5.575469	0.661086	-1.978121
H	-6.095832	1.315827	-2.680500
H	-5.297004	-0.250745	-2.514408
C	-4.303096	1.337621	-1.411483
C	-4.404857	2.867989	-1.342168
H	-5.348178	3.190960	-0.889076
H	-4.351840	3.278319	-2.354849
H	-3.577550	3.278296	-0.757763
C	-3.016487	0.887897	-2.097954
H	-2.877129	-0.194603	-2.029714
H	-2.145509	1.377146	-1.659635
H	-3.065591	1.164154	-3.155795
N	-4.327611	0.828999	0.028496
H	-5.608592	-0.034558	1.389063

O	-3.314619	1.041481	0.826547
H	-2.338450	-0.042383	0.808277
C	0.197365	2.156919	-0.129875
C	0.098216	1.142964	0.826407
C	0.537858	3.451108	0.263049
C	0.351565	1.429730	2.170933
C	0.775829	3.763724	1.608732
C	0.674964	2.731375	2.552360
H	0.053768	1.921372	-1.178394
H	0.336167	0.639215	2.911287
H	0.878182	2.940179	3.599373
C	1.180629	5.158176	2.024265
H	0.631706	4.225606	-0.493539
H	0.840012	5.388583	3.038358
H	0.771371	5.912925	1.345916
H	2.272476	5.264343	2.012254

TS2-10Ph,N1

C	-0.730049	0.848128	-0.346572
C	1.372873	0.984164	0.700108
C	1.364308	1.811796	2.013491
H	0.363737	2.232394	2.162714
H	1.622590	1.212014	2.887532
C	2.414411	2.876517	1.678408
H	3.414187	2.523974	1.959162
H	2.241026	3.827372	2.188936
C	2.318617	3.021355	0.129857
C	3.674828	3.258030	-0.558295
H	4.378021	2.451386	-0.326345
H	4.105949	4.200788	-0.205992
H	3.554182	3.313429	-1.643719
C	1.349177	4.167492	-0.269857
H	0.390664	4.070803	0.241743
H	1.160826	4.151080	-1.344981
H	1.814433	5.119942	0.004679
N	0.226521	0.153301	0.372638
N	1.751864	1.760099	-0.358429
O	-0.459005	1.909194	-0.881857
Cl	-4.944337	-0.554963	-0.471299
Cl	-2.942183	1.199605	1.709057
Cl	-2.192679	-0.834088	-2.496309
Au	-2.676419	0.152481	-0.399855
C	5.468353	-0.094379	0.433709
C	6.462266	-0.350002	-0.649641
H	6.930550	0.573588	-1.004618
H	7.273035	-0.985317	-0.266532
C	5.611005	-1.055646	-1.735296
H	6.160461	-1.849211	-2.246248
H	5.299328	-0.326391	-2.488745
C	4.365060	-1.612049	-1.004218
C	4.530744	-3.064733	-0.535798

H	5.484820	-3.216817	-0.019959
H	4.500080	-3.728974	-1.404432
H	3.718845	-3.341458	0.141252
C	3.062689	-1.412396	-1.774038
H	2.881653	-0.357191	-1.998118
H	2.211705	-1.799662	-1.211074
H	3.123900	-1.959832	-2.719746
N	4.360575	-0.742927	0.251307
H	5.598933	0.495359	1.333507
O	3.351720	-0.780112	1.082490
H	2.323502	0.197054	0.780111
C	-0.194663	-2.247280	0.196713
C	-0.020115	-1.119117	1.005114
C	-0.429863	-3.491391	0.784972
C	-0.088749	-1.232420	2.397242
C	-0.472638	-3.614486	2.175613
C	-0.302982	-2.483249	2.978090
H	-0.189363	-2.138300	-0.882311
H	-0.014279	-0.351454	3.022492
H	-0.364520	-2.566304	4.058867
H	-0.657482	-4.582345	2.631914
H	-0.589389	-4.359296	0.152511

TS2-10Xyl,N1

C	-0.983051	0.813574	-0.514256
C	1.228861	1.045469	0.244339
C	1.263073	1.950520	1.507123
H	0.252895	2.333989	1.685727
H	1.581643	1.410085	2.399468
C	2.239367	3.042323	1.054994
H	3.270548	2.779055	1.322357
H	2.025434	4.018239	1.498473
C	2.086612	3.062778	-0.496956
C	3.416888	3.249073	-1.250293
H	4.133253	2.465062	-0.982054
H	3.853907	4.218123	-0.987814
H	3.258409	3.218466	-2.331699
C	1.092203	4.163579	-0.954352
H	0.155048	4.101392	-0.400157
H	0.864029	4.053332	-2.016462
H	1.556663	5.140245	-0.781074
N	0.092347	0.154425	0.064955
N	1.518875	1.764795	-0.866379
O	-0.842426	1.880748	-1.081266
Cl	-5.169372	-0.487415	0.334482
Cl	-2.828691	1.526682	1.786959
Cl	-2.951481	-1.098582	-2.143290
Au	-2.922326	0.144450	-0.143695
C	5.180361	0.426062	1.223226
C	6.597393	0.389106	0.757005
H	7.005010	1.392775	0.599503

H	7.224274	-0.085343	1.524683
C	6.512575	-0.444415	-0.547761
H	7.360609	-1.122702	-0.662866
H	6.502998	0.225598	-1.412471
C	5.174559	-1.220907	-0.473132
C	5.320859	-2.638032	0.099786
H	5.912382	-2.641472	1.021316
H	5.826009	-3.272315	-0.634509
H	4.338578	-3.066609	0.313147
C	4.386917	-1.223397	-1.779999
H	4.200423	-0.206664	-2.138649
H	3.429073	-1.731545	-1.657183
H	4.966422	-1.753745	-2.541894
N	4.425563	-0.399912	0.570718
H	4.765800	0.998598	2.044371
O	3.163357	-0.659335	0.814200
H	2.233903	0.276180	0.375328
C	0.388369	-2.110772	-0.792263
C	0.127954	-1.273299	0.314828
C	0.435964	-3.492330	-0.576104
C	-0.053295	-1.787511	1.612400
C	0.235074	-4.026143	0.696486
C	-0.002912	-3.179776	1.775823
C	0.590868	-1.558970	-2.183525
C	-0.268977	-0.913444	2.823504
H	-0.162914	-3.596279	2.766460
H	0.257657	-5.102208	0.844666
H	0.616022	-4.152443	-1.420269
H	-0.847834	-0.017106	2.596886
H	0.693230	-0.605074	3.252832
H	-0.804489	-1.467981	3.598799
H	1.063714	-2.309020	-2.824601
H	1.203303	-0.653420	-2.189184
H	-0.372919	-1.297855	-2.633525

TS2-14

C	-0.952737	1.088959	-0.054256
C	1.461797	1.034996	0.511742
H	2.129508	0.225426	0.808129
C	0.423797	-1.086507	-0.531774
C	-0.774338	-1.542964	-1.375146
H	-1.009454	-0.832883	-2.171698
H	-1.674819	-1.698254	-0.781296
H	-0.517466	-2.500650	-1.836675
C	1.684129	-1.203998	-1.418752
H	2.606611	-0.922367	-0.906801
H	1.591034	-0.594049	-2.319070
H	1.778781	-2.253356	-1.710033
C	0.574229	-1.966971	0.724757
H	1.460790	-1.712253	1.314674
H	0.687354	-3.007052	0.402964

H	-0.299103	-1.891217	1.373813
C	1.280346	2.108745	1.597220
H	0.373627	1.957113	2.186198
H	2.126177	2.025391	2.286428
C	1.306575	3.445600	0.820846
H	1.919954	4.196711	1.326667
H	0.303054	3.856236	0.702303
C	1.880966	3.076393	-0.565952
C	3.465539	3.241070	-0.573826
H	3.932719	2.744973	0.280023
H	3.648886	4.317924	-0.503175
H	3.894748	2.858512	-1.500511
C	1.306210	3.847040	-1.757481
H	0.225903	3.697689	-1.800138
H	1.751809	3.506903	-2.696394
H	1.512722	4.914932	-1.638151
N	0.259254	0.370568	-0.103213
N	1.837704	1.643667	-0.721446
O	-1.015914	2.265628	-0.302287
Cl	-4.674616	-0.614451	1.746642
Cl	-1.556341	0.161957	2.861476
Cl	-3.711974	0.382830	-1.341820
Au	-2.674490	0.206521	0.767813

TS2-20

C	-0.343399	0.976589	0.242995
C	1.808570	0.635518	0.978808
C	0.514113	-1.437715	-0.017795
C	-0.931673	-1.952420	0.099557
H	-1.604830	-1.479882	-0.617853
H	-1.323464	-1.823938	1.110494
H	-0.923353	-3.023651	-0.122654
C	1.015899	-1.676664	-1.457868
H	2.073531	-1.428495	-1.573038
H	0.437571	-1.089981	-2.175559
H	0.897193	-2.735366	-1.709363
C	1.373721	-2.218871	0.994294
H	2.435867	-1.969812	0.930884
H	1.279528	-3.285913	0.775393
H	1.026053	-2.053065	2.017934
C	3.183392	0.532287	0.278545
H	3.866502	-0.123676	0.822815
H	3.072208	0.137140	-0.731549
C	3.676857	1.992861	0.232849
H	4.391168	2.168041	-0.576175
H	4.163339	2.262894	1.175981
C	2.393873	2.830985	0.045826
C	1.917345	2.821992	-1.417531
H	1.816020	1.812767	-1.825711
H	2.645462	3.361391	-2.031559
H	0.953225	3.324649	-1.518715

C	2.532989	4.269828	0.551065
H	2.849005	4.281339	1.597721
H	1.578211	4.799688	0.476597
H	3.270237	4.815121	-0.047831
N	0.617254	0.036885	0.305407
N	1.507700	2.080698	1.000546
O	0.101356	2.181202	0.638245
Cl	-4.657111	0.927597	0.740430
Cl	-1.348645	0.353098	3.141182
Cl	-1.310610	1.167139	-1.503132
Au	-2.315611	0.807107	1.031878
H	1.837277	0.255574	2.004464

TS2-6

Au	-0.972910	-1.302552	1.114405
Cl	-0.419632	-0.580293	3.279244
Cl	-1.397193	-1.947720	-1.102347
Cl	-2.491111	-2.870873	1.943830
C	0.519978	0.175355	0.336228
N	1.760933	-0.057800	0.263794
O	-0.198099	1.149696	0.203313
C	2.457061	1.844502	-0.204193
N	1.360959	2.556915	-0.514052
C	1.229243	3.666229	0.467802
C	3.169594	2.343056	1.045100
H	2.985494	1.379853	-1.032221
C	1.854416	4.891241	-0.257650
C	-0.229217	3.987585	0.803955
C	2.092005	3.237432	1.681183
H	4.055966	2.915188	0.737949
H	3.515086	1.540272	1.697383
H	2.508461	4.091371	2.222207
H	1.483459	2.657565	2.383011
H	1.313325	5.097621	-1.184590
H	2.908267	4.730803	-0.505606
H	1.784181	5.767651	0.394829
H	-0.695931	3.171813	1.357991
H	-0.804975	4.156295	-0.110628
H	-0.273855	4.895886	1.413694
C	2.127521	-2.454586	0.836483
C	2.522709	-1.583009	-1.512648
C	2.602830	-1.255100	-0.010931
C	4.049660	-0.924156	0.399990
H	4.461268	-0.085131	-0.166594
H	4.676153	-1.796718	0.197367
H	4.117717	-0.698626	1.467708
H	2.851403	-3.267662	0.724650
H	1.158215	-2.823148	0.492656
H	2.059087	-2.191943	1.894904
H	3.149586	-2.453102	-1.732570
H	2.879557	-0.746496	-2.121979

H	1.494715	-1.812132	-1.804414

TS2-6N5

Au	3.516510	-1.511248	-2.208440
Cl	2.111510	-2.936539	-3.437526
Cl	5.440919	-2.422705	-3.191641
Cl	4.787827	-0.053177	-0.870187
C	1.666549	-0.534076	-1.351911
N	1.325994	-0.853481	-0.163589
O	1.418145	0.333672	-2.151829
C	0.047817	0.727586	0.327926
N	-0.131569	1.476242	-0.775627
H	-0.749992	0.025343	0.530622
C	0.814375	1.498663	1.384605
O	0.569768	2.625181	-0.658982
C	1.458848	2.567286	0.506112
H	0.110957	1.925942	2.110740
H	1.544747	0.893701	1.919328
H	1.482669	3.572513	0.926529
H	2.450778	2.278405	0.144985
C	1.114293	-2.160069	0.532055
C	2.402933	-3.010545	0.482977
C	0.809642	-1.866996	2.013415
C	-0.056958	-2.903560	-0.133215
H	1.643070	-1.348695	2.495585
H	0.663099	-2.818865	2.530001
H	-0.102562	-1.280931	2.150144
H	-0.230745	-3.854127	0.381058
H	0.165262	-3.113893	-1.182554
H	-0.981691	-2.319376	-0.082664
H	2.272032	-3.876596	1.139254
H	3.266500	-2.437437	0.828758
H	2.593873	-3.383191	-0.525330

TS34-32

C	2.717136	1.152751	-2.001262
C	0.868163	-0.882278	-0.755184
C	1.456192	-2.114288	-1.372144
H	2.259925	-2.486121	-0.728977
H	1.865977	-1.946381	-2.369457
C	0.160053	-3.002478	-1.353120
H	-0.323173	-2.944532	-2.332972
H	0.372957	-4.055550	-1.146649
C	-0.788956	-2.372076	-0.265819
C	-2.242704	-2.303997	-0.695684
H	-2.864731	-1.857105	0.084097
H	-2.598831	-3.324942	-0.878836
H	-2.363018	-1.718900	-1.611039
C	-0.602389	-2.973807	1.123101
H	-1.092255	-2.358603	1.882266
H	0.456040	-3.065613	1.386105
H	-1.047451	-3.975197	1.132503

C	2.683383	2.119842	0.308697
N	2.481992	1.153502	-0.810234
N	-0.188610	-0.927761	-0.207323
O	2.897776	1.001228	-3.157558
Cl	-1.156108	0.307480	2.932350
Cl	-2.204941	1.553976	-1.465417
Au	-1.612338	0.859980	0.695285
C	2.590604	1.326218	1.618059
C	1.582840	3.187802	0.231253
C	4.078950	2.749673	0.154740
H	1.601494	0.878796	1.745884
H	2.761414	1.997249	2.464956
H	3.348807	0.536875	1.648327
H	1.685086	3.881988	1.071433
H	0.590294	2.731955	0.281794
H	1.652793	3.758937	-0.699934
H	4.860450	1.983843	0.179472
H	4.258140	3.449034	0.977260
H	4.161340	3.305811	-0.785194

TS4-2

C	-0.443959	0.931060	-1.134252
C	2.178591	1.036967	-1.101351
H	2.169200	0.353605	-1.939626
C	-0.018300	-1.222773	0.067965
C	-1.367003	-1.818509	-0.371159
H	-1.426184	-1.915157	-1.458649
H	-2.209218	-1.215813	-0.023610
H	-1.470097	-2.815899	0.068517
C	1.116173	-2.187697	-0.324672
H	2.093268	-1.802267	-0.015313
H	1.130442	-2.354676	-1.406553
H	0.968191	-3.154457	0.165171
C	-0.012446	-0.971710	1.587526
H	0.950097	-0.565474	1.917461
H	-0.182615	-1.913475	2.119035
H	-0.803753	-0.269066	1.862881
C	3.286870	1.146198	-0.099941
H	3.415013	0.214733	0.456879
H	4.230197	1.326356	-0.633171
C	2.850686	2.338382	0.784666
H	3.698968	2.945249	1.109000
H	2.342543	1.965410	1.678181
C	1.849944	3.174240	-0.067701
C	2.519919	4.375532	-0.751168
H	3.421618	4.074558	-1.294532
H	2.802185	5.119067	0.000699
H	1.833555	4.847542	-1.460028
C	0.607073	3.601618	0.711041
H	0.074712	2.751668	1.143278
H	-0.093744	4.149989	0.077796

H	0.920310	4.262311	1.525507
N	0.287406	0.070269	-0.590709
N	1.513427	2.176027	-1.154505
O	0.215318	2.092177	-1.647683
Cl	-4.734200	1.301439	-2.069747
Cl	-2.782250	1.891240	0.650091
Cl	-1.929059	0.297002	-3.717603
Au	-2.439902	1.113143	-1.561922

TS4-2Bz

C	-2.630251	0.223045	-0.812315
C	-0.126282	1.036441	-0.813577
H	-0.106393	0.769649	-1.861588
C	1.051141	1.011793	0.105624
H	1.443655	-0.004108	0.203156
H	1.853907	1.626439	-0.323247
C	0.483257	1.576731	1.431362
H	1.197666	2.227134	1.940859
H	0.240104	0.749807	2.103418
C	-0.819490	2.350611	1.065426
C	-0.599780	3.867200	0.966993
H	0.250803	4.107175	0.320561
H	-0.402294	4.276085	1.962713
H	-1.488478	4.361170	0.563451
C	-1.993333	2.017887	1.985054
H	-2.202197	0.946704	2.016385
H	-2.905588	2.531979	1.674730
H	-1.741854	2.348716	2.997559
N	-1.053827	1.842600	-0.341487
O	-2.352770	1.615757	-0.797868
Cl	-6.914099	-0.545369	-1.467785
Cl	-4.869622	-0.351441	1.241073
Cl	-4.194380	0.095907	-3.410348
Au	-4.625519	-0.118144	-1.101705
N	-1.645973	-0.550191	-0.699826
C	-1.695328	-2.014414	-0.680668
H	-1.238487	-2.368333	-1.611099
H	-2.737776	-2.350785	-0.671604
C	-0.942720	-2.570143	0.512558
C	0.330228	-3.133157	0.357008
C	-1.517372	-2.524576	1.791702
C	1.025504	-3.638365	1.460656
C	-0.824232	-3.028584	2.894333
C	0.449629	-3.584066	2.732258
H	0.775192	-3.192119	-0.633881
H	2.007939	-4.081519	1.324683
H	0.983801	-3.982564	3.589910
H	-1.283441	-2.997844	3.878237
H	-2.511408	-2.102267	1.917559

TS4-2Cy

C	-0.269431	0.674737	-0.895441

C	2.282470	1.349380	-0.667974
H	2.382289	1.014287	-1.691552
C	3.367111	1.317810	0.359707
H	3.693131	0.291785	0.553073
H	4.242769	1.858125	-0.024295
C	2.717098	1.999561	1.590249
H	3.418784	2.649238	2.117908
H	2.372360	1.237279	2.293957
C	1.492807	2.806501	1.059405
C	1.794166	4.304261	0.905108
H	2.711858	4.470361	0.331374
H	1.917776	4.758783	1.892958
H	0.971674	4.812963	0.394104
C	0.222481	2.576493	1.877386
H	-0.045678	1.519424	1.936234
H	-0.629120	3.115271	1.456622
H	0.393997	2.946240	2.893189
N	1.364740	2.229071	-0.332940
O	0.113623	2.061886	-0.909191
Cl	-4.534738	0.400494	-1.965150
Cl	-2.752657	0.416986	0.930796
Cl	-1.585723	0.714132	-3.640211
Au	-2.254804	0.563626	-1.380809
N	0.638266	-0.148706	-0.644767
H	-1.382145	-4.074099	0.653362
C	-0.364692	-4.280879	0.294401
C	0.644232	-3.513990	1.163882
C	-0.258137	-3.868007	-1.182027
H	-0.207124	-5.360876	0.399124
C	0.513716	-1.993073	0.981204
C	-0.416812	-2.348278	-1.356238
C	0.631053	-1.608014	-0.507010
H	0.716246	-4.184396	-1.583073
H	-1.020749	-4.380821	-1.778546
H	-0.319318	-2.060776	-2.408030
H	-1.422732	-2.054912	-1.033500
H	1.624528	-1.924836	-0.858162
H	-0.458169	-1.645506	1.352578
H	1.287010	-1.472349	1.560192
H	0.507947	-3.767628	2.221653
H	1.664996	-3.826118	0.897352

TS4-2Me

C	-0.333907	0.630490	-0.150923
C	2.155693	1.464961	-0.320128
H	2.121104	1.150674	-1.354562
C	3.382481	1.496328	0.532725
H	3.810238	0.495718	0.640504
H	4.145380	2.113310	0.039198
C	2.875146	2.099090	1.866272
H	3.606661	2.772109	2.318722

H	2.672390	1.295074	2.578850
C	1.547177	2.847158	1.538796
C	1.746440	4.360732	1.372451
H	2.560870	4.583870	0.675469
H	1.989046	4.808931	2.340879
H	0.833460	4.831183	0.996183
C	0.424823	2.540001	2.529432
H	0.220528	1.469824	2.606603
H	-0.504757	3.040638	2.250030
H	0.726461	2.905223	3.516060
N	1.246583	2.282487	0.166631
O	-0.071021	2.024717	-0.210495
Cl	-4.634977	-0.194191	-0.568531
Cl	-2.444304	0.064850	2.021902
Cl	-2.027751	0.444329	-2.665169
Au	-2.335805	0.262497	-0.332991
N	0.660825	-0.130018	-0.045944
C	0.620975	-1.581696	0.031126
H	1.141880	-1.907121	0.936002
H	1.138652	-2.000049	-0.837547
H	-0.404032	-1.961979	0.056075

TS4-2N2

C	2.658300	-0.549607	1.352812
C	0.225167	0.523523	1.856997
H	0.149862	-0.180738	2.672811
C	1.352333	-2.361118	0.243825
C	2.514385	-3.363119	0.347770
H	2.771982	-3.571377	1.389346
H	3.408407	-3.001303	-0.166509
H	2.215078	-4.301964	-0.129383
C	0.083152	-2.979430	0.858914
H	-0.765382	-2.289147	0.797893
H	0.246488	-3.240966	1.909342
H	-0.187441	-3.892072	0.319781
C	1.107619	-1.976391	-1.227744
H	0.262742	-1.285021	-1.320944
H	0.875635	-2.873112	-1.811046
H	1.996000	-1.502557	-1.654347
C	-0.899536	1.047555	1.019151
H	-1.138453	0.305761	0.248899
H	-1.808251	1.198496	1.609898
C	-0.320062	2.360638	0.417366
H	-0.678951	3.221294	0.987913
H	-0.607871	2.502081	-0.625530
C	1.204009	2.216137	0.574015
H	1.727541	3.141897	0.814577
H	1.695202	1.737302	-0.280454
N	1.600751	-1.101615	0.985413
N	1.286390	1.290077	1.727561
O	2.517453	0.732497	2.011720

Cl	6.977486	-1.331448	0.999783
Cl	4.560800	0.193792	-0.885872
Cl	4.565099	-1.952467	3.327445
Au	4.666276	-0.913778	1.213127

TS4-2N3

C	1.870723	-1.124561	1.567705
C	0.171522	0.953773	1.411819
H	-0.621200	0.292099	1.725299
C	0.697319	-1.856902	-0.510311
C	1.025054	-3.338447	-0.260274
H	0.566391	-3.699345	0.664166
H	2.102986	-3.511654	-0.207965
H	0.634764	-3.932345	-1.093147
C	-0.820805	-1.689095	-0.710050
H	-1.082263	-0.641923	-0.896756
H	-1.370726	-2.040601	0.169403
H	-1.151990	-2.277290	-1.570940
C	1.458811	-1.341341	-1.745880
H	1.211930	-0.294031	-1.951567
H	1.180923	-1.932484	-2.624347
H	2.538873	-1.429251	-1.597131
O	-0.131510	1.959116	0.621117
C	0.983553	2.923450	0.655030
H	0.604685	3.801702	1.182325
H	1.224905	3.173866	-0.377709
C	2.139520	2.214686	1.409818
C	2.758207	3.087275	2.504424
H	1.997717	3.442877	3.205298
H	3.257604	3.952076	2.056282
H	3.506125	2.516434	3.061094
C	3.203063	1.661872	0.455720
H	2.760495	1.089453	-0.362053
H	3.910938	1.014429	0.977173
H	3.758572	2.503161	0.029447
N	1.061583	-0.977267	0.625990
N	1.327367	1.118049	2.051240
O	1.971650	-0.035123	2.495686
Cl	4.551083	-4.306818	3.029142
Cl	4.798367	-1.747208	0.797039
Cl	1.349962	-3.301613	3.635313
Au	3.126121	-2.594118	2.248770

TS4-2N4

C	2.555925	-1.051204	0.372336
C	0.542915	-0.711582	2.079376
H	0.273679	-1.741840	1.900072
C	0.721988	-0.902996	-1.320403
C	1.516941	-1.715654	-2.356644
H	1.717133	-2.730113	-2.001916
H	2.467195	-1.235842	-2.603778
H	0.929780	-1.781553	-3.278240

C	-0.661867	-1.545958	-1.114024
H	-1.257200	-0.983666	-0.386146
H	-0.565028	-2.579889	-0.767109
H	-1.213244	-1.556560	-2.058562
C	0.574265	0.557987	-1.784313
H	-0.015999	1.144165	-1.071520
H	0.060177	0.586970	-2.750218
H	1.555295	1.027232	-1.899089
C	-0.395311	0.389285	2.476925
H	-0.860199	0.842398	1.590421
H	-1.188101	0.041181	3.147077
O	0.433071	1.315497	3.182381
C	1.810067	1.110812	2.849924
C	2.655554	1.268498	4.101613
H	2.296524	0.605013	4.891379
H	2.593418	2.302808	4.449234
H	3.700958	1.037362	3.879933
C	2.259386	1.998988	1.695089
H	1.586033	1.913558	0.840026
H	3.269236	1.747168	1.362667
H	2.251334	3.035414	2.041745
N	1.371097	-0.879988	0.013414
N	1.752570	-0.351491	2.449136
O	2.821830	-0.921631	1.782807
Cl	6.352458	-2.151253	-1.571937
Cl	4.675135	0.745569	-0.984566
Cl	3.830461	-3.796206	0.013983
Au	4.330265	-1.552411	-0.524562

TS4-2Ph

C	0.500313	1.472781	1.108307
C	1.029941	1.679334	-1.464672
H	0.022876	1.315459	-1.621730
C	2.179260	1.460588	-2.391661
H	2.390479	0.392613	-2.499207
H	1.910668	1.829807	-3.390430
C	3.331926	2.257280	-1.730678
H	3.947770	2.776412	-2.468202
H	3.980085	1.574237	-1.175185
C	2.671435	3.265614	-0.740649
C	2.583315	4.687462	-1.313268
H	2.131092	4.690571	-2.310433
H	3.586991	5.117129	-1.388370
H	1.983529	5.329576	-0.661773
C	3.325446	3.262217	0.640642
H	3.329885	2.268719	1.093999
H	2.819769	3.943492	1.328184
H	4.362214	3.595172	0.530356
N	1.261017	2.716690	-0.688263
O	0.537433	2.754929	0.506599
Cl	-1.143581	1.709039	5.180093

Cl	1.963720	1.665085	3.812941
Cl	-2.405784	1.525202	2.022241
Au	-0.254000	1.598015	3.003921
N	0.885858	0.506424	0.396881
C	-0.308399	-1.523866	1.077794
C	0.874824	-0.876096	0.693877
C	-0.289449	-2.899690	1.313039
C	2.058948	-1.606869	0.525949
C	0.891512	-3.631300	1.160831
C	2.064971	-2.980580	0.767972
H	-1.222650	-0.951443	1.195483
H	2.969169	-1.091609	0.235103
H	2.988095	-3.541041	0.654566
H	0.898629	-4.700387	1.349457
H	-1.203925	-3.397247	1.621248

TS4-2PhCl

C	0.520875	1.478972	-0.657761
C	3.133194	1.676305	-0.817637
H	3.027953	1.317668	-1.833515
C	4.326727	1.454158	0.051181
H	4.483070	0.386067	0.228462
H	5.221759	1.819398	-0.469867
C	3.993715	2.255423	1.335035
H	4.869340	2.772010	1.733884
H	3.625801	1.576834	2.109215
C	2.869585	3.267944	0.953996
C	3.406452	4.687420	0.721108
H	4.249069	4.686633	0.021998
H	3.746077	5.113130	1.670319
H	2.623629	5.334721	0.315489
C	1.704657	3.269724	1.943272
H	1.266591	2.277387	2.070392
H	0.910188	3.949783	1.628485
H	2.078639	3.607811	2.914675
N	2.451695	2.722124	-0.395680
O	1.105746	2.758027	-0.779295
Cl	-3.837802	1.685660	-1.188844
Cl	-1.711082	1.672154	1.456005
Cl	-1.117486	1.494115	-3.226890
Au	-1.506679	1.589799	-0.894461
N	1.312731	0.513873	-0.469416
C	0.353065	-1.517006	-1.454264
C	1.022485	-0.867171	-0.407084
C	0.128196	-2.891782	-1.386890
C	1.480056	-1.602491	0.694346
C	0.579122	-3.611375	-0.279573
C	1.253322	-2.975739	0.764930
H	0.005618	-0.948437	-2.310639
H	1.990788	-1.093945	1.505745
H	1.590894	-3.546278	1.622912

Cl	0.299079	-5.341752	-0.197981
H	-0.397699	-3.397272	-2.189116

TS4-2PhCl$_3$

C	-0.511800	0.803605	0.303184
C	1.892995	1.320976	-0.556150
H	1.538599	1.109275	-1.557197
C	3.299964	1.125163	-0.092213
H	3.573078	0.066267	-0.119926
H	3.978235	1.643363	-0.783047
C	3.300743	1.724022	1.336892
H	4.218812	2.276834	1.547315
H	3.213931	0.919101	2.069621
C	2.052776	2.654388	1.434522
C	2.410057	4.137926	1.261698
H	3.011337	4.301758	0.361467
H	2.985061	4.481353	2.127271
H	1.505381	4.748205	1.186461
C	1.227814	2.429286	2.702250
H	0.893738	1.394613	2.804255
H	0.349282	3.078331	2.726352
H	1.853188	2.674171	3.566403
N	1.295124	2.234381	0.192168
O	-0.105871	2.138260	0.238250
Cl	-4.796906	0.493958	1.248480
Cl	-1.918235	-0.107885	2.898439
Cl	-2.984074	1.534877	-1.394646
Au	-2.509783	0.673061	0.747870
N	0.387181	-0.061193	0.066821
C	-0.208805	-2.104998	-1.149554
C	0.273515	-1.457172	0.006910
C	-0.289916	-3.493459	-1.231753
C	0.752792	-2.274224	1.049043
C	0.147690	-4.259334	-0.153515
C	0.681925	-3.663595	0.987100
Cl	-0.693675	-1.161845	-2.534563
Cl	1.487868	-1.552630	2.460577
H	1.038051	-4.264019	1.814670
Cl	0.047683	-6.002945	-0.242842
H	-0.682924	-3.962004	-2.125364

TS4-2PhMe

C	0.501955	1.467067	1.093589
C	1.047244	1.692014	-1.483088
H	0.044948	1.317993	-1.645285
C	2.205494	1.486417	-2.402228
H	2.424128	0.420300	-2.513346
H	1.943476	1.859453	-3.401322
C	3.347471	2.287003	-1.726483
H	3.967203	2.813488	-2.455488
H	3.993945	1.605477	-1.167425
C	2.670807	3.286324	-0.738618

C	2.569704	4.707568	-1.311102
H	2.122043	4.705709	-2.310320
H	3.568942	5.148294	-1.381580
H	1.960125	5.342892	-0.662071
C	3.315518	3.289541	0.647117
H	3.324248	2.297050	1.103071
H	2.798854	3.968283	1.329020
H	4.350340	3.630999	0.544523
N	1.267313	2.721392	-0.695104
O	0.535078	2.752795	0.492931
Cl	-1.131947	1.704273	5.170583
Cl	1.972295	1.605030	3.794131
Cl	-2.403442	1.569260	2.013983
Au	-0.248457	1.592206	2.990286
N	0.892286	0.502766	0.383667
C	-0.297335	-1.526881	1.085263
C	0.879177	-0.879346	0.680786
C	-0.279057	-2.900702	1.320004
C	2.050346	-1.622030	0.491397
C	0.889977	-3.659854	1.157506
C	2.050575	-2.995015	0.736191
H	-1.211624	-0.956520	1.213428
H	2.960198	-1.119307	0.177881
H	2.970842	-3.557249	0.600813
C	0.899449	-5.141268	1.451641
H	-1.195581	-3.389364	1.640364
H	1.754309	-5.637060	0.982555
H	-0.014027	-5.626186	1.092523
H	0.962190	-5.325432	2.531315

TS4-2Xyl

C	-2.044226	-0.830106	0.536131
C	-0.286175	0.952209	1.356318
H	0.350875	0.606194	0.554315
C	0.199461	1.531172	2.645180
H	0.759567	0.784999	3.216902
H	0.897077	2.352112	2.432364
C	-1.101080	1.998132	3.347599
H	-0.969056	2.954107	3.859007
H	-1.403276	1.259694	4.094671
C	-2.196118	2.100155	2.242063
C	-2.413926	3.543093	1.762240
H	-1.467681	4.021217	1.488507
H	-2.878617	4.130283	2.560383
H	-3.074532	3.565201	0.890692
C	-3.519101	1.444950	2.636109
H	-3.395726	0.397062	2.915218
H	-4.247401	1.492437	1.823646
H	-3.929446	1.984382	3.495433
N	-1.518912	1.354655	1.114297
O	-2.270074	0.542089	0.262216

Cl	-5.000658	-3.237402	-1.683328
Cl	-4.835608	-1.929535	1.411186
Cl	-2.038965	-1.788832	-2.387383
Au	-3.436163	-1.941876	-0.492540
N	-1.062461	-1.104053	1.276124
C	0.483261	-2.957807	0.938611
C	-0.539524	-2.355776	1.704763
C	1.012099	-4.171850	1.391479
C	-0.972153	-2.905134	2.930590
C	0.569082	-4.756780	2.577014
C	-0.406062	-4.118302	3.340916
C	1.015511	-2.320271	-0.322199
C	-2.005308	-2.220735	3.790076
H	-0.741526	-4.562744	4.273712
H	0.990080	-5.700906	2.909423
H	1.784181	-4.658002	0.801924
H	-1.704233	-1.194754	4.033651
H	-2.135585	-2.760501	4.731471
H	-2.977575	-2.168911	3.290598
H	1.765960	-2.965206	-0.786052
H	1.503415	-1.360184	-0.108169
H	0.228240	-2.135683	-1.058516

TS4-6

Au	-2.569995	0.754659	-0.002431
Cl	-2.932291	0.430857	2.304514
Cl	-4.860109	0.454376	-0.502068
Cl	-2.024904	1.139029	-2.269957
C	-0.449984	0.736522	0.424371
N	0.412517	-0.144406	0.529260
O	-0.407274	2.039330	0.521350
C	1.990673	2.255313	1.695066
N	1.216468	2.675002	0.777608
H	1.626133	1.623092	2.498576
C	3.403416	2.732491	1.497680
C	1.863749	3.453739	-0.316503
C	3.253712	3.752195	0.338148
H	3.817403	3.161031	2.415616
H	4.029333	1.868439	1.238453
H	3.261267	4.770753	0.736515
H	4.058794	3.671724	-0.395209
C	1.966053	2.554811	-1.558132
C	1.041267	4.712124	-0.603988
H	0.054629	4.449527	-0.993969
H	1.557177	5.320052	-1.353791
H	0.911397	5.315006	0.299927
H	2.553954	1.655270	-1.352258
H	2.453784	3.113569	-2.362696
H	0.974361	2.249497	-1.902344
C	0.342301	-1.619179	0.451473
C	-0.761324	-2.120598	-0.495039

C	1.717344	-2.077352	-0.070184
C	0.113846	-2.150080	1.879334
H	1.896819	-1.695510	-1.080458
H	1.763153	-3.170318	-0.103153
H	2.519079	-1.718712	0.583774
H	0.115754	-3.245110	1.873007
H	-0.845482	-1.804323	2.273623
H	0.909109	-1.810689	2.551624
H	-0.683323	-3.207616	-0.599988
H	-0.670329	-1.669955	-1.487228
H	-1.758508	-1.897931	-0.105014

TS4-6Bz

Au	-4.418715	-1.160159	1.418862
Cl	-3.692283	-1.612579	3.611896
Cl	-6.555718	-2.066171	1.832614
Cl	-4.959891	-0.653184	-0.817597
C	-2.376437	-0.637533	0.942152
N	-1.440120	-1.344491	0.533955
O	-2.513317	0.616173	1.214192
C	0.128619	1.187860	1.284400
N	-1.014551	1.555025	0.864089
H	0.235829	0.431024	2.055366
C	1.244811	1.905307	0.575910
C	-1.007936	2.514719	-0.276744
C	0.484530	2.985205	-0.237246
H	1.977750	2.311150	1.279857
H	1.775016	1.178528	-0.053766
H	0.551097	3.950140	0.273446
H	0.884530	3.109707	-1.245772
C	-1.357787	1.746492	-1.560497
C	-2.009717	3.639522	-0.006889
H	-3.030596	3.250008	0.024783
H	-1.949684	4.381590	-0.809160
H	-1.796871	4.139308	0.942977
H	-0.643559	0.939508	-1.749697
H	-1.335257	2.438493	-2.407892
H	-2.359051	1.312345	-1.497282
C	-1.489200	-2.791285	0.300907
H	-1.433269	-2.951267	-0.780641
H	-2.439882	-3.209772	0.649938
C	1.839189	-4.585279	0.875600
C	0.766897	-3.948543	0.242543
C	1.825948	-4.762712	2.261029
C	-0.326508	-3.485019	0.983817
C	0.735921	-4.304101	3.008720
C	-0.334000	-3.669601	2.374623
H	2.678011	-4.946085	0.286984
H	0.777409	-3.817828	-0.837078
H	-1.182900	-3.320389	2.957380
H	0.714617	-4.449178	4.085095

H	2.654564	-5.262267	2.754835

TS4-6Cy

Au	-1.865580	0.363318	0.236378
Cl	-2.155699	0.079669	2.559787
Cl	-4.086859	-0.298337	-0.222336
Cl	-1.397734	0.728272	-2.050344
C	0.233120	0.679615	0.634629
N	1.212790	-0.067410	0.754268
O	0.091213	1.975970	0.696183
C	2.450599	2.489851	1.838709
N	1.619067	2.829951	0.936897
H	2.164201	1.835943	2.656046
C	3.808404	3.093574	1.606291
C	2.174913	3.647007	-0.180777
H	-0.302290	-4.266333	1.852991
C	0.688480	-4.343283	1.384168
C	1.707058	-3.553853	2.221390
C	0.608633	-3.803614	-0.052553
H	0.950695	-5.408125	1.375425
C	1.419180	-2.044191	2.190319
C	0.300831	-2.296768	-0.074442
C	1.350996	-1.523950	0.741172
H	1.562596	-3.989942	-0.567782
H	-0.160653	-4.339251	-0.620262
H	0.268658	-1.918600	-1.101522
H	-0.691684	-2.130056	0.363135
H	2.330815	-1.703861	0.275689
H	0.461360	-1.829941	2.681216
H	2.194181	-1.495562	2.739954
H	1.704812	-3.906949	3.259425
H	2.718877	-3.738752	1.830975
C	3.536711	4.089737	0.449345
H	4.205666	3.561009	2.512479
H	4.502731	2.288432	1.331519
H	3.444565	5.104099	0.847938
H	4.333724	4.091805	-0.297143
C	2.352114	2.740620	-1.408729
C	1.230962	4.814044	-0.478167
H	0.270100	4.449802	-0.850748
H	1.675951	5.456682	-1.244289
H	1.052878	5.416420	0.417801
H	3.026436	1.905487	-1.195953
H	2.775794	3.330200	-2.227531
H	1.392468	2.333643	-1.737672

TS4-6Me

Au	-3.206934	1.044110	-0.286850
Cl	-2.907285	1.161484	2.044416
Cl	-5.538562	0.754267	-0.079624
Cl	-3.291907	0.911648	-2.639736
C	-1.065566	0.989082	-0.459893

N	-0.298109	0.011202	-0.444082
O	-0.903611	2.265587	-0.586266
C	1.744511	2.316029	-0.094272
N	0.806155	2.717070	-0.852807
H	1.539464	1.850169	0.864786
C	3.098963	2.556139	-0.703449
C	1.224146	3.239529	-2.184974
C	2.758877	3.427753	-1.940443
H	3.782700	3.035080	0.004120
H	3.538081	1.583968	-0.963911
H	2.969083	4.478841	-1.722873
H	3.335592	3.144577	-2.823459
C	0.912765	2.171417	-3.244443
C	0.487035	4.548483	-2.476064
H	-0.587438	4.374157	-2.575845
H	0.855796	4.972632	-3.415151
H	0.649672	5.279910	-1.678704
H	1.442027	1.236462	-3.037750
H	1.225943	2.540626	-4.225739
H	-0.158781	1.958886	-3.281676
C	-0.725951	-1.377356	-0.294874
H	0.164193	-2.005554	-0.225678
H	-1.313592	-1.697125	-1.161600
H	-1.324577	-1.512103	0.611730

TS4-6N2

Au	3.217990	-1.688905	-2.563844
Cl	1.328748	-2.566836	-3.659200
Cl	4.689484	-2.956874	-3.893612
Cl	4.997504	-0.699005	-1.371426
C	1.874727	-0.735804	-1.156578
N	1.348184	-1.102909	-0.094867
O	1.849306	0.386425	-1.806748
C	0.050580	1.288261	-0.134349
N	1.060677	1.641950	-0.853258
H	-0.697006	0.603376	-0.516245
C	0.004163	2.008207	1.185872
C	2.019945	2.483253	-0.114977
C	1.165113	3.030127	1.053991
H	-0.973003	2.467060	1.365405
H	0.168128	1.276824	1.987134
H	0.768922	4.016755	0.798946
H	1.746703	3.127209	1.972742
H	2.847013	1.845161	0.213471
H	2.419390	3.252723	-0.777420
C	1.331834	-2.389255	0.636018
C	2.659440	-3.155949	0.508638
C	1.083745	-2.030850	2.113159
C	0.162065	-3.228570	0.089040
H	1.900451	-1.417612	2.507803
H	1.018955	-2.942623	2.714376

H	0.143916	-1.480499	2.228327
H	0.086374	-4.166699	0.648571
H	0.311100	-3.462734	-0.968298
H	-0.785757	-2.690250	0.194538
H	2.637245	-4.029704	1.167855
H	3.510447	-2.529828	0.789894
H	2.819146	-3.515645	-0.511607

TS4-6N3

Au	3.809721	-2.541946	-1.235925
Cl	2.531578	-2.918468	-3.178680
Cl	5.238937	-4.353594	-1.721695
Cl	5.001732	-2.022242	0.735470
C	2.344169	-1.066763	-0.677440
N	1.258822	-1.102801	-0.078850
O	3.000761	-0.069102	-1.212757
C	0.958755	1.526231	-0.918512
N	2.254025	1.479591	-0.957869
H	0.286479	0.914754	-1.503072
O	0.439508	2.479117	-0.161897
C	2.831653	2.368289	0.098076
C	1.572851	3.236046	0.396721
H	1.589012	4.197769	-0.121993
H	1.373392	3.376796	1.458826
C	3.262157	1.547819	1.321306
C	3.990332	3.180885	-0.481904
H	4.819901	2.518129	-0.741716
H	4.350591	3.902923	0.258044
H	3.684089	3.722637	-1.381393
H	2.423166	0.980219	1.733205
H	3.635962	2.228524	2.092961
H	4.057428	0.844876	1.064453
C	0.465969	-2.208023	0.502493
C	1.335358	-3.380862	0.986454
C	-0.291833	-1.598631	1.697178
C	-0.530032	-2.680161	-0.573539
H	0.407253	-1.250908	2.464669
H	-0.948183	-2.349380	2.147757
H	-0.907091	-0.751078	1.378230
H	-1.175944	-3.462880	-0.162576
H	-0.001900	-3.082679	-1.442038
H	-1.166920	-1.852998	-0.905016
H	0.702610	-4.110250	1.502475
H	2.110387	-3.044036	1.680432
H	1.818406	-3.895955	0.151335

TS4-6N4

Au	4.566008	-1.177207	-1.567205
Cl	3.440571	-2.323823	-3.290382
Cl	6.665176	-1.964116	-2.292149
Cl	5.537674	0.056125	0.195580
C	2.630018	-0.690240	-0.761317

N	1.836120	-1.259674	0.000321
O	2.564147	0.470033	-1.376367
C	0.039377	0.795472	-0.793163
N	1.166440	1.376603	-0.950728
H	-0.235843	-0.111276	-1.317049
C	-0.810347	1.594012	0.153054
C	1.326885	2.557309	-0.042160
O	-0.037232	2.769752	0.380734
H	-1.779926	1.867315	-0.277762
H	-0.986667	1.024217	1.078539
C	2.226598	2.201389	1.137833
C	1.799014	3.770260	-0.827185
H	2.812854	3.605189	-1.201212
H	1.804796	4.642575	-0.168780
H	1.130459	3.966781	-1.668595
H	1.836410	1.334812	1.677638
H	2.253723	3.056660	1.817765
H	3.243349	1.975944	0.806544
C	1.866173	-2.574039	0.679655
C	3.292135	-3.049013	1.006007
C	1.071599	-2.390387	1.986283
C	1.154123	-3.585830	-0.237747
H	1.559118	-1.659919	2.639903
H	1.007575	-3.341284	2.523821
H	0.053171	-2.046050	1.777649
H	1.103670	-4.561585	0.256203
H	1.692075	-3.699514	-1.182622
H	0.131047	-3.261300	-0.456081
H	3.239624	-3.965274	1.602851
H	3.843402	-2.296452	1.576397
H	3.857664	-3.279026	0.098654

TS4-6Ph

Au	-2.123613	1.284879	1.327991
Cl	-0.601396	1.410424	3.122190
Cl	-3.957069	0.970530	2.775183
Cl	-3.505358	1.245840	-0.585140
C	-0.424062	1.318248	0.036049
N	0.306313	0.416201	-0.422518
O	-0.348857	2.605122	-0.090326
C	2.036971	3.574816	-0.326383
N	1.068434	3.107226	-1.001201
H	2.088611	3.429946	0.750501
C	3.039334	4.283212	-1.192514
C	1.090230	3.390385	-2.470227
C	2.290707	4.396311	-2.547830
H	3.321947	5.249224	-0.761463
H	3.955568	3.681524	-1.248859
H	1.910532	5.413192	-2.679216
H	2.936139	4.167594	-3.398287
C	1.367011	2.081854	-3.222574

C	-0.247180	4.008693	-2.886623
H	-1.068797	3.301500	-2.748305
H	-0.199851	4.282798	-3.945070
H	-0.466222	4.909070	-2.305234
H	2.322027	1.641672	-2.920182
H	1.404532	2.290998	-4.296140
H	0.582030	1.346983	-3.034233
C	-1.013234	-1.645474	-0.681700
C	0.172209	-0.984330	-0.325277
C	-1.069978	-3.038623	-0.619094
C	1.297516	-1.725268	0.063604
C	0.044516	-3.779353	-0.214383
C	1.227567	-3.117004	0.126478
H	-1.877217	-1.070092	-0.997589
H	2.210160	-1.200557	0.327881
H	2.098174	-3.683684	0.443614
H	-0.008728	-4.862689	-0.164666
H	-1.993425	-3.544428	-0.885226

TS4-6PhCl

Au	-1.654301	1.303531	1.754356
Cl	0.126557	1.353554	3.293093
Cl	-3.251909	0.999613	3.456775
Cl	-3.310809	1.325993	0.071574
C	-0.179113	1.326719	0.209343
N	0.444449	0.416813	-0.376834
O	-0.105664	2.611616	0.081535
C	2.159198	3.649235	-0.608246
N	1.111163	3.113189	-1.085607
H	2.412534	3.541853	0.444030
C	2.947364	4.381437	-1.657159
C	0.853981	3.357534	-2.541403
C	1.948480	4.437653	-2.843306
H	3.265088	5.365990	-1.298826
H	3.860980	3.816225	-1.882416
H	1.484179	5.426724	-2.890059
H	2.431199	4.247288	-3.803980
C	1.088893	2.050601	-3.310803
C	-0.575651	3.872121	-2.727485
H	-1.309416	3.114462	-2.441256
H	-0.729465	4.122096	-3.781827
H	-0.756745	4.769562	-2.128920
H	2.114798	1.691176	-3.184038
H	0.913114	2.230114	-4.375838
H	0.410769	1.267205	-2.967645
C	-0.948233	-1.616206	-0.370248
C	0.298314	-0.979753	-0.267437
C	-1.029386	-3.007392	-0.315700
C	1.460982	-1.752072	-0.134958
C	0.135690	-3.761064	-0.167700
C	1.383343	-3.142392	-0.076170

H	-1.850442	-1.025923	-0.491473
H	2.423052	-1.255012	-0.065615
H	2.281028	-3.739579	0.039547
Cl	0.032750	-5.514397	-0.103339
H	-1.992903	-3.500053	-0.385687

TS4-6PhCl$_3$

Au	0.611625	1.355364	2.328315
Cl	2.759301	0.398338	2.446950
Cl	0.432574	1.435432	4.670682
Cl	-1.487662	2.393828	2.069329
C	0.720326	1.013200	0.211909
N	0.597630	-0.013330	-0.494161
O	0.966999	2.226733	-0.134195
C	2.320866	2.320439	-2.399228
N	1.158873	2.396578	-1.895895
H	3.163269	1.951710	-1.818829
C	2.339030	2.752389	-3.838670
C	0.079525	2.914307	-2.788991
C	0.932040	3.383877	-4.019003
H	3.163637	3.445657	-4.033959
H	2.507306	1.872124	-4.472272
H	1.009800	4.474518	-4.016133
H	0.460955	3.083389	-4.957034
C	-0.870361	1.757724	-3.129764
C	-0.656347	4.059132	-2.086867
H	-1.172220	3.705478	-1.190542
H	-1.398526	4.479634	-2.772541
H	0.035458	4.855118	-1.795573
H	-0.339922	0.937815	-3.623183
H	-1.649684	2.125374	-3.804230
H	-1.347344	1.363177	-2.229958
C	-0.807966	-1.896916	0.243454
C	0.433273	-1.349116	-0.139653
C	-0.960701	-3.255759	0.514083
C	1.507038	-2.250049	-0.295828
C	0.140249	-4.098025	0.381500
C	1.379370	-3.610046	-0.028782
Cl	-2.205131	-0.860679	0.377345
Cl	3.054162	-1.659355	-0.861177
H	2.229584	-4.270830	-0.141721
Cl	-0.039649	-5.807328	0.720711
H	-1.924220	-3.642594	0.821518

TS4-6PhMe

Au	-1.616672	1.397036	2.081409
Cl	0.078835	1.446470	3.716398
Cl	-3.308452	1.121457	3.700271
Cl	-3.180865	1.431432	0.313072
C	-0.057726	1.402261	0.626005
N	0.593065	0.488736	0.078621
O	0.044092	2.688980	0.501398

C	2.343981	3.719487	0.000277
N	1.352150	3.158641	-0.562354
H	2.499084	3.632780	1.073244
C	3.214558	4.447975	-0.984033
C	1.232106	3.375355	-2.041223
C	2.320782	4.481525	-2.251706
H	3.492098	5.439225	-0.611188
H	4.148640	3.888687	-1.124214
H	1.837969	5.459134	-2.338409
H	2.887875	4.303958	-3.167715
C	1.581573	2.065814	-2.761332
C	-0.185498	3.843869	-2.376559
H	-0.921546	3.066815	-2.155502
H	-0.240004	4.078562	-3.444179
H	-0.452691	4.740803	-1.810476
H	2.598815	1.739095	-2.523775
H	1.512609	2.226022	-3.841744
H	0.894878	1.267137	-2.475900
C	-0.808062	-1.534806	-0.044466
C	0.432049	-0.909170	0.158650
C	-0.894013	-2.925175	-0.011829
C	1.573218	-1.695093	0.362358
C	0.235530	-3.727932	0.213945
C	1.468080	-3.085794	0.396285
H	-1.693169	-0.933896	-0.225987
H	2.533360	-1.208956	0.504338
H	2.361753	-3.680351	0.568077
C	0.116670	-5.232782	0.274995
H	-1.863233	-3.394072	-0.163248
H	1.096383	-5.714377	0.203981
H	-0.509765	-5.618018	-0.536712
H	-0.342107	-5.553662	1.218488

TS4-6Xyl

Au	0.543902	0.594951	3.028574
Cl	2.666093	0.174253	3.954535
Cl	-0.515996	0.191053	5.095061
Cl	-1.505798	1.175018	2.011121
C	1.472001	0.682833	1.080818
N	1.732446	-0.174250	0.218190
O	1.660672	1.970688	1.115450
C	3.418097	2.175804	-0.906518
N	2.366482	2.632822	-0.357102
H	4.036838	1.430190	-0.417548
C	3.646327	2.782343	-2.263653
C	1.563961	3.591002	-1.170129
C	2.590777	3.918502	-2.305276
H	4.677511	3.128992	-2.382155
H	3.481103	2.006382	-3.022762
H	3.071456	4.878957	-2.099130
H	2.094494	3.991630	-3.275144

C	0.313273	2.863651	-1.685994
C	1.192737	4.803076	-0.312512
H	0.527523	4.511707	0.504272
H	0.674630	5.541018	-0.932787
H	2.083902	5.273851	0.113364
H	0.578566	2.001705	-2.305783
H	-0.277686	3.557080	-2.291958
H	-0.307740	2.517019	-0.856075
C	0.356131	-2.114441	-0.333968
C	1.554192	-1.578739	0.184533
C	0.239983	-3.507583	-0.411712
C	2.639315	-2.404420	0.549508
C	1.281203	-4.344459	-0.012125
C	2.473130	-3.790590	0.454611
C	-0.763553	-1.222676	-0.809332
C	3.948033	-1.816187	1.015876
H	3.293996	-4.438606	0.749527
H	1.169147	-5.422778	-0.075759
H	-0.682570	-3.934953	-0.795150
H	4.370886	-1.145350	0.256428
H	4.678739	-2.607213	1.204107
H	3.828613	-1.236478	1.936333
H	-1.556655	-1.818052	-1.269378
H	-0.404544	-0.502230	-1.554230
H	-1.204348	-0.644852	0.008614

TS6-7

Au	-0.528120	0.553934	0.154116
Cl	-0.419552	1.986689	-1.691016
Cl	-0.595927	-1.057050	1.880461
Cl	-2.767334	1.041679	0.437397
N	2.889558	-1.736224	0.819673
C	2.159899	-1.045640	0.195331
O	1.523961	-0.265798	-0.468517
C	3.237932	-3.028283	1.423169
C	2.341354	-4.116976	0.810546
C	4.721102	-3.290765	1.116198
C	3.004720	-2.906055	2.938638
H	4.892088	-3.356117	0.037635
H	5.026730	-4.236912	1.572587
H	5.349168	-2.491743	1.520406
H	3.271784	-3.849641	3.424546
H	1.955747	-2.685186	3.152334
H	3.623944	-2.110534	3.363036
H	2.591213	-5.087522	1.250473
H	2.491572	-4.182755	-0.271440
H	1.286313	-3.907955	1.008643
C	1.047012	1.901530	3.040232
N	1.108971	2.090769	1.779453
C	1.868356	3.345988	1.485070
C	1.750450	2.926335	3.896644

C	2.871228	3.085178	0.356821
C	0.850365	4.421912	1.065611
C	2.560573	3.702515	2.837913
H	1.006034	3.548522	4.412622
H	2.364495	2.463081	4.676874
H	3.598312	3.351238	2.829449
H	2.578427	4.781022	3.016850
H	2.355157	2.804672	-0.565327
H	3.561351	2.278724	0.628016
H	3.462149	3.987376	0.162720
H	0.279495	4.095414	0.193023
H	1.371961	5.351502	0.812421
H	0.144857	4.634459	1.876414
H	0.490876	1.055427	3.442088

4’

Au	-0.895881	-2.379317	0.279140
Cl	-0.307625	-2.276997	-2.016156
Cl	-1.370059	-2.221021	2.587526
C	0.734725	-1.124299	0.665770
Cl	-2.682850	-3.887625	-0.125295
N	1.922597	-1.380300	0.766322
C	0.208461	0.386310	0.952319
O	2.413641	0.960958	1.336440
C	1.249679	2.123198	-0.444254
N	1.351832	1.220042	0.769541
C	2.867671	-2.504722	0.717515
C	3.559602	-2.445442	-0.656769
C	2.147932	-3.852044	0.913049
C	3.884804	-2.269470	1.849078
C	-0.279816	2.286723	-0.506400
C	1.828642	1.372962	-1.659856
C	2.019473	3.412444	-0.160777
C	-0.864382	0.946729	0.005628
H	-0.073342	0.307512	2.007001
H	2.894676	-4.651655	0.945650
H	1.463839	-4.062618	0.086943
H	1.587361	-3.867797	1.851808
H	4.376988	-1.300370	1.731642
H	4.644363	-3.056668	1.827138
H	3.392631	-2.291833	2.825941
H	2.831610	-2.571494	-1.462734
H	4.297998	-3.250405	-0.723179
H	4.078442	-1.491365	-0.790022
H	-1.031863	0.256890	-0.823721
H	-1.816594	1.080838	0.521008
H	-0.585884	3.113775	0.143158
H	-0.615741	2.516333	-1.520228
H	1.892965	4.095109	-1.005994
H	3.086604	3.212325	-0.034276
H	1.647101	3.908081	0.740717

H	1.784680	2.036435	-2.528738
H	1.267809	0.463962	-1.893229
H	2.873663	1.105743	-1.481695

TS1-4’

Au	-1.609963	-0.178384	-0.509946
Cl	-0.482943	0.480778	-2.483489
Cl	-2.578875	-0.745431	1.568920
C	0.203646	-0.085292	0.467761
Cl	-3.655757	-0.424681	-1.649674
N	1.179318	-0.757729	0.594772
C	0.184193	1.480141	1.592857
O	2.327656	0.866923	2.133209
C	1.979444	2.938857	0.908732
N	1.524717	1.711904	1.689520
C	1.942285	-1.981225	0.342308
C	3.284106	-1.570037	-0.285438
C	1.137295	-2.883305	-0.612395
C	2.160564	-2.662925	1.704363
C	0.662998	3.741910	0.871703
C	2.454698	2.488997	-0.482842
C	3.104083	3.615400	1.692187
C	-0.482067	2.699853	0.989925
H	-0.270116	0.915347	2.402843
H	1.706286	-3.797825	-0.807059
H	0.951158	-2.379268	-1.564561
H	0.177691	-3.163563	-0.168753
H	2.699721	-2.000865	2.386423
H	2.746930	-3.575068	1.558496
H	1.204825	-2.935803	2.160972
H	3.128077	-1.068429	-1.244908
H	3.888225	-2.465347	-0.459393
H	3.832853	-0.901265	0.382812
H	-0.908750	2.463940	0.010961
H	-1.301950	3.053006	1.619500
H	0.629627	4.431878	1.720861
H	0.585837	4.334743	-0.042444
H	3.393553	4.536567	1.177734
H	3.979344	2.964393	1.759431
H	2.783301	3.873411	2.706022
H	2.828973	3.363057	-1.024373
H	1.648129	2.042729	-1.071314
H	3.269898	1.765839	-0.394363