

A Novel Approach for Estimating the Strength of Argentophilic and Auophilic Interactions using QTAIM Parameters

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1. Regression plots for the argentophilic interaction at the PBE0-D4/def2-TZVP level of theory

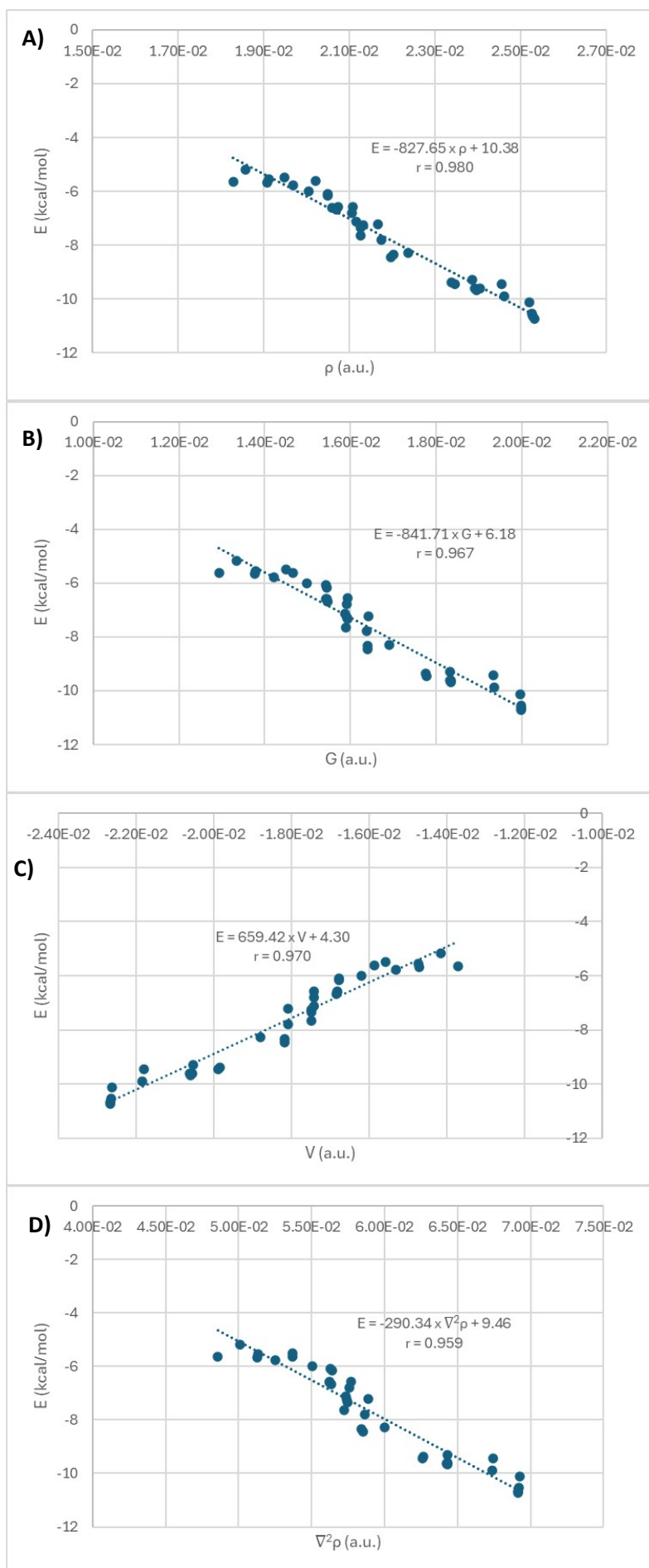


Figure S1 Regression plots and energy equations for the argentophilic interaction at the PBE0-D4/def2-TZVP level of theory for electron density (ρ), A); Lagrangian kinetic energy (G), B); potential energy density (V), C); and Laplacian of the electron density ($\nabla^2 \rho$), D)

2. Regression plots for the aurophilic interaction at the PBE0-D4/def2-TZVP level of theory

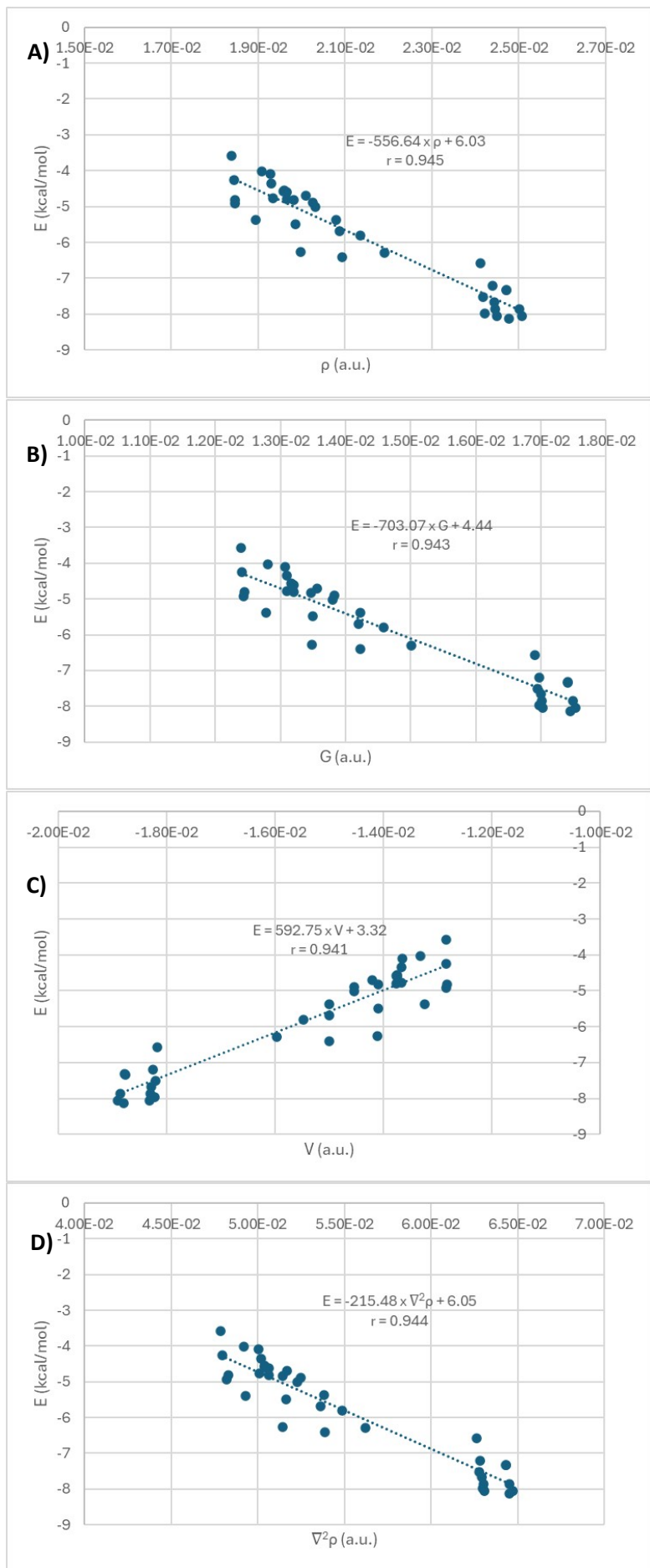


Figure S2 Regression plots and energy equations for the aurophilic interaction at the PBE0-D4/def2-TZVP level of theory for electron density (ρ), A); Lagrangian kinetic energy (G), B); potential energy density (V), C); and Laplacian of the electron density ($\nabla^2 \rho$), D)

3. Tetrameric assemblies including the counterions in HAMMIS, UJOQAN and FAZGET

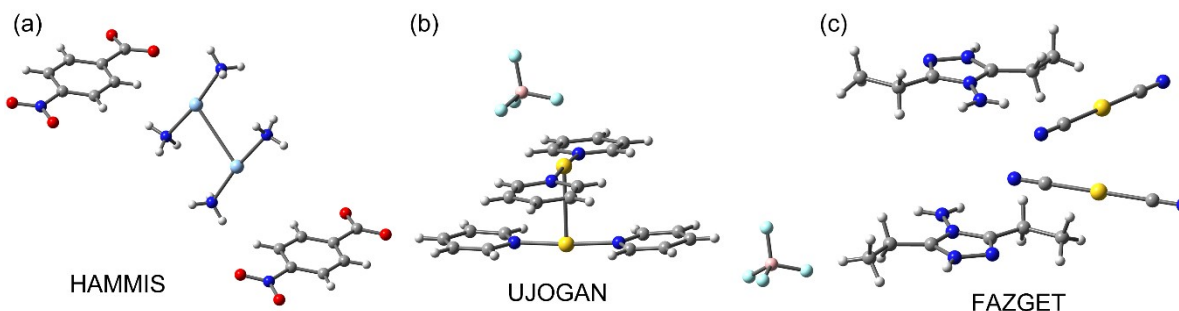


Figure S3. Tetrameric assemblies used to compute the interactions considering the counterions in HAMMIS (a), UJOQAN (b) and FAZGET (c)

4. Tables of the parameters obtained from the multivariable statistical analyses

Table S1: Parameters obtained from the multivariable analyses combining 2 of either ρ , $\nabla^2\rho$, G, V or H variables obtained at the PBE0-D4/x2c-TZVPall level of theory.

R_{adj}	Int	ρ		$\nabla^2\rho$		G		V		H	
Coef ₁	Coef ₂										
ρ				0.956	25.24	0.953	27.21	0.949	27.85	0.943	-3.650
				-3298	760.9	-3281	2832	-3120	-2497	56.81	12810
$\nabla^2\rho$		0.961	12.19			0.946	-7.950	0.946	-7.950	0.946	-7.950
		167.1	-1373			4878	-19016	2501	9508	123.6	19016
G		0.971	15.02	0.966	-8.551			0.946	-7.950	0.946	-7.950
		678.9	-1539	-4873	1311			20004	19510	494.3	19510
V		0.971	17.75	0.966	-8.551	0.966	-8.551			0.946	-7.950
		-670.0	-1687	2436	702.0	5244	5616			-494.3	20004
H		0.968	19.86	0.966	-8.551	0.966	-8.551	0.966	-8.551		
		-2098	-1340	4873	92.89	5244	371.6	-371.6	5616		

R_{adj} refers to the adjusted value for Pearson's R; Int refers to the interception coefficient of the regression; Coef₁ refers to the coefficient of variable in the same row while Coef₂ refers to the variable in the same column. The light-blue cells contain the values of the double-variable plots for the Ag complexes while the yellow cells contain the values for the Au complexes. PBE0-D4/x2c-TZVPall level of theory.

Table S2: Parameters obtained from the multivariable analyses combining 2 of either ρ , $\nabla^2\rho$, G, V or H variables obtained at the PBE0-D4/def2-TZVP level of theory.

R_{adj}	Int	ρ		$\nabla^2\rho$		G		V		H	
Coef ₁	Coef ₂										
ρ				0.941	6.041	0.942	7.496	0.944	11.57	0.954	25.00
				-375.5	-70.21	-1080	662.6	-1714	-1238	-1777	-8377
$\nabla^2\rho$		0.987	10.82			0.947	16.48	0.947	16.51	0.947	16.55
		319.8	-1714			-1632	4633	-1055	-2317	-476.6	-4636
G		0.986	15.32	0.991	-18.91			0.947	16.58	0.947	16.58
		1074	-1865	-7014	2147			-8455	-6546	-1910	-6546
V		0.984	18.13	0.991	-18.92	0.991	-18.92			0.947	16.58
		-876.4	-1913	3507	1270	8586	10158			1910	-8455
H		0.980	-0.118	0.991	-18.92	0.991	-18.92	0.991	-18.83		
		2468	-153.6	7014	393.1	8586	1572	10158	-1564		

R_{adj} refers to the adjusted value for Pearson's R; Int refers to the interception coefficient of the regression; Coef₁ refers to the coefficient of variable in the same row while Coef₂ refers to the variable in the same column. The light-blue cells contain the values of the double-variable plots for the Ag complexes while the yellow cells contain the values for the Au complexes. PBE0-D4/def2-TZVP level of theory.

5. Tables of the QTAIM parameters from the dimers plotted in figure 6

Table S3: QTAIM parameters obtained at the bCP Ag...Ag of the dimers of complex 4 from figure 6 at the PBE0-D4/x2c-TZVPall level of theory.

	ρ	$\nabla^2\rho$	G	V
b)	0.00151	0.00335	0.00068	-0.00052
c)	0.00359	0.00732	0.00163	-0.00143
d)	0.02131	0.06073	0.01596	-0.01674

6. Coordinates of the dimers 1 to 84 at their energetic minimum (PBE0-D4/x2c-TZVPall)

1.
Ag 0.73586603 -0.38433013 0.00000058
N 2.80515863 -0.38433323 -0.00000232
C 3.94608123 -0.38433513 -0.00000412
Cl -1.52726117 -0.38432983 0.00000088
H 5.01596113 -0.38433893 -0.00000762
Ag 0.73587059 2.65316987 -0.00000044
N 0.73586769 2.65316915 -2.06929304
C 0.73586589 2.65316856 -3.21021564
Cl 0.73587089 2.65316757 2.26312676
H 0.73586239 2.65316599 -4.28009554

2.
Ag 0.74433466 -0.87938554 0.00000177
N 2.83283976 -0.87938934 -0.00000173
C 3.97677626 -0.87939134 -0.00000363
F 5.22244266 -0.87939474 -0.00000683
Cl -1.52059714 -0.87938514 0.00000207
Ag 0.74434013 2.13311446 -0.00000120
N 0.74433663 2.13311238 -2.08850630
C 0.74433473 2.13311133 -3.23244280
F 0.74433153 2.13310895 -4.47810920
Cl 0.74434043 2.13311299 2.26493060

3.
Ag 0.77045421 1.65757624 -0.49995676
N 2.83543331 1.65770794 -0.49992436
C 3.97770091 1.65805404 -0.49995156
C 5.46928201 1.65779194 -0.49999556
F 5.91021881 2.79364064 -1.01059256
F 5.90967951 1.53187054 0.73909664
F 5.90923561 0.64743324 -1.22848286
Cl -1.48922249 1.65757564 -0.50000916
Ag 0.77061159 -1.11040298 0.72025470
N 0.77052882 -0.27744062 2.60978172
C 0.77041409 0.18356781 3.65488775
C 0.77056009 0.78496114 5.01985672
F 0.77953540 2.10232515 4.92107244
F -0.31242633 0.39973664 5.67093133
F 1.84473802 0.38537001 5.67677858
Cl 0.77065978 -2.02177520 -1.34748307

4.
Ag 0.78076180 -0.68630836 1.03097000
N 2.84012770 -0.68631836 1.03095910
C 3.98464260 -0.68630956 1.03096990
N 5.40873780 -0.68633056 1.03094610
O 5.91790740 -1.38770396 0.19836960
O 5.91791100 0.01507934 1.86356710
Cl -1.47534160 -0.68630276 1.03097660
Ag 0.78076257 1.60661577 -0.92291208
N 0.78074779 0.27092843 -2.49037093
C 0.78076172 -0.47139428 -3.36150315
N 0.78072998 -1.39505054 -4.44543408
O -0.30787936 -1.72060389 -4.83697802
O 1.86939688 -1.72998635 -4.82898762
Cl 0.78077123 3.06990493 0.79429128

5.
Ag 0.78342714 -0.48396373 -0.75735072
N 2.85187824 -0.48396973 -0.75735502
C 3.99650354 -0.48397043 -0.75735622
C 5.43988034 -0.48397213 -0.75736412
H 5.80845294 0.45262617 -1.17835482
H 5.80845444 -0.58768583 0.26425608
H 5.80844544 -1.31686773 -1.35798672
Cl -1.48377986 -0.48396013 -0.75734942
Ag 0.78343794 1.94405873 1.06778302
N 0.78343811 3.18692288 -0.58563122
C 0.78343757 3.87469277 -1.50058458
C 0.78343228 4.74196959 -2.65434691
H -0.11585551 5.35968011 -2.65110543
H 1.66238336 5.38784897 -2.62993274
H 0.80378110 4.14276496 -3.56585256
Cl 0.78343682 0.58176516 2.88006992

6.
Ag 0.80166312 0.50940667 1.10336733
N 2.87065552 0.50940357 1.10336313
C 4.02191782 0.50939587 1.10336123
N 5.33076092 0.50943417 1.10335923
H 5.83850212 1.37660007 1.10335823

H	5.83851222	-0.35784773	1.10335113
Cl	-1.46786008	0.50940757	1.10336823
Ag	0.80165697	0.54836802	-1.93388279
N	0.80165382	-1.52045417	-1.96042133
C	0.80164609	-2.67162177	-1.97518783
N	0.80168436	-3.98035720	-1.99197595
H	1.66877889	-4.48791396	-2.00961241
H	-0.06552627	-4.48820933	-1.98737057
Cl	0.80165788	2.81770456	-1.90477576

7.

Ag	0.76789195	-0.59786394	1.39734518
N	2.84736385	-0.59086954	1.40385968
C	3.99416985	-0.56137514	1.43121818
O	5.26845465	-0.59476284	1.40018648
H	5.66330265	0.05362456	2.00207958
Cl	-1.49967315	-0.58757024	1.40687558
Ag	0.76899356	1.28198377	-0.97263296
N	0.77852178	-0.34720966	-2.26489173
C	0.81863018	-1.24737099	-2.97544314
O	0.77318934	-2.24321266	-3.77049908
H	1.65519129	-2.59534050	-3.96198021
Cl	0.78298016	3.05735757	0.43800538

8.

Ag	1.16991377	-2.34199847	-0.07444816
N	3.25648267	-2.34200167	-0.07445116
C	4.39739597	-2.34200347	-0.07445286
H	5.46735137	-2.34200717	-0.07445626
Br	-1.21984763	-2.34199817	-0.07444786
Ag	1.16991816	-2.31735405	2.93795103
N	1.16992133	-0.23087265	2.91884297
C	1.16992312	0.90999281	2.90839483
H	1.16992679	1.97990333	2.89859467
Br	1.16991787	-4.70701528	2.95983246

9.

Ag	-0.49011192	-1.22910374	0.00000007
N	1.61544078	-1.22910774	-0.00000373
C	2.75950258	-1.22910964	-0.00000553
Br	-2.88132872	-1.22910334	0.00000037
F	4.00507948	-1.22911274	-0.00000843
Ag	-0.49010627	1.75839626	-0.00000123
N	-0.49011007	1.75839536	-2.10555393
C	-0.49011187	1.75839515	-3.24961573
Br	-0.49010597	1.75839313	2.39121557
F	-0.49011477	1.75839389	-4.49519263

10.

Ag	0.45572475	-1.11187529	-0.12810244
N	2.53862025	-1.11192399	-0.12820814
C	3.68086415	-1.11190409	-0.12849894
Br	-1.93053975	-1.11180709	-0.12812074
C	5.17269055	-1.11186649	-0.12832804
F	5.61319815	-1.94706559	-1.05216884
F	5.61244355	-1.49445349	1.05714276
F	5.61292785	0.10595871	-0.38953094
Ag	0.45575975	1.81489895	-0.78688356
N	0.45564594	1.35750820	-2.81893852
C	0.45536661	1.10677287	-3.93332307
Br	0.45575688	2.33894929	1.54112621
C	0.45554159	0.77919333	-5.38873973
F	-0.62916116	0.08546966	-5.68412711
F	1.52805564	0.06451155	-5.67863647
F	0.46815557	1.89758649	-6.09171319

11.

Ag	0.05159019	-0.77593114	-0.23786783
N	2.12838489	-0.77590374	-0.23787223
C	3.27294179	-0.77593934	-0.23787373
Br	-2.33082431	-0.77595644	-0.23786673
N	4.69692949	-0.77594794	-0.23787833
O	5.20621899	-1.86468394	-0.23788463
O	5.20622609	0.31277746	-0.23787563
Ag	0.05159690	-0.80403926	2.76200049
N	0.05156955	1.27266428	2.78145875
C	0.05160516	2.41717093	2.79218393
Br	0.05162219	-3.18634915	2.73967476
N	0.05161380	3.84109614	2.80552447
O	1.14030210	4.35026776	2.82048892
O	-1.03706386	4.35046592	2.80010232

12.

Ag	-0.11177950	-0.34318612	-0.05772892
N	1.97166470	-0.34318982	-0.05773222
C	3.11632980	-0.34319232	-0.05773552

Br	-2.50553310	-0.34318602	-0.05772972
C	4.55978830	-0.34319822	-0.05774202
H	4.92819970	0.66084568	-0.27319982
H	4.92819770	-0.65862972	0.91951568
H	4.92818960	-1.03181422	-0.81954072
Ag	-0.11177524	2.60348825	-0.68404065
N	-0.11177924	2.17033122	-2.72195986
C	-0.11178299	1.93235026	-3.84161305
Br	-0.11177600	3.10115691	1.65740809
C	-0.11179057	1.63224668	-5.25353028
H	-0.11379394	2.56011388	-5.82738708
H	0.77853295	1.05511816	-5.50750239
H	-1.00011030	1.05172539	-5.50677299

13.

Ag	-0.18056846	-0.59293706	-0.44774720
N	1.90270254	-0.59294176	-0.44775160
C	3.05406314	-0.59293986	-0.44775350
Br	-2.57664126	-0.59293596	-0.44774640
N	4.36284624	-0.59298246	-0.44775530
H	4.87053964	0.27433314	-0.44775640
H	4.87051584	-1.46020056	-0.44776350
Ag	-0.18056199	-0.56629854	2.57713551
N	-0.18055733	1.51689169	2.55878998
C	-0.18055925	2.66820765	2.54865154
Br	-0.18056309	-2.96227847	2.59823131
N	-0.18051667	3.97694001	2.53712685
H	-1.04779863	4.48468098	2.54029526
H	0.68666772	4.48452261	2.52501076

14.

Ag	-0.07751117	-0.09962542	0.28030044
N	2.01692093	-0.09238952	0.28702554
C	3.16389573	-0.06300852	0.31422024
Br	-2.47130607	-0.08896022	0.29015284
O	4.43807633	-0.09614892	0.28348024
H	4.83294823	0.55301448	0.88483134
Ag	-0.07646137	1.78258873	-2.07181033
N	-0.06660985	0.14728804	-3.38041187
C	-0.02667922	-0.74980774	-4.09509969
Br	-0.06197902	3.65045715	-0.57470555
O	-0.07175979	-1.74232020	-4.89414049
H	0.81079914	-2.09069493	-5.09082513

15.

Ag	1.14979180	-2.69573824	0.00000047
N	3.26054490	-2.69574174	-0.00000283
C	4.40150220	-2.69574334	-0.00000433
H	5.47154850	-2.69574684	-0.00000763
I	-1.40209100	-2.69573794	0.00000067
Ag	1.14979679	0.30426176	-0.00000011
N	1.14979349	0.30426136	-2.11075321
C	1.14979199	0.30426143	-3.25171051
H	1.14978869	0.30425950	-4.32175681
I	1.14979699	0.30425832	2.55188269

16.

Ag	0.22355937	-1.33698151	0.00000004
N	2.35339427	-1.33698571	-0.00000396
C	3.49768207	-1.33698741	-0.00000566
I	-2.32916333	-1.33698101	0.00000044
F	4.74334987	-1.33699031	-0.00000826
Ag	0.22356521	1.63801849	-0.00000093
N	0.22356121	1.63801777	-2.12983583
C	0.22355951	1.63801794	-3.27412363
I	0.22356561	1.63801481	2.55272177
F	0.22355691	1.63801708	-4.51979143

17.

Ag	0.34394577	0.80757081	-0.08504746
N	2.45280017	0.80749801	-0.08510266
C	3.59507977	0.80721761	-0.08521216
I	-2.20478243	0.80754741	-0.08502426
C	5.08701327	0.80734811	-0.08514126
F	5.52757777	-0.09015919	-0.94852526
F	5.52699827	0.50848481	1.12408574
F	5.52673697	2.00412711	-0.43079376
Ag	0.34402247	3.67224500	-0.93286704
N	0.34394888	3.07377535	-2.95501959
C	0.34376430	2.74940909	-4.05027722
I	0.34403807	4.39545541	1.51110148
C	0.34386932	2.32615221	-5.48091316
F	-0.73873665	1.61087774	-5.72869350
F	1.41855080	1.59741845	-5.72410617
F	0.35209240	3.39583763	-6.25603770

18.			
Ag	-0.37833231	-0.07159915	-0.18447660
N	1.72232949	-0.07158865	-0.18448120
C	2.86712739	-0.07162545	-0.18448270
I	-2.92268471	-0.07160485	-0.18447540
N	4.29025139	-0.07164765	-0.18448700
O	4.80010559	-1.16064605	-0.18449330
O	4.80003989	1.01741575	-0.18448430
Ag	-0.37832563	-0.09569131	2.80292625
N	-0.37833609	2.00490218	2.81986669
C	-0.37829928	3.14966284	2.82910007
I	-0.37831994	-2.63996094	2.78240332
N	-0.37827705	4.57274057	2.84057567
O	0.71068601	5.08250742	2.85346148
O	-1.46730508	5.08258329	2.83591076

19.			
Ag	0.11177002	-0.26846280	0.08018578
N	2.21689772	-0.26846570	0.08018278
C	3.36166062	-0.26847030	0.08017908
I	-2.44381358	-0.26846450	0.08018458
C	4.80518222	-0.26847460	0.08017448
H	5.17359102	0.71807180	-0.20481182
H	5.17359162	-0.51494760	1.07704228
H	5.17358352	-1.00855750	-0.63171352
Ag	0.11177283	2.61923555	-0.73295519
N	0.11176916	2.04864703	-2.75927978
C	0.11176435	1.73836023	-3.86118913
I	0.11177122	3.31191522	1.72696400
C	0.11175876	1.34709657	-5.25067369
H	0.10484200	2.23566250	-5.88361822
H	1.00450368	0.75879075	-5.46775110
H	-0.77407824	0.74726392	-5.46449688

20.			
Ag	0.01719569	-0.47647672	-0.54663323
N	2.12089709	-0.47648152	-0.54663783
C	3.27243609	-0.47647922	-0.54663953
I	-2.54042401	-0.47647602	-0.54663243
N	4.58127789	-0.47650682	-0.54664123
H	5.08900209	0.39077018	-0.54664243
H	5.08898609	-1.34373272	-0.54664953
Ag	0.01720229	-0.48054046	2.46586403
N	0.01720709	1.62315903	2.46870185
C	0.01720480	2.77469698	2.47025604
I	0.01720159	-3.03815782	2.46240911
N	0.01723240	4.08353759	2.47202281
H	-0.85004381	4.59126290	2.47153959
H	0.88445752	4.59124376	2.47386846

21.			
Ag	-0.31856891	-0.76259561	0.45921488
N	1.79766789	-0.75418451	0.46703608
C	2.94486169	-0.72584621	0.49326648
I	-2.87426961	-0.75097191	0.46995098
O	4.21899489	-0.75840931	0.46304288
H	4.61204139	-0.10885871	1.06497068
Ag	-0.31628399	0.95175867	-2.00269173
N	-0.30491211	-0.78490641	-3.21201186
C	-0.26667069	-1.72890185	-3.86389752
I	-0.30061314	3.04669803	-0.53884748
O	-0.31065899	-2.77038350	-4.59790722
H	0.56626454	-3.16337974	-4.72151020

22.			
Ag	0.70834879	-0.57045602	-0.01676630
C	-1.29652421	-0.57045542	-0.01676580
N	-2.45269311	-0.57045542	-0.01676570
N	2.79171459	-0.57045922	-0.01676930
C	3.93187499	-0.57046072	-0.01677070
H	5.00224239	-0.57046372	-0.01677350
Ag	0.70835359	2.50418293	0.03035373
C	0.70835408	2.47345855	2.03499130
N	0.70835418	2.45574008	3.19102442
N	0.70835064	2.53610759	-2.05276745
C	0.70834926	2.55357921	-3.19279398
H	0.70834650	2.56997971	-4.26303572

23.			
Ag	0.70228546	0.17038301	0.00000025
C	-1.30211244	0.17038371	0.00000085
N	-2.45826294	0.17038371	0.00000085
N	2.82118836	0.19133507	-0.00000350
C	3.96465816	0.19133347	-0.00000500

F	5.20857086	0.19133117	-0.00000720
Ag	0.67200442	3.23273330	-0.00000155
C	0.67131874	3.30214161	2.00319414
N	0.67092288	3.34217639	3.15865120
N	0.67271922	3.16006979	-2.09704949
C	0.67310925	3.12047249	-3.23983342
F	0.67353299	3.07739638	-4.48299997

24.

Ag	4.03570315	0.02893779	0.04968015
C	2.03104845	0.02892468	0.04957826
N	0.87501195	0.02891461	0.04953319
N	6.11840285	0.02909809	0.04971895
C	7.25974265	0.02951879	0.04968795
C	8.75410945	0.02919089	0.04962885
F	9.19176805	1.16504439	-0.46101435
F	9.19113285	-0.09681061	1.28879625
F	9.19056265	-0.98132091	-0.67892945
Ag	4.03551235	2.81074277	-1.20094411
C	4.03541404	3.63273286	0.62743571
N	4.03536881	4.10674771	1.68182193
N	4.03559894	1.95692502	-3.10058442
C	4.03559410	1.48932813	-4.14174237
C	4.03556932	0.87629772	-5.50457983
F	3.52487446	1.73279712	-6.36948689
F	5.27475359	0.58225661	-5.85151476
F	3.30707593	-0.22436374	-5.48831859

25.

Ag	0.74580695	0.33244808	0.16117131
C	-1.25853165	0.33245358	0.16117761
N	-2.41456455	0.33245388	0.16117791
N	2.82796255	0.33243238	0.16115341
C	3.97109595	0.33244278	0.16116621
N	5.40033795	0.33244338	0.16116791
O	5.90589175	-0.36890542	-0.67137939
O	5.90591235	1.03379158	0.99371561
Ag	0.74580762	2.66398909	-1.80514924
C	0.74581598	3.95617646	-0.27295310
N	0.74581641	4.70146523	0.61076445
N	0.74578382	1.32163323	-3.39683159
C	0.74580031	0.58466050	-4.27068808
N	0.74580199	-0.33676529	-5.36325716
O	-0.34278645	-0.66223415	-5.75010988
O	1.83439035	-0.66316637	-5.74935064

26.

Ag	0.75032791	0.14087902	-0.00000027
C	-1.25479879	0.14088312	0.00000123
N	-2.41121569	0.14088372	0.00000133
N	2.82903331	0.14087342	-0.00000417
C	3.97328981	0.14087362	-0.00000607
C	5.41620271	0.14087132	-0.00001117
H	5.78385061	1.07776882	-0.42113717
H	5.78385151	0.03712642	1.02193063
H	5.78384401	-0.69228698	-0.60082597
Ag	0.75033617	3.21587902	-0.00000191
C	0.75033728	3.07539410	2.00019736
N	0.75033715	2.99437046	3.15377233
N	0.75033267	3.36151772	-2.07359914
C	0.75033099	3.44169014	-3.21504355
C	0.75032617	3.54278540	-4.65441055
H	0.32920337	4.50314103	-4.95551128
H	1.77226770	3.46505131	-5.02842475
H	0.14950866	2.73743540	-5.07952347

27.

Ag	0.78065374	0.59368499	0.56312669
C	-1.22426762	0.59330225	0.56314934
N	-2.38080770	0.59308065	0.56316182
N	2.85760101	0.59407859	0.56310021
C	4.00870049	0.59429873	0.56308649
N	5.31620176	0.59453464	0.56307139
H	5.82380932	1.46207949	0.55104908
H	5.82413059	-0.27279226	0.57507289
Ag	0.73805693	0.40128941	-2.50555290
C	0.73767349	2.40228197	-2.63100595
N	0.73745151	3.55655567	-2.70337424
N	0.73845142	-1.67158810	-2.37559615
C	0.73867200	-2.82043195	-2.30356961
N	0.73890840	-4.12537113	-2.22175691
H	1.60600817	-4.63008941	-2.15977720
H	-0.12797263	-4.63419971	-2.22020004

28.

Ag	0.74093523	0.34337508	0.19078138
C	-1.26357027	0.34920488	0.19616348
N	-2.41991077	0.35352818	0.20016308
N	2.82824463	0.35530168	0.20187588
C	3.97503733	0.37978848	0.22456968
O	5.24721693	0.34408208	0.19136948
H	5.64621353	0.99145298	0.79233628
Ag	0.74163843	2.36237359	-2.11194543
C	0.74957000	3.86914410	-0.78994506
N	0.75545743	4.73832944	-0.02729165
N	0.75792039	0.79290057	-3.48803235
C	0.79129335	-0.06982366	-4.24357272
O	0.74255799	-1.02525049	-5.08357425
H	1.62551369	-1.34187531	-5.32767756

29.

Ag	0.70313311	0.52322960	-0.01249502
N	2.83314291	0.52323620	-0.01244262
C	3.51738911	-0.62332590	0.02774968
C	3.51733751	1.67002510	-0.05264982
C	4.89879131	-0.66721420	0.02920298
H	2.93073301	-1.53304970	0.05969648
C	4.89875351	1.71379540	-0.05425942
H	2.93064101	2.57962870	-0.08450602
C	5.60474031	0.52341940	-0.01263162
H	5.40369701	-1.62388210	0.06277018
H	5.40359891	2.67060690	-0.08778472
Cl	-1.56508719	0.52316380	-0.01249652
H	6.68812151	0.52339220	-0.01278642
Ag	0.70306089	0.61287549	2.91113092
N	0.70305590	2.74188469	2.84585000
C	1.85031108	3.42596419	2.82992154
C	-0.44442643	3.42560186	2.81979654
C	1.89422331	4.80671974	2.78765856
H	2.76058654	2.83970905	2.85198693
C	-0.48822549	4.80635964	2.77715626
H	-1.35457896	2.83905915	2.83380806
C	0.70286700	5.51217236	2.76065400
H	2.85147047	5.311151838	2.77642459
H	-1.44561490	5.31083840	2.75746454
Cl	0.70312662	-1.65427767	2.98070018
H	0.70288945	6.59503904	2.72726813

30.

Ag	0.70594776	0.48272433	-1.50854761
N	2.83557766	0.48278343	-1.50849081
C	3.52122886	-0.66332007	-1.46829451
C	3.52118366	1.62895113	-1.54865891
C	4.90033516	-0.71674777	-1.46651081
H	2.93800946	-1.57518247	-1.43629911
C	4.90028416	1.68238983	-1.55060351
H	2.93793276	2.54078413	-1.58062011
C	5.58298606	0.48285253	-1.50873301
H	5.42814126	-1.66005167	-1.43338521
H	5.42802966	2.62575403	-1.58363371
F	6.90596616	0.48283953	-1.50911091
Cl	-1.56009714	0.48266573	-1.50853511
Ag	0.70586760	0.56196668	1.41537880
N	0.70581006	2.69081492	1.35768413
C	1.85258162	3.37646245	1.34825014
C	-0.44102491	3.37592108	1.32996117
C	1.90603802	4.75507068	1.31118737
H	2.76497593	2.79365565	1.37136870
C	-0.49449667	4.75450087	1.29206416
H	-1.35338891	2.79268749	1.33850927
C	0.70573443	5.43720636	1.28293753
H	2.84989290	5.28288833	1.30445499
H	-1.43840924	5.28184924	1.27026820
F	0.70573720	6.75968963	1.24668191
Cl	0.70592651	-1.70324451	1.47684215

31.

Ag	0.70710770	0.51954190	-0.08337466
N	2.84052190	0.52014990	-0.08756946
C	3.52407510	-0.62583160	-0.04093926
C	3.52321350	1.66700430	-0.12068976
C	4.90470310	-0.67100730	-0.02324746
H	2.93976210	-1.53700240	-0.01428496
C	4.90412020	1.71443470	-0.10628556
H	2.93825560	2.57732340	-0.15737476
C	5.60508670	0.52231880	-0.05482566
H	5.41656480	-1.62291800	0.02296094
H	5.41506950	2.66764670	-0.12652866
C	7.11240480	0.51998370	-0.07402366
F	7.61028400	1.62758820	0.47678814

F	7.56645710	0.45424860	-1.33019546
F	7.60685750	-0.52701820	0.58793634
Cl	-1.55829510	0.51949950	-0.07250806
Ag	0.71281765	0.64560870	2.83890177
N	0.71202942	2.77704459	2.74695333
C	1.85895074	3.45980691	2.71378627
C	-0.43515008	3.45992685	2.73742422
C	1.90488285	4.83990887	2.67259962
H	2.77039500	2.87539194	2.72342172
C	-0.48187816	4.84034415	2.69711298
H	-1.34619986	2.87564737	2.76585325
C	0.71134837	5.54061786	2.66597350
H	2.85791075	5.35146828	2.65481202
H	-1.43503240	5.35179921	2.69878802
C	0.71282197	7.04586575	2.58468082
F	-0.36884201	7.56802321	3.16383510
F	0.72190145	7.44777328	1.30920441
F	1.78858410	7.56516627	3.17793481
Cl	0.71334091	-1.61742869	2.94296630

32.

Ag	0.71085702	0.57700564	1.31418573
N	2.84520202	0.57708874	1.31426543
C	3.52541702	-0.57178066	1.35459413
C	3.52544272	1.72587064	1.27397073
C	4.90683712	-0.62335276	1.35623963
H	2.93956622	-1.48165196	1.38656953
C	4.90687952	1.77750114	1.27204833
H	2.93959302	2.63578044	1.24204813
C	5.58288122	0.57700134	1.31392913
H	5.44107242	-1.56225616	1.38915363
H	5.44107842	2.71637224	1.23909653
N	7.05875112	0.57684874	1.31317213
O	7.60491492	1.65368024	1.27603403
O	7.60467182	-0.50003636	1.34961713
Cl	-1.55263538	0.57692144	1.31418973
Ag	0.71097080	0.45831134	-1.60840501
N	0.71105060	-1.67427565	-1.52179489
C	-0.43850876	-2.35418967	-1.50058295
C	1.86052116	-2.35369767	-1.48782303
C	-0.49010514	-3.73449237	-1.44502989
H	-1.34892797	-1.76902353	-1.52933770
C	1.91218713	-3.73399164	-1.43164286
H	2.77097668	-1.76812436	-1.50651521
C	0.71097693	-4.40971797	-1.41114760
H	-1.42957061	-4.26850130	-1.42861711
H	2.85162186	-4.26754014	-1.40477995
N	0.71085521	-5.88440547	-1.35207720
O	1.78830653	-6.42985143	-1.32330956
O	-0.36662151	-6.43017438	-1.33726545
Cl	0.71088650	2.71994295	-1.70016730

33.

Ag	0.69989848	0.45250729	-1.09296624
N	2.82856288	0.45255359	-1.09639934
C	3.51938888	-0.68994171	-1.05083294
C	3.51912218	1.59546029	-1.13095344
C	4.89860748	-0.72998581	-1.03695894
H	2.93792468	-1.60329601	-1.02153454
C	4.89844828	1.63663989	-1.11993004
H	2.93752428	2.50856709	-1.16568354
C	5.62772408	0.45365149	-1.07283724
H	5.40040088	-1.68921381	-0.99419104
H	5.40007688	2.59659059	-1.14445854
C	7.12037168	0.45301219	-1.08330904
H	7.48938428	0.40079489	-2.11209974
H	7.52190298	1.36291659	-0.63616424
H	7.52129078	-0.40796961	-0.54726234
Cl	-1.57011222	0.45277509	-1.08498524
Ag	0.70462189	0.64348568	1.83831525
N	0.70435249	2.76764935	1.69992248
C	1.84734711	3.45513893	1.62553336
C	-0.43831542	3.45946364	1.69771191
C	1.88823008	4.83229051	1.54923100
H	2.76062273	2.87283795	1.63085443
C	-0.47866562	4.83688547	1.62396429
H	-1.35170895	2.88069836	1.76071469
C	0.70483394	5.56267289	1.54596488
H	2.84817761	5.33172548	1.49622604
H	-1.43811656	5.34001025	1.63155319
C	0.70477806	7.05165145	1.44084702
H	0.68834383	7.35461087	0.38953700
H	-0.17331585	7.48451081	1.92113415
H	1.59955887	7.48203932	1.89196279
Cl	0.70488050	-1.62145078	1.99022024

34.

Ag	0.71523406	0.56671211	1.05770358
N	2.84051326	0.56676211	1.05774858
C	3.54135416	-0.57312669	1.09769398
C	3.54134536	1.70672051	1.01781558
C	4.91350356	-0.62490629	1.09936498
H	2.96497956	-1.48978529	1.12991728
C	4.91354136	1.75844681	1.01589758
H	2.96497636	2.62329801	0.98573298
C	5.64887886	0.56679151	1.05739588
H	5.41237036	-1.58588029	1.13313638
H	5.41233666	2.71945821	0.98224738
N	6.99901566	0.56667491	1.05706178
H	7.51496996	-0.29214599	1.08597718
H	7.51521646	1.42512211	1.02652078
Cl	-1.55790364	0.56663681	1.05769928
Ag	0.71529877	0.44765142	-1.86487226
N	0.71534690	-1.67586641	-1.77836383
C	-0.42522301	-2.37639201	-1.75635808
C	1.85598584	-2.37585279	-1.74333094
C	-0.47702770	-3.74742331	-1.70097457
H	-1.34243343	-1.80070351	-1.78493795
C	1.90774734	-3.74690505	-1.68731664
H	2.77310950	-1.79974642	-1.76151029
C	0.71539064	-4.48192133	-1.66446369
H	-1.43857980	-4.24609655	-1.68606882
H	2.86933187	-4.24506298	-1.66151258
N	0.71528774	-5.83095417	-1.60987517
H	-0.14399824	-6.34672889	-1.59496531
H	1.57426654	-6.34654675	-1.58443259
Cl	0.71522371	2.71890695	-1.95735632

35.

Ag	0.70742531	0.48335542	-1.18211006
N	2.83677091	0.47702042	-1.18180556
C	3.52237091	-0.66805098	-1.14171056
C	3.53773731	1.61704912	-1.22178086
C	4.89935521	-0.72544518	-1.13989886
H	2.93869751	-1.57975648	-1.10964406
C	4.91270221	1.66186892	-1.22352166
H	2.96140381	2.53329532	-1.25381776
C	5.61869951	0.46426752	-1.18181306
H	5.39906471	-1.68670278	-1.10618396
H	5.44012241	2.60563662	-1.25663096
O	6.95508281	0.51832372	-1.18417526
H	7.32661591	-0.36915498	-1.15369306
Cl	-1.56245479	0.47860802	-1.18200156
Ag	0.70733133	0.59225588	1.74086200
N	0.71367327	2.72012519	1.66158471
C	1.85944364	3.40515483	1.63351089
C	-0.42705343	3.42069643	1.63792294
C	1.91686551	4.78117071	1.58187595
H	2.77171097	2.82181711	1.65339158
C	-0.47190696	4.79470371	1.58661527
H	-1.34385722	2.84484028	1.66146597
C	0.72641707	5.50010376	1.55744006
H	2.87871196	5.28045617	1.56119063
H	-1.41625309	5.32183291	1.56898124
O	0.67231041	6.83554590	1.50729286
H	1.56030878	7.20672587	1.49089814
Cl	0.71207947	-1.67605031	1.82537649

36.

Ag	0.69462153	0.52344678	-0.01247469
C	-1.30807747	0.52339640	-0.01250547
N	-2.46466407	0.52337552	-0.01249749
N	2.82946783	0.52350368	-0.01243599
C	3.51333563	-0.62346782	0.02775031
C	3.51327273	1.67051998	-0.05267119
C	4.89457533	-0.66715152	0.02918561
H	2.92650793	-1.53326012	0.05971531
C	4.89450563	1.71424798	-0.05429059
H	2.92640343	2.58027938	-0.08451259
C	5.60014153	0.52357438	-0.01262139
H	5.39989483	-1.62347192	0.06270291
H	5.39979453	2.67060468	-0.08784239
H	6.68363833	0.52361408	-0.01271649
Ag	0.69456678	0.56300623	2.94976117
C	0.69461674	-1.43951414	2.97650866
N	0.69463155	-2.59599727	2.99197881
N	0.69450902	2.69766219	2.92125371
C	1.84191398	3.38180239	2.93699483
C	-0.45294227	3.38107177	2.88717594
C	1.88561205	4.76293002	2.91937764

H	2.75205202	2.79529291	2.96467020
C	-0.49668886	4.76216729	2.86767021
H	-1.36304500	2.79399083	2.87531825
C	0.69443407	5.46808571	2.88402017
H	2.84229404	5.26848258	2.93338057
H	-1.45340826	5.26713232	2.84011953
H	0.69439241	6.55148437	2.86943723

37.

Ag	0.69312673	0.49002569	-1.06344413
C	-1.30875247	0.48997179	-1.06348023
N	-2.46526007	0.48995609	-1.06347393
N	2.82972853	0.49007609	-1.06339703
C	3.51546753	-0.65620151	-1.02323903
C	3.51544183	1.63639649	-1.10361173
C	4.89453333	-0.70982991	-1.02148693
H	2.93200563	-1.56798311	-0.99118203
C	4.89445583	1.69007359	-1.10560873
H	2.93191233	2.54815939	-1.13550243
C	5.57693713	0.49012709	-1.06365023
H	5.42302123	-1.65280871	-0.98843593
H	5.42294933	2.63306299	-1.13869353
F	6.89892253	0.49016839	-1.06383823
Ag	0.69305927	0.58355678	1.89757903
C	0.69311200	-1.41732422	1.96078952
N	0.69312789	-2.57325427	1.99733452
N	0.69301038	2.71909346	1.83012294
C	1.83998432	3.40461569	1.81242963
C	-0.45400812	3.40433713	1.80443070
C	1.89364130	4.78299489	1.76891810
H	2.75232340	2.82154855	1.83413748
C	-0.50772150	4.78265312	1.76055913
H	-1.36632327	2.82100069	1.81975883
C	0.69295142	5.46492263	1.74307509
H	2.83719341	5.31132273	1.75550378
H	-1.45128528	5.31077795	1.74054528
F	0.69290421	6.78624216	1.70112120

38.

Ag	0.69799328	0.51033510	-0.18384499
C	-1.30326402	0.51012990	-0.17563989
N	-2.45965622	0.51013730	-0.17246219
N	2.83591088	0.51097590	-0.18768609
C	3.51856368	-0.63555390	-0.14025949
C	3.51790188	1.65821120	-0.21990459
C	4.89909368	-0.68075510	-0.12190169
H	2.93406708	-1.54670970	-0.11393849
C	4.89864558	1.70550110	-0.20482789
H	2.93286818	2.56868510	-0.25683089
C	5.59900638	0.51295240	-0.15379779
H	5.41093698	-1.63262030	-0.07537419
H	5.40980358	2.65863900	-0.22463679
C	7.10703068	0.51049590	-0.17412289
F	7.60450178	1.61818910	0.37591841
F	7.55798308	0.44436670	-1.43091549
F	7.60103978	-0.53627730	0.48769591
Ag	0.70326011	0.72487491	2.78340457
C	0.70406467	-1.27084966	2.93233724
N	0.70428843	-2.42415390	3.01684937
N	0.70234398	2.85722963	2.62923145
C	1.84924649	3.53555592	2.54389221
C	-0.44413425	3.54123681	2.63375104
C	1.89568476	4.91371846	2.46170513
H	2.75985499	2.94961557	2.54404550
C	-0.49017672	4.91986334	2.55510119
H	-1.35484991	2.95979683	2.70527204
C	0.70288521	5.61586724	2.46870952
H	2.84838770	5.42260771	2.40183379
H	-1.44217171	5.43332197	2.56967930
C	0.70383810	7.11871667	2.34222195
F	-0.36018934	7.65930448	2.93603807
F	0.67693620	7.48003640	1.05537187
F	1.79664732	7.65248870	2.88870039

39.

Ag	0.70033775	0.47635814	-1.15076380
C	-1.30093365	0.47626694	-1.15081580
N	-2.45728095	0.47624634	-1.15080760
N	2.84108875	0.47639904	-1.15067870
C	3.51990935	-0.67317346	-1.11035510
C	3.51995335	1.62595354	-1.19107530
C	4.90138735	-0.72443466	-1.10880710
H	2.93263275	-1.58225576	-1.07831870
C	4.90146495	1.67710304	-1.19304740
H	2.93272625	2.53504794	-1.22292730

C	5.57636965	0.47634174	-1.15113460
H	5.43684725	-1.66247776	-1.07597030
H	5.43694105	2.61514794	-1.22602720
N	7.05323645	0.47624464	-1.15177670
O	7.59831105	1.55318274	-1.18869990
O	7.59821445	-0.60078446	-1.11542920
Ag	0.70021774	0.59801818	1.80923706
C	0.70030673	-1.40156392	1.89144799
N	0.70032765	-2.55693351	1.93898947
N	0.70018037	2.73696326	1.72132352
C	1.85043934	3.41492755	1.68655198
C	-0.45006360	3.41553355	1.70021086
C	1.90172089	4.79521498	1.62920747
H	2.76007059	2.82793003	1.70541094
C	-0.50125094	4.79588268	1.64354877
H	-1.35969937	2.82902773	1.72981699
C	0.70021893	5.46991333	1.60842642
H	2.84032140	5.32998899	1.60152583
H	-1.43985911	5.33113359	1.62706460
N	0.70028960	6.94550526	1.54707164
O	-0.37725661	7.49041883	1.53194959
O	1.77790312	7.48969912	1.51680626

40.

Ag	0.69334153	0.47416075	-0.89303432
C	-1.30886537	0.47425465	-0.89022872
N	-2.46544767	0.47424975	-0.89073062
N	2.82364593	0.47412765	-0.89809432
C	3.51362603	-0.66920085	-0.85513692
C	3.51335613	1.61763425	-0.93530642
C	4.89256583	-0.70920905	-0.84479092
H	2.93144403	-1.58228185	-0.82369622
C	4.89241543	1.65854905	-0.92779312
H	2.93106723	2.53063055	-0.96788892
C	5.62124273	0.47498195	-0.88020752
H	5.39487903	-1.66815455	-0.80412212
H	5.39459223	2.61800525	-0.95438472
C	7.11353623	0.47456795	-0.88600612
H	7.48582473	0.42239305	-1.91356832
H	7.51256073	1.38473565	-0.43711522
H	7.51192173	-0.38649205	-0.34819612
Ag	0.70036998	0.63789946	2.06492891
C	0.70042668	-1.36135535	2.17365130
N	0.70039613	-2.51634464	2.23433573
N	0.70012336	2.76495352	1.94718595
C	1.84403097	3.45274352	1.88770280
C	-0.44362312	3.45522585	1.93941922
C	1.88457675	4.83017662	1.82276619
H	2.75740289	2.87024792	1.89729028
C	-0.48402908	4.83287589	1.87631005
H	-1.35698285	2.87482057	1.99029095
C	0.70031721	5.55958020	1.81706979
H	2.84427493	5.33100489	1.78154210
H	-1.44342005	5.33587608	1.87845851
C	0.70040470	7.04947657	1.73232038
H	0.69326700	7.36681539	0.68520522
H	-0.18237383	7.47443016	2.21111611
H	1.59103439	7.47307738	2.19784807

41.

Ag	0.70766928	0.52031906	-1.30023924
C	-1.29565142	0.52024406	-1.30027734
N	-2.45243552	0.52022266	-1.30027414
N	2.83411718	0.52036826	-1.30018544
C	3.53463128	-0.62046474	-1.26025664
C	3.53465608	1.66116456	-1.34018594
C	4.90622608	-0.67180444	-1.25864644
H	2.95793678	-1.53717984	-1.22800224
C	4.90626998	1.71249476	-1.34213944
H	2.95797668	2.57790676	-1.37221824
C	5.64144328	0.52030476	-1.30057864
H	5.40681918	-1.63169714	-1.22498274
H	5.40686058	2.67236776	-1.37577964
N	6.99036928	0.52022786	-1.30075514
H	7.50667288	-0.33848624	-1.27185984
H	7.50681168	1.37882936	-1.33155664
Ag	0.70759414	0.52789269	1.66225108
C	0.70766904	-1.47542144	1.66738507
N	0.70769045	-2.63220167	1.67037486
N	0.70754508	2.65433364	1.65681483
C	1.84847549	3.35494104	1.69204715
C	-0.43334881	3.35477438	1.61789340
C	1.89981910	4.72653509	1.68998614
H	2.76526929	2.77832574	1.72346996
C	-0.48468379	4.72637900	1.61252853

H	-1.35016916	2.77802019	1.58967060
C	0.70760758	5.46164937	1.64917337
H	2.85979393	5.22720716	1.71992756
H	-1.44463887	5.22688736	1.58002566
N	0.70768404	6.81057041	1.64551395
H	1.56646853	7.32694128	1.67090253
H	-0.15099267	7.32693718	1.61555250

42.

Ag	0.69864547	0.50460512	-1.01362811
C	-1.30383253	0.50185642	-1.01358921
N	-2.46046143	0.49977792	-1.01351561
N	2.83048277	0.49838612	-1.01332791
C	3.51588197	-0.64725968	-0.97322131
C	3.53125517	1.63891892	-1.05332801
C	4.89242737	-0.70496058	-0.97140851
H	2.93211527	-1.55918988	-0.94114351
C	4.90578607	1.68338712	-1.05506731
H	2.95544057	2.55576112	-1.08538031
C	5.61170947	0.48526792	-1.01334191
H	5.39176037	-1.66639758	-0.93769231
H	5.43356067	2.62697982	-1.08817111
O	6.94678037	0.54094052	-1.01575841
H	7.32182847	-0.34526178	-0.98528581
Ag	0.69842026	0.57037214	1.94814178
C	0.70116914	-1.43160946	1.99272674
N	0.70324875	-2.58795074	2.01851921
N	0.70464439	2.70168407	1.90081581
C	1.85089710	3.38724178	1.90029502
C	-0.43649420	3.40195386	1.87045183
C	1.90862399	4.76345754	1.87016697
H	2.76331377	2.80388489	1.92519051
C	-0.48098999	4.77612686	1.83907812
H	-1.35382112	2.82602017	1.87152111
C	0.71775909	5.48221387	1.83855751
H	2.87057160	5.26294368	1.87147810
H	-1.42508411	5.30349830	1.81510472
O	0.66204666	6.81692711	1.80763376
H	1.54870622	7.19212403	1.81013550

43.

Cl	-0.98180983	-3.12884800	0.00000065
Au	1.24014037	-3.12884860	0.00000015
N	3.20334967	-3.12885110	-0.00000225
C	4.34536047	-3.12885310	-0.00000405
H	5.41425067	-3.12885720	-0.00000785
Cl	1.24014494	0.04614961	2.22194973
Au	1.24014444	0.04615140	-0.00000047
N	1.24014204	0.04615102	-1.96320977
C	1.24014024	0.04615025	-3.10522057
H	1.24013644	0.04614730	-4.17411077

44.

Cl	-0.97566008	-2.64138890	0.00000084
Au	1.24679582	-2.64138960	0.00000024
N	3.23273942	-2.64139280	-0.00000276
C	4.37577322	-2.64139490	-0.00000466
F	5.62264572	-2.64139860	-0.00000816
Cl	1.24680149	0.50860844	2.22245483
Au	1.24680089	0.50861040	-0.00000107
N	1.24679789	0.50860958	-1.98594467
C	1.24679599	0.50860884	-3.12897847
F	1.24679249	0.50860664	-4.37585097

45.

Cl	-0.92106274	-2.26123344	-0.23671637
Au	1.29693946	-2.26128254	-0.23672557
N	3.25163346	-2.26131024	-0.23682457
C	4.39550666	-2.26129964	-0.23703817
C	5.88291986	-2.26127654	-0.23689667
F	6.32749126	-3.09640314	-1.16067937
F	6.32687726	-2.64383374	0.94842213
F	6.32728206	-1.04357604	-0.49810657
Cl	1.29702701	-5.37330134	2.04099184
Au	1.29707734	-3.27880850	2.77080928
N	1.29713607	-1.43293158	3.41390107
C	1.29719492	-0.35268603	3.79008650
C	1.29712828	1.05186051	4.27962410
F	2.38423459	1.67155545	3.85226864
F	1.27968976	1.06130986	5.60175702
F	0.22734066	1.68128673	3.82370747

46.

Cl	-0.87842450	-3.12002002	0.78036603
Au	1.33505540	-3.12001832	0.78036763

N	3.28421250	-3.12002502	0.78036143
C	4.43042740	-3.12004352	0.78034443
N	5.84720580	-3.12001742	0.78036843
O	6.36035820	-2.32159662	1.52046253
O	6.36037900	-3.91845822	0.04025583
Cl	1.33505363	0.68945184	0.09622398
Au	1.33505596	-0.87745811	-1.46719743
N	1.33504684	-2.25725572	-2.84392252
C	1.33502174	-3.06865554	-3.65351434
N	1.33505716	-4.07158399	-4.65421188
O	2.42299679	-4.40656750	-5.04499809
O	0.24709032	-4.46313133	-4.98833749

47.

Cl	-0.91943083	-2.61276766	0.05718242
Au	1.30690057	-2.61276926	0.05718152
N	3.27806207	-2.61277166	0.05717892
C	4.42290027	-2.61277386	0.05717632
C	5.86566797	-2.61277986	0.05717062
H	6.23522037	-1.60888876	-0.15825548
H	6.23521787	-2.92816376	1.03427832
H	6.23520997	-3.30129186	-0.70451358
Cl	1.23117746	1.00316065	1.56986759
Au	1.23240202	0.49315731	-0.59726106
N	1.23348428	0.04160714	-2.51600516
C	1.23411162	-0.22065093	-3.63039953
C	1.23489926	-0.55116097	-5.03480016
H	1.20720413	0.36325267	-5.62965761
H	2.13790996	-1.11172341	-5.28201468
H	0.36019063	-1.15898155	-5.27189054

48.

Cl	-0.91731660	-2.64543866	0.33174433
Au	1.31103740	-2.64544016	0.33174283
N	3.28824020	-2.64544366	0.33173953
C	4.43888740	-2.64544546	0.33173783
N	5.74730530	-2.64545156	0.33173233
H	6.25552510	-3.28141136	-0.25776907
H	6.25553630	-2.00949256	0.92123273
Cl	1.31103942	1.14256065	-0.50326396
Au	1.31103730	-0.50019741	-2.00888925
N	1.31103249	-1.95780506	-3.34481995
C	1.31103002	-2.80607018	-4.12227430
N	1.31102181	-3.77064503	-5.00632903
H	0.44388117	-4.14200593	-5.35331943
H	2.17816117	-4.14861862	-5.34612102

49.

Cl	-0.95192800	-2.97593988	0.78191673
Au	1.27416070	-2.97630788	0.78161663
N	3.25803320	-2.96993548	0.78754223
C	4.40399330	-2.94505648	0.81056053
O	5.67863670	-2.98446048	0.77401183
H	6.07650530	-2.33621948	1.37449573
Cl	1.27558114	0.74367385	-0.27403047
Au	1.27510649	-0.98566254	-1.67576745
N	1.28378798	-2.52720951	-2.92452018
C	1.31760830	-3.41885685	-3.64437750
O	1.26398537	-4.40678890	-4.44980852
H	2.14565251	-4.75291468	-4.65464197

50.

N	2.76351490	-1.76775006	-0.00000244
C	3.90546800	-1.76775196	-0.00000414
H	4.97451060	-1.76775596	-0.00000784
Br	-1.56382740	-1.76774686	0.00000066
Au	0.78498290	-1.76774746	0.00000006
N	0.78498040	1.38224976	-1.97853223
C	0.78497870	1.38224775	-3.12048533
H	0.78497500	1.38224365	-4.18952793
Br	0.78498350	1.38225336	2.34881007
Au	0.78498290	1.38225254	-0.00000023

51.

N	1.70973602	-1.15160620	-0.00000312
C	2.85296082	-1.15160810	-0.00000492
Br	-2.64125668	-1.15160200	0.00000078
F	4.09961932	-1.15161150	-0.00000802
Au	-0.29234788	-1.15160280	0.00000008
N	-0.29234577	1.97339665	-2.00208467
C	-0.29234757	1.97339638	-3.14530947
Br	-0.29234187	1.97339465	2.34890803
F	-0.29235067	1.97339476	-4.39196797
Au	-0.29234257	1.97339720	-0.00000077

52.

N	-0.11177968	-0.14477952	-0.00851810
C	1.03205952	-0.14476732	-0.00873520
Br	-4.42715158	-0.14470172	-0.00842260
C	2.51994402	-0.14474462	-0.00859620
F	2.96411152	-0.97988282	-0.93239540
F	2.96349712	-0.52730732	1.17673560
F	2.96390212	1.07297338	-0.26981370
Au	-2.08203698	-0.14475152	-0.00842770
N	-2.08211749	2.52694096	-2.59037910
C	-2.08232732	2.28925650	-3.70925096
Br	-2.08200791	3.42392071	1.63074183
C	-2.08218663	1.98000190	-5.16464158
F	-3.15939590	1.27644578	-5.46923070
F	-1.00225899	1.28078232	-5.46952403
F	-2.08459324	3.10594829	-5.85775732
Au	-2.08202325	2.93645579	-0.66315015

53.

N	1.63746516	-0.95105781	-0.34157029
C	2.78377066	-0.95106361	-0.34157189
Br	-2.66707154	-0.95105171	-0.34156539
N	4.20063076	-0.95105581	-0.34157689
O	4.71375996	-2.03990231	-0.34158329
O	4.71376766	0.13775699	-0.34157429
Au	-0.32674174	-0.95105401	-0.34156699
N	-0.32673263	1.02171060	2.81560180
C	-0.32672683	2.16801190	2.81249760
Br	-0.32673871	-3.28281032	2.82725734
N	-0.32673464	3.58486679	2.80865776
O	0.76210784	4.09798611	2.80431180
O	-1.41554344	4.09800981	2.81022214
Au	-0.32673642	-0.94248910	2.82092141

54.

N	1.67606263	-0.95938935	0.02389308
C	2.82091303	-0.95939135	0.02389018
Br	-2.66244107	-0.95938525	0.02389628
C	4.26369473	-0.95939695	0.02388468
H	4.63297583	0.04456605	-0.19155702
H	4.63297323	-1.27480405	1.00106278
H	4.63296513	-1.64795915	-0.73785462
Au	-0.30954437	-0.95938675	0.02389558
N	-0.30954416	1.70903849	-2.57314928
C	-0.30954741	1.47104985	-3.69299027
Br	-0.30954018	2.61091405	1.67057960
C	-0.30955396	1.17112543	-5.10425367
H	-0.31158711	2.09874670	-5.67891878
H	0.58071108	0.59388703	-5.35910516
H	-1.19778999	0.59044546	-5.35836548
Au	-0.30954117	2.12180119	-0.63091806

55.

N	1.99106931	-0.76430090	-0.66738487
C	3.14184611	-0.76430250	-0.66738697
Br	-2.35463709	-0.76429580	-0.66738007
N	4.45011681	-0.76430990	-0.66738927
H	4.95826141	0.10290820	-0.66738997
H	4.95825261	-1.63152520	-0.66739717
Au	-0.00000119	-0.76429730	-0.66738137
N	0.00000797	1.24248577	2.47263192
C	0.00000956	2.39324820	2.46688256
Br	0.00000289	-3.10316641	2.49434023
N	0.00001695	3.70150258	2.46034641
H	-0.86719033	4.20966248	2.46214202
H	0.86722138	4.20961035	2.45346667
Au	0.00000439	-0.74855988	2.48257932

56.

N	1.59444907	0.11614457	0.39864530
C	2.74064717	0.14105427	0.42168830
Br	-2.75659293	0.11098217	0.39379130
O	4.01503087	0.10242697	0.38585240
H	4.41256307	0.75080347	0.98648570
Au	-0.40425363	0.11005177	0.39297640
N	-0.39516776	0.56475775	-3.29917039
C	-0.36128942	-0.32047734	-4.02727248
Br	-0.40223903	3.92079038	-0.52994457
O	-0.41388984	-1.30138658	-4.84083278
H	0.46846794	-1.64042272	-5.05456985
Au	-0.40347515	2.10657326	-2.02731441

57.

N	3.14698100	-0.41164512	-0.00000259
C	4.28890230	-0.41164702	-0.00000439

H	5.35813730	-0.41165082	-0.00000789
I	-1.36686710	-0.41164182	0.00000051
Au	1.14334460	-0.41164232	0.00000001
N	1.14334638	2.71335755	-2.00363660
C	1.14334458	2.71335717	-3.14555790
H	1.14334108	2.71335480	-4.21479290
I	1.14334948	2.71335483	2.51021150
Au	1.14334898	2.71335768	-0.00000020

58.

N	1.39268064	-2.23019498	-0.00000330
C	2.53622694	-2.23019698	-0.00000510
I	-3.14561126	-2.23019088	0.00000060
F	3.78281394	-2.23020028	-0.00000820
Au	-0.63628546	-2.23019148	0.00000000
N	-0.63628344	0.85730803	-2.02896684
C	-0.63628524	0.85730773	-3.17251314
I	-0.63627954	0.85730540	2.50932506
F	-0.63628834	0.85730628	-4.41910014
Au	-0.63628014	0.85730852	-0.00000074

59.

N	1.79780582	-0.13276290	0.16025814
C	2.94161772	-0.13299800	0.16016534
I	-2.70488698	-0.13265990	0.16035424
C	4.42994742	-0.13284100	0.16025024
F	4.87401862	-1.03029210	-0.70307126
F	4.87350892	-0.43169900	1.36934494
F	4.87327222	1.06379450	-0.18538216
Au	-0.19778718	-0.13266050	0.16032014
N	-0.19775005	2.28468314	-2.63726765
C	-0.19790582	1.95959656	-3.73390999
I	-0.19762866	3.56372563	1.67994125
C	-0.19777981	1.53696296	-5.16097206
F	-1.28050904	0.82099013	-5.41201400
F	0.87657247	0.80684929	-5.40729319
F	-0.18917513	2.60525740	-5.93982258
Au	-0.19766152	2.85160153	-0.72389498

60.

N	1.96254199	-1.82619293	0.07458221
C	3.10906939	-1.82619903	0.07458061
I	-2.52771181	-1.82617873	0.07458731
N	4.52534789	-1.82616993	0.07457591
O	5.03885809	-2.91533253	0.07456951
O	5.03883949	-0.73703783	0.07457851
Au	-0.02579521	-1.82618193	0.07458571
N	-0.02577854	0.20342027	3.17294411
C	-0.02577246	1.34984686	3.15774072
I	-0.02579267	-4.28643875	3.23248528
N	-0.02580162	2.76600081	3.13895810
O	1.06326510	3.27927426	3.11769928
O	-1.11483789	3.27963883	3.14659579
Au	-0.02578949	-1.78474210	3.19931094

61.

N	0.03439364	0.66934503	0.06509088
C	1.17930264	0.66934103	0.06508818
I	-4.48835976	0.66934663	0.06509338
C	2.62220034	0.66933423	0.06508208
H	2.99142004	1.65578663	-0.21987562
H	2.99142074	0.42288763	1.06185318
H	2.99141194	-0.07067307	-0.64673442
Au	-1.97492256	0.66934713	0.06509318
N	-1.97492318	3.12652944	-2.72152335
C	-1.97492687	2.81374245	-3.82287748
I	-1.97492034	4.36212618	1.62917763
C	-1.97493460	2.41954459	-5.21088390
H	-1.97955630	3.30639085	-5.84656838
H	-1.08341094	1.82866699	-5.42689663
H	-2.86183994	1.82096988	-5.42470151
Au	-1.97492039	3.67546694	-0.78864487

62.

N	1.75605736	-0.82116718	0.00120003
C	2.90702846	-0.82116928	0.00119813
I	-2.77250104	-0.82116208	0.00120503
N	4.21531886	-0.82117298	0.00119593
H	4.72339596	0.04607562	0.00119513
H	4.72338886	-1.68842808	0.00118803
Au	-0.25795354	-0.82116348	0.00120373
N	-0.25794413	1.16342284	3.14497250
C	-0.25794201	2.31434322	3.15577742
I	-0.25794928	-3.36493599	3.10245751
N	-0.25793829	3.62257597	3.16805917

H	-1.12514869	4.13070711	3.16468952
H	0.60927868	4.13054722	3.18096108
Au	-0.25794787	-0.85049932	3.12606603

63.

N	2.29840673	0.17734839	0.22967992
C	3.44487763	0.20244709	0.25290202
I	-2.23719767	0.17374669	0.22626222
O	4.71921523	0.16512729	0.21825852
H	5.11578303	0.81371169	0.81930052
Au	0.27510723	0.17129879	0.22404762
N	0.28382143	0.68041666	-3.45320522
C	0.31799685	-0.18665740	-4.20325811
I	0.27886126	4.10793433	-0.48271200
O	0.26710606	-1.14847566	-5.03922763
H	1.15086772	-1.46755902	-5.27656780
Au	0.27556107	2.20953515	-2.12823820

64.

Au	1.17755124	-2.67946743	-0.00000027
N	3.18005824	-2.67947003	-0.00000267
C	4.32042054	-2.67947173	-0.00000427
H	5.39021474	-2.67947513	-0.00000747
C	-0.76660716	-2.67946673	0.00000043
N	-1.92188456	-2.67946663	0.00000043
Au	1.17755537	0.48303257	-0.00000054
N	1.17755297	0.48303240	-2.00250754
C	1.17755137	0.48303209	-3.14286984
H	1.17754817	0.48302999	-4.21266404
C	1.17755607	0.48303090	1.94415786
N	1.17755607	0.48302960	3.09943526

65.

Au	1.18369732	-3.16492148	0.00000009
N	3.20607062	-3.16492488	-0.00000301
C	4.34830282	-3.16492658	-0.00000461
C	-0.75711918	-3.16492058	0.00000089
N	-1.91236908	-3.16492058	0.00000099
F	5.59216502	-3.16492928	-0.00000711
Au	1.18370261	-0.01492148	-0.00000127
N	1.18369951	-0.01492232	-2.02237457
C	1.18369791	-0.01492258	-3.16460677
C	1.18370341	-0.01492304	1.94081523
N	1.18370351	-0.01492450	3.09606513
F	1.18369541	-0.01492370	-4.40846897

66.

Au	1.23505397	-2.39948925	0.01264748
N	3.23173297	-2.39952205	0.01253578
C	4.37359777	-2.39950215	0.01227658
C	-0.70931233	-2.39943975	0.01264188
N	-1.86444393	-2.39941665	0.01263038
C	5.86604517	-2.39946245	0.01247398
F	6.30455667	-1.18163225	-0.24873562
F	6.30406607	-2.78205095	1.19794158
F	6.30483477	-3.23466875	-0.91137952
Au	1.23506731	0.69147421	-0.65619566
N	1.23495120	0.26919278	-2.60770928
C	1.23470207	0.02777493	-3.72376154
C	1.23507230	1.10273236	1.24417984
N	1.23506595	1.34705301	2.37317782
C	1.23490340	-0.28786233	-5.18245012
F	1.23716891	0.83675113	-5.87445635
F	2.31263842	-0.99102469	-5.47845625
F	0.15530571	-0.98753775	-5.47999725

67.

Au	1.26416596	-2.69540268	0.37109154
N	3.25668146	-2.69541008	0.37108464
C	4.40045306	-2.69539848	0.37109554
C	-0.67953924	-2.69540338	0.37109094
N	-1.83474754	-2.69540368	0.37109064
N	5.82526676	-2.69545468	0.37104334
O	6.33268066	-1.89692808	1.11123544
O	6.33271306	-3.49387038	-0.36904606
Au	1.26416615	-0.52107868	-1.90812218
N	1.26415604	-1.96278302	-3.28347909
C	1.26417195	-2.79037017	-4.07298082
C	1.26416523	0.88530837	-0.56645704
N	1.26416481	1.72117075	0.23093892
N	1.26409526	-3.82130889	-5.05647430
O	2.35280327	-4.17767214	-5.41802381
O	0.17553838	-4.19925621	-5.39544546

68.

Au	1.24175434	-2.58195606	0.04637123
N	3.24870394	-2.58195936	0.04636803
C	4.39264504	-2.58196096	0.04636573
C	-0.70198996	-2.58195466	0.04637193
N	-1.85756366	-2.58195446	0.04637193
C	5.83482114	-2.58196616	0.04636053
H	6.20259054	-1.57752856	-0.16918267
H	6.20258834	-2.89752176	1.02400053
H	6.20258044	-3.27085306	-0.71573837
Au	1.24175853	0.52337856	-0.55221305
N	1.24175476	0.14351186	-2.52288501
C	1.24175220	-0.07300798	-3.64614829
C	1.24175948	0.89128075	1.35639636
N	1.24175952	1.11000143	2.49108215
C	1.24174611	-0.34597900	-5.06225518
H	1.22021601	0.59292495	-5.61777650
H	2.14198664	-0.90153852	-5.32970354
H	0.36303270	-0.93815338	-5.32263766

69.

Au	1.24890151	-2.95950501	0.66590291
N	3.25911011	-2.95950861	0.66589951
C	4.40935701	-2.95951011	0.66589811
C	-0.69368479	-2.95950341	0.66590441
N	-1.84945789	-2.95950331	0.66590451
N	5.71584231	-2.95951571	0.66589311
H	6.22379791	-3.59585731	0.07603781
H	6.22380851	-2.32317451	1.25574771
Au	1.24890145	-0.79949435	-1.66110783
N	1.24889650	-2.27280994	-3.02868957
C	1.24889445	-3.11584519	-3.81122359
C	1.24890364	0.62425974	-0.33953081
N	1.24890379	1.47134524	0.44676278
N	1.24888694	-4.07339029	-4.70004934
H	0.38121215	-4.44608768	-5.04518106
H	2.11656097	-4.44527887	-5.04606799

70.

Au	1.21339808	-1.73559285	-0.59608879
N	3.23108851	-1.72998660	-0.58442434
C	4.37680573	-1.70996886	-0.56224681
C	-0.72810682	-1.73811995	-0.59845839
N	-1.88351612	-1.73446185	-0.59508609
O	5.64819216	-1.75386094	-0.59889288
H	6.05421413	-1.10865171	0.00010457
Au	1.20683313	-3.98917643	1.62263251
N	1.19459778	-2.57022364	3.05708901
C	1.16475815	-1.76368817	3.87082769
C	1.21028599	-5.35425730	0.24205453
N	1.20531200	-6.16639059	-0.57977890
O	1.22166552	-0.87175189	4.77686528
H	0.34224829	-0.55626184	5.03578242

71.

Cl	-1.00691230	-2.34833937	-0.26598595
N	3.27108860	-2.34820997	-0.26593185
C	3.95423550	-3.49885877	-0.22559135
C	3.95417780	-1.19754607	-0.30626875
C	5.33430410	-3.53805077	-0.22430185
H	3.36329610	-4.40424937	-0.19379475
C	5.33424110	-1.15827417	-0.30771985
H	3.36319330	-0.29217007	-0.33797825
C	6.04106530	-2.34815347	-0.26611425
H	5.83837420	-4.49507167	-0.19072255
H	5.83826470	-0.20123367	-0.34125445
H	7.12427380	-2.34812187	-0.26628535
Au	1.22556600	-2.34827107	-0.26596235
Cl	1.22558560	-4.50012704	2.85372362
N	1.22545766	-0.22358126	2.74215369
C	2.37676697	0.45960281	2.73466318
C	0.07413334	0.45900570	2.71399852
C	2.41597926	1.83920849	2.69892012
H	3.28267871	-0.13092169	2.75826950
C	0.03483696	1.83858795	2.67756109
H	-0.83176154	-0.13198901	2.72131921
C	1.22539642	2.54544758	2.66969492
H	3.37355023	2.34333205	2.69439034
H	-0.92275243	2.34221604	2.65583152
H	1.22536037	3.62828282	2.64126023
Au	1.22551794	-2.26840821	2.79549615

72.

Cl	-1.00797779	-2.37417052	-0.59387490
N	3.27179451	-2.37404372	-0.59381010
C	3.95644411	-3.52399492	-0.55349820

C	3.95638881	-1.22407402	-0.63412670
C	5.33450951	-3.57318842	-0.55188280
H	3.36799011	-4.43103012	-0.52162970
C	5.33446221	-1.17481482	-0.63594950
H	3.36790891	-0.31705592	-0.66587930
C	6.01778511	-2.37400312	-0.59405560
H	5.86144501	-4.51701162	-0.51876500
H	5.86135401	-0.23098132	-0.66902470
Au	1.22339021	-2.37409962	-0.59384250
F	7.34048841	-2.37397222	-0.59432720
Cl	1.22340601	-4.43265056	2.59943333
N	1.22328297	-0.15937964	2.36362273
C	2.37370884	0.52295667	2.30283314
C	0.07283837	0.52544647	2.34894196
C	2.42291663	1.89886694	2.22578523
H	3.28112240	-0.06560269	2.31715337
C	0.02355355	1.90147440	2.27388049
H	-0.83455174	-0.06113279	2.39960375
C	1.22322891	2.58242361	2.21203331
H	3.36713117	2.42395874	2.17785238
H	-0.92066892	2.42861044	2.26377406
Au	1.22333700	-2.20467228	2.47648637
F	1.22318310	3.90310152	2.13886266

73.

Cl	-0.99502541	-2.34263603	-0.01959045
N	3.27857069	-2.34177963	-0.03477645
C	3.96138579	-3.49210323	0.01215235
C	3.96060669	-1.19065763	-0.06784005
C	5.34051009	-3.53243243	0.03008785
H	3.37210029	-4.39849023	0.03850965
C	5.33991119	-1.14807153	-0.05284915
H	3.37062129	-0.28503683	-0.10444935
C	6.04183939	-2.33963473	-0.00118145
H	5.85153219	-4.48469463	0.07595475
H	5.85009919	-0.19452103	-0.07341365
Au	1.23424409	-2.34239423	-0.03159875
C	7.54836439	-2.34199893	-0.02124595
F	8.04334399	-3.38892803	0.64060175
F	8.00193919	-2.40789963	-1.27771015
F	8.04669269	-1.23432613	0.52919005
Cl	1.22912707	-0.14863881	-3.11116863
N	1.23014609	-4.42206554	-3.07020671
C	0.07941114	-5.10435970	-3.02585678
C	2.38154355	-5.10432249	-3.08275687
C	0.03890731	-6.48313484	-2.99021243
H	-0.82719613	-4.51490049	-3.01633810
C	2.42398039	-6.48330536	-3.04922241
H	3.28748469	-4.51474732	-3.11802454
C	1.23196042	-7.18465427	-3.00029694
H	-0.91376596	-6.99363819	-2.94719364
H	3.37769047	-6.99359148	-3.05351488
Au	1.22949471	-2.37787367	-3.09388954
C	1.22980130	-8.69131315	-3.00059296
F	0.17628483	-9.17769709	-2.34283810
F	1.17651290	-9.16136151	-4.25158863
F	2.33189622	-9.18221973	-2.43257234

74.

Cl	-0.95802222	-2.38732133	-1.12790999
N	3.31062518	-2.38720893	-1.12779479
C	3.99046978	-3.54068013	-1.08732569
C	3.99044338	-1.23364633	-1.16831039
C	5.36991098	-3.58719623	-1.08593469
H	3.39883308	-4.44530253	-1.05546199
C	5.37001828	-1.18724643	-1.17011249
H	3.39892188	-0.32908543	-1.20000539
C	6.04749028	-2.38724283	-1.12824739
H	5.90333658	-4.52644753	-1.05302649
H	5.90338508	-0.24800263	-1.20310979
Au	1.26887478	-2.38721953	-1.12784539
N	7.52102158	-2.38745423	-1.12893209
O	8.06749808	-3.46435983	-1.09256389
O	8.06775478	-1.31039193	-1.16591679
Cl	1.26889709	-4.48717713	2.03519000
N	1.26878946	-0.22206298	1.86154698
C	2.42295229	0.45695512	1.82741728
C	0.11453343	0.45745300	1.84028657
C	2.46948648	1.83523255	1.77076384
H	3.32812219	-0.13439235	1.84656326
C	0.06809863	1.83588792	1.78421440
H	-0.79056817	-0.13337029	1.86946899
C	1.26880494	2.51251517	1.74968498
H	3.40929912	2.36800002	1.74374827
H	-0.87171014	2.36902499	1.76771511

Au	1.26879800	-2.26212313	1.94460898
N	1.26898833	3.98479692	1.68901021
O	2.34648212	4.53051739	1.65932571
O	0.19131289	4.53135522	1.67358462

75.

Cl	-1.00904268	-2.33659765	0.15536216
N	3.26986522	-2.33677135	0.14364586
C	3.95906092	-3.48343435	0.18925736
C	3.95881232	-1.18967355	0.10884376
C	5.33700552	-3.51884705	0.20292996
H	3.37274662	-4.39211225	0.21874136
C	5.33685292	-1.15316485	0.11999986
H	3.37236022	-0.28123295	0.07462476
C	6.06671602	-2.33568905	0.16729806
H	5.83797252	-4.47837695	0.24532426
H	5.83768932	-0.19296195	0.09507706
Au	1.22467972	-2.33680735	0.14689366
C	7.55893682	-2.33632225	0.15689236
H	7.95957652	-3.19728505	0.69315276
H	7.92780522	-2.38853645	-0.87194534
H	7.96014422	-1.42639295	0.60424146
Cl	1.21977170	-0.20030329	-2.97938913
N	1.21995861	-4.47726419	-2.84979165
C	0.07244678	-5.16571168	-2.81567708
C	2.36758583	-5.16585055	-2.82758255
C	0.03664517	-6.54248837	-2.75756914
H	-0.83670779	-4.57964204	-2.83269615
C	2.40374869	-6.54273516	-2.76983960
H	3.27664159	-4.57995001	-2.85403050
C	1.22034139	-7.27180764	-2.73376695
H	-0.92372140	-7.04273107	-2.72730137
H	3.36426891	-7.04317204	-2.74954938
Au	1.21982052	-2.43308706	-2.91408868
C	1.22002286	-8.76355863	-2.69490189
H	0.34343614	-9.14712913	-2.17162976
H	1.19854611	-9.16623872	-3.71209642
H	2.11619321	-9.14888114	-2.20759786

76.

Cl	-0.98775482	-2.37361787	-1.07324269
N	3.29457828	-2.37349467	-1.07317169
C	3.99238898	-3.51780617	-1.03309769
C	3.99241398	-1.22916387	-1.11327739
C	5.36344068	-3.56490697	-1.03162429
H	3.41021718	-4.42923087	-1.00102929
C	5.36346388	-1.18211277	-1.11506899
H	3.41023338	-0.31775197	-1.14514089
C	6.09912148	-2.37350027	-1.07356469
H	5.86213918	-4.52565647	-0.99788809
H	5.86215278	-0.22131607	-1.14872509
Au	1.24868418	-2.37352867	-1.07320189
N	7.44896928	-2.37364767	-1.07382609
H	7.96505748	-3.23230657	-1.04491639
H	7.96527848	-1.51512467	-1.10446789
Cl	1.24872540	-4.51706096	2.05502089
N	1.24860439	-0.23665611	1.92652552
C	2.39360301	0.46101220	1.91130712
C	0.10358552	0.46069190	1.89981085
C	2.44072681	1.83144763	1.87020357
H	3.30557949	-0.12075552	1.93350148
C	0.05650185	1.83111233	1.85826791
H	-0.80837202	-0.12136176	1.91277858
C	1.24859820	2.56661100	1.84193092
H	3.40205593	2.33006859	1.86013415
H	-0.90487204	2.32943159	1.83847385
Au	1.24863746	-2.28162885	1.98791893
N	1.24873769	3.91584231	1.80113838
H	2.10787738	4.43179222	1.78878532
H	0.38968189	4.43177229	1.78076079

77.

Cl	-1.00560360	-2.37451439	-1.21077432
N	3.27504610	-2.37802059	-1.21053532
C	3.95881970	-3.52700219	-1.17028272
C	3.97337150	-1.23362479	-1.25064462
C	5.33455370	-3.57958459	-1.16861092
H	3.36986740	-4.43383019	-1.13839942
C	5.34717460	-1.19278239	-1.25221942
H	3.39119640	-0.32245109	-1.28252582
C	6.05403100	-2.39002909	-1.21052632
H	5.83363100	-4.54106669	-1.13485582
H	5.87231170	-0.24785729	-1.28534932
Au	1.22797600	-2.37317049	-1.21076052
O	7.39010180	-2.33619039	-1.21290202

H	7.76149020	-3.22383259	-1.18248442
Cl	1.22918397	-4.52072901	1.91270976
N	1.23269547	-0.24173579	1.79363455
C	2.38235170	0.44200482	1.78292717
C	0.08762725	0.45608694	1.76586619
C	2.43496025	1.81721108	1.74482405
H	3.28971532	-0.14653255	1.80602263
C	0.04675687	1.82934489	1.72716542
H	-0.82408034	-0.12604539	1.77550950
C	1.24469959	2.53616213	1.71591515
H	3.39700886	2.31629111	1.73797136
H	-0.89872377	2.35408657	1.70565883
Au	1.22784098	-2.28801437	1.85055532
O	1.19081569	3.87169017	1.67782561
H	2.07896022	4.24309502	1.67324330

78.

Cl	-1.00560360	-2.37451439	-1.21077432
N	3.27504610	-2.37802059	-1.21053532
C	3.95881970	-3.52700219	-1.17028272
C	3.97337150	-1.23362479	-1.25064462
C	5.33455370	-3.57958459	-1.16861092
H	3.36986740	-4.43383019	-1.13839942
C	5.34717460	-1.19278239	-1.25221942
H	3.39119640	-0.32245109	-1.28252582
C	6.05403100	-2.39002909	-1.21052632
H	5.83363100	-4.54106669	-1.13485582
H	5.87231170	-0.24785729	-1.28534932
Au	1.22797600	-2.37317049	-1.21076052
O	7.39010180	-2.33619039	-1.21290202
H	7.76149020	-3.22383259	-1.18248442
Cl	1.22918397	-4.52072901	1.91270976
N	1.23269547	-0.24173579	1.79363455
C	2.38235170	0.44200482	1.78292717
C	0.08762725	0.45608694	1.76586619
C	2.43496025	1.81721108	1.74482405
H	3.28971532	-0.14653255	1.80602263
C	0.04675687	1.82934489	1.72716542
H	-0.82408034	-0.12604539	1.77550950
C	1.24469959	2.53616213	1.71591515
H	3.39700886	2.31629111	1.73797136
H	-0.89872377	2.35408657	1.70565883
Au	1.22784098	-2.28801437	1.85055532
O	1.19081569	3.87169017	1.67782561
H	2.07896022	4.24309502	1.67324330

79.

N	3.26063797	-2.31481753	0.66615382
C	3.94399267	-3.46465443	0.70644062
C	3.94390397	-1.16487143	0.62581742
C	5.32182327	-3.51472153	0.70807272
H	3.35539167	-4.37209503	0.73833922
C	5.32181067	-1.11477753	0.62395102
H	3.35531627	-0.25750743	0.59406992
C	6.00451427	-2.31475373	0.66590092
H	5.84961897	-4.45797383	0.74114962
H	5.84952647	-0.17153663	0.59087342
Au	1.18442387	-2.31484773	0.66611722
C	-0.75846333	-2.31489903	0.66607852
N	-1.91430903	-2.31492413	0.66607822
F	7.32595107	-2.31471533	0.66569512
N	1.18450855	-4.51157125	-2.32398242
C	0.03397897	-5.19460312	-2.30228653
C	2.33514922	-5.19408423	-2.29146213
C	-0.01611344	-6.57136149	-2.24793871
H	-0.87401245	-4.60663260	-2.32984282
C	2.38527772	-6.57089939	-2.23662689
H	3.24305809	-4.60578845	-2.31049804
C	1.18458235	-7.25329381	-2.21528740
H	-0.95993509	-7.09891710	-2.23141435
H	3.32908801	-7.09802301	-2.21124356
Au	1.18447983	-2.43699584	-2.40645578
C	1.18443011	-0.49564231	-2.48363836
N	1.18440504	0.65929190	-2.52953225
F	1.18462890	-8.57369670	-2.16302400

80.

N	3.27044065	-2.33581200	0.12950776
C	3.95116355	-3.48604140	0.17659216
C	3.95044795	-1.18489900	0.09672666
C	5.33049145	-3.52739360	0.19473246
H	3.36161385	-4.39290760	0.20273046
C	5.33003735	-1.14142490	0.11185666
H	3.36035375	-0.27873040	0.05995116
C	6.03056285	-2.33382010	0.16328716

H	5.84239555	-4.47914870	0.24066876
H	5.84119925	-0.18842180	0.09149586
Au	1.19548345	-2.33644350	0.13154046
C	-0.74735675	-2.33669310	0.13960286
N	-1.90308255	-2.33666120	0.14545536
C	7.53827565	-2.33629130	0.14269376
F	7.98823155	-2.40255860	-1.11442594
F	8.03565525	-1.22856490	0.69249736
F	8.03216635	-3.38304810	0.80444946
N	1.19321991	-4.52950435	-2.86037462
C	0.04203287	-5.20955118	-2.82983006
C	2.34454849	-5.20853384	-2.82233902
C	0.00002328	-6.58712116	-2.75827104
H	-0.86517254	-4.62080242	-2.86163573
C	2.38741834	-6.58635660	-2.75055852
H	3.25145941	-4.61900238	-2.84823087
C	1.19393095	-7.28608093	-2.71648364
H	-0.95278904	-7.09822866	-2.72807961
H	3.34050807	-7.09647979	-2.71436099
Au	1.19250978	-2.45611817	-2.94112843
C	1.19195256	-0.51450297	-3.01057773
N	1.19176124	0.64053650	-3.05082891
C	1.19224451	-8.79341853	-2.67700455
F	1.17373594	-9.29322070	-3.91678551
F	2.27830701	-9.26681148	-2.06618903
F	0.12112716	-9.26212668	-2.03624818

81.

N	3.28676164	-2.33377510	0.25108548
C	3.96401294	-3.48701910	0.29154528
C	3.96404824	-1.18064980	0.21057418
C	5.34411224	-3.53440150	0.29296208
H	3.37227944	-4.39214940	0.32343798
C	5.34415804	-1.13322210	0.20873348
H	3.37234274	-0.27545200	0.17885778
C	6.01954484	-2.33390990	0.25063178
H	5.87950594	-4.47228570	0.32581628
H	5.87956184	-0.19541070	0.17577958
Au	1.21215014	-2.33383650	0.25102568
C	-0.73051126	-2.33391270	0.25096858
N	-1.88613996	-2.33395090	0.25097298
N	7.49554634	-2.33400510	0.24997228
O	8.04046244	-3.41110940	0.28632608
O	8.04064284	-1.25690810	0.21303988
N	1.21230103	-4.49885694	-2.76100429
C	0.05836395	-5.17562740	-2.73475585
C	2.36612101	-5.17602970	-2.74711965
C	0.01096037	-6.55511892	-2.69380186
H	-0.84731442	-4.58400693	-2.74734391
C	2.41358247	-6.55554469	-2.70660265
H	3.27186160	-4.58472686	-2.76946513
C	1.21217978	-7.23045066	-2.68038211
H	-0.92748600	-7.09012983	-2.67296160
H	3.35195903	-7.09086291	-2.69577498
Au	1.21224144	-2.42516056	-2.82261791
C	1.21216697	-0.48335614	-2.88031443
N	1.21212865	0.67176392	-2.91459774
N	1.21210423	-8.70582203	-2.63725208
O	0.13441025	-9.25037015	-2.61676934
O	2.28982311	-9.25082381	-2.62597290

82.

N	3.26112581	-2.33610555	0.33178792
C	3.94890931	-3.48305195	0.37448662
C	3.94869201	-1.18907765	0.29406802
C	5.32687991	-3.51957895	0.38403652
H	3.36243841	-4.39212955	0.40627052
C	5.32669731	-1.15172785	0.30102992
H	3.36208471	-0.27998025	0.26210282
C	6.05543241	-2.33531645	0.34844802
H	5.83026671	-4.47798625	0.42435322
H	5.83002101	-0.19277915	0.27412212
Au	1.18868921	-2.33612655	0.33566302
C	-0.75488899	-2.33604535	0.33865512
N	-1.91081949	-2.33601065	0.33920272
C	7.54755471	-2.33570055	0.34342032
H	7.94571751	-3.19671135	0.88138962
H	7.92135391	-2.38784205	-0.68360858
H	7.94634431	-1.42554455	0.79248582
N	1.18304643	-4.45680298	-2.69362969
C	0.03561796	-5.14401040	-2.65478086
C	2.33049167	-5.14464153	-2.70314978
C	-0.00103404	-6.52160511	-2.62134697
H	-0.87381693	-4.55729671	-2.64608267
C	2.36774541	-6.52229823	-2.67127101

H	3.23994479	-4.55846408	-2.73279788
C	1.18361254	-7.25037647	-2.62749061
H	-0.95990917	-7.02443962	-2.58551145
H	3.32697814	-7.02577892	-2.67587003
Au	1.18296407	-2.38462262	-2.72644763
C	1.18299668	-0.44129606	-2.75786551
N	1.18301969	0.71446296	-2.77778291
C	1.18330391	-8.74235400	-2.60610490
H	0.31486506	-9.13114670	-2.07324621
H	1.14551256	-9.13428904	-3.62698279
H	2.08710077	-9.13290311	-2.13738372

83.

N	3.26942515	-2.32354503	0.52354042
C	3.96679355	-3.46799813	0.56361032
C	3.96684235	-1.17925953	0.48343012
C	5.33718835	-3.51610393	0.56511592
H	3.38479065	-4.38007623	0.59570332
C	5.33717875	-1.13106213	0.48159552
H	3.38480495	-0.26708413	0.45154872
C	6.07245375	-2.32364413	0.52315752
H	5.83639065	-4.47671533	0.59882752
H	5.83641475	-0.17049153	0.44794322
Au	1.19830525	-2.32362853	0.52350502
C	-0.74583835	-2.32369323	0.52346802
N	-1.90210145	-2.32372733	0.52346672
N	7.42084015	-2.32375403	0.52294032
H	7.93738185	-3.18228553	0.55186272
H	7.93757325	-1.46526893	0.49223902
N	1.19844421	-4.49735688	-2.47983772
C	0.05329071	-5.19428122	-2.45491559
C	2.34343157	-5.19442586	-2.45775424
C	0.00516150	-6.56390010	-2.40880653
H	-0.85935095	-4.61256662	-2.47327648
C	2.39166343	-6.56398927	-2.41173317
H	3.25616333	-4.61275543	-2.47844637
C	1.19835810	-7.29880316	-2.38566633
H	-0.95604044	-7.06277605	-2.39071543
H	3.35282259	-7.06298141	-2.39608516
Au	1.19836195	-2.42741705	-2.54974293
C	1.19829854	-0.48438129	-2.61536569
N	1.19826450	0.67122364	-2.65437345
N	1.19825559	-8.64642957	-2.34040061
H	0.33923706	-9.16268023	-2.32306297
H	2.05728782	-9.16292565	-2.32466026

84.

N	3.26351050	-2.33073444	0.34228520
C	3.94644380	-3.47973064	0.38252480
C	3.96116990	-1.18637494	0.30216590
C	5.32189400	-3.53401304	0.38423770
H	3.35780870	-4.38731604	0.41444580
C	5.33449200	-1.14530664	0.30056410
H	3.38011060	-0.27394634	0.27025540
C	6.04094390	-2.34340654	0.34228640
H	5.82047760	-4.49566004	0.41798490
H	5.86140970	-0.20139774	0.26746380
Au	1.18943730	-2.32537504	0.34203590
C	-0.75411830	-2.32607554	0.34200620
N	-1.91013010	-2.32842984	0.34208400
O	7.37541660	-2.28648574	0.33981510
H	7.75273360	-3.17169574	0.37021070
N	1.18411980	-4.52223672	-2.64647608
C	0.03443661	-5.20486663	-2.62516083
C	2.32916524	-5.21907128	-2.61198804
C	-0.01987063	-6.57920978	-2.56998467
H	-0.87369696	-4.61691050	-2.65384024
C	2.37026471	-6.59126582	-2.55634876
H	3.24213760	-4.63828286	-2.63043819
C	1.17145805	-7.29741559	-2.53458853
H	-0.98209540	-7.07759646	-2.55503021
H	3.31473974	-7.11754327	-2.52987446
Au	1.18948490	-2.44986389	-2.73044315
C	1.18878618	-0.50790279	-2.80915433
N	1.18643066	0.64716130	-2.85595423
O	1.22843224	-8.63080173	-2.48074801
H	0.34271750	-9.00803141	-2.47095403

7. Coordinates of the dimers 1 to 84 at their energetic minimum (PBE0-D4//def2-TZVP)

1.
 Ag 0.73586603 -0.38433013 0.00000058
 N 2.80515863 -0.38433323 -0.00000232
 C 3.94608123 -0.38433513 -0.00000412
 Cl -1.52726117 -0.38432983 0.00000088
 H 5.01596113 -0.38433893 -0.00000762
 Ag 0.73587059 2.65316987 -0.00000044
 N 0.73586769 2.65316915 -2.06929304
 C 0.73586589 2.65316856 -3.21021564
 Cl 0.73587089 2.65316757 2.26312676
 H 0.73586239 2.65316599 -4.28009554

2.
 Ag 0.74433466 -0.87938554 0.00000177
 N 2.83283976 -0.87938934 -0.00000173
 C 3.97677626 -0.87939134 -0.00000363
 F 5.22244266 -0.87939474 -0.00000683
 Cl -1.52059714 -0.87938514 0.00000207
 Ag 0.74434013 2.13311446 -0.00000120
 N 0.74433663 2.13311238 -2.08850630
 C 0.74433473 2.13311133 -3.23244280
 F 0.74433153 2.13310895 -4.47810920
 Cl 0.74434043 2.13311299 2.26493060

3.
 Ag 0.77045421 1.65757624 -0.49995676
 N 2.83543331 1.65770794 -0.49992436
 C 3.97770091 1.65805404 -0.49995156
 C 5.46928201 1.65779194 -0.49999556
 F 5.91021881 2.79364064 -1.01059256
 F 5.90967951 1.53187054 0.73909664
 F 5.90923561 0.64743324 -1.22848286
 Cl -1.48922249 1.65757564 -0.50000916
 Ag 0.77061159 -1.11040298 0.72025470
 N 0.77052882 -0.27744062 2.60978172
 C 0.77041409 0.18356781 3.65488775
 C 0.77056009 0.78496114 5.01985672
 F 0.77953540 2.10232515 4.92107244
 F -0.31242633 0.39973664 5.67093133
 F 1.84473802 0.38537001 5.67677858
 Cl 0.77065978 -2.02177520 -1.34748307

4.
 Ag 0.78076180 -0.69582257 1.03907739
 N 2.84012770 -0.69583257 1.03906649
 C 3.98464260 -0.69582377 1.03907729
 N 5.40873780 -0.69584477 1.03905349
 O 5.91790740 -1.39721817 0.20647699
 O 5.91791100 0.00556513 1.87167449
 Cl -1.47534160 -0.69581697 1.03908399
 Ag 0.78076257 1.60661577 -0.92291208
 N 0.78074779 0.27092843 -2.49037093
 C 0.78076172 -0.47139428 -3.36150315
 N 0.78072998 -1.39505054 -4.44543408
 O -0.30787936 -1.72060389 -4.83697802
 O 1.86939688 -1.72998635 -4.82898762
 Cl 0.78077123 3.06990493 0.79429128

5.
 Ag 0.78342714 -0.48396373 -0.75735072
 N 2.85187824 -0.48396973 -0.75735502
 C 3.99650354 -0.48397043 -0.75735622
 C 5.43988034 -0.48397213 -0.75736412
 H 5.80845294 0.45262617 -1.17835482
 H 5.80845444 -0.58768583 0.26425608
 H 5.80844544 -1.31686773 -1.35798672
 Cl -1.48377986 -0.48396013 -0.75734942
 Ag 0.78343794 1.94405873 1.06778302
 N 0.78343811 3.18692288 -0.58563122
 C 0.78343757 3.87469277 -1.50058458
 C 0.78343228 4.74196959 -2.65434691
 H -0.11585551 5.35968011 -2.65110543
 H 1.66238336 5.38784897 -2.62993274
 H 0.80378110 4.14276496 -3.56585256
 Cl 0.78343682 0.58176516 2.88006992

6.
 Ag 0.80166312 0.50940667 1.10336733
 N 2.87065552 0.50940357 1.10336313
 C 4.02191782 0.50939587 1.10336123
 N 5.33076092 0.50943417 1.10335923
 H 5.83850212 1.37660007 1.10335823

H	5.83851222	-0.35784773	1.10335113
Cl	-1.46786008	0.50940757	1.10336823
Ag	0.80165694	0.54852835	-1.94638176
N	0.80165379	-1.52029384	-1.97292030
C	0.80164606	-2.67146144	-1.98768680
N	0.80168433	-3.98019687	-2.00447492
H	1.66877886	-4.48775363	-2.02211138
H	-0.06552630	-4.48804900	-1.99986954
Cl	0.80165785	2.81786489	-1.91727473

7.

Ag	0.76789195	-0.59786394	1.39734518
N	2.84736385	-0.59086954	1.40385968
C	3.99416985	-0.56137514	1.43121818
O	5.26845465	-0.59476284	1.40018648
H	5.66330265	0.05362456	2.00207958
Cl	-1.49967315	-0.58757024	1.40687558
Ag	0.76899356	1.28198377	-0.97263296
N	0.77852178	-0.34720966	-2.26489173
C	0.81863018	-1.24737099	-2.97544314
O	0.77318934	-2.24321266	-3.77049908
H	1.65519129	-2.59534050	-3.96198021
Cl	0.78298016	3.05735757	0.43800538

8.

Ag	1.16991375	-2.34210073	-0.08694775
N	3.25648265	-2.34210393	-0.08695075
C	4.39739595	-2.34210573	-0.08695245
H	5.46735135	-2.34210943	-0.08695585
Br	-1.21984765	-2.34210043	-0.08694745
Ag	1.16991816	-2.31735405	2.93795103
N	1.16992133	-0.23087265	2.91884297
C	1.16992312	0.90999281	2.90839483
H	1.16992679	1.97990333	2.89859467
Br	1.16991787	-4.70701528	2.95983246

9.

Ag	-0.49011197	-1.24160374	0.00000004
N	1.61544073	-1.24160774	-0.00000376
C	2.75950253	-1.24160964	-0.00000556
Br	-2.88132877	-1.24160334	0.00000034
F	4.00507943	-1.24161274	-0.00000846
Ag	-0.49010627	1.75839626	-0.00000123
N	-0.49011007	1.75839536	-2.10555393
C	-0.49011187	1.75839515	-3.24961573
Br	-0.49010597	1.75839313	2.39121557
F	-0.49011477	1.75839389	-4.49519263

10.

Ag	0.45572518	-1.07529061	-0.13633721
N	2.53862068	-1.07533931	-0.13644291
C	3.68086458	-1.07531941	-0.13673371
Br	-1.93053932	-1.07522241	-0.13635551
C	5.17269098	-1.07528181	-0.13656281
F	5.61319858	-1.91048091	-1.06040361
F	5.61244398	-1.45786881	1.04890799
F	5.61292828	0.14254339	-0.39776571
Ag	0.45576035	1.86367852	-0.79786324
N	0.45564654	1.40628777	-2.82991820
C	0.45536721	1.15555244	-3.94430275
Br	0.45575748	2.38772886	1.53014653
C	0.45554219	0.82797290	-5.39971941
F	-0.62916056	0.13424923	-5.69510679
F	1.52805624	0.11329112	-5.68961615
F	0.46815617	1.94636606	-6.10269287

11.

Ag	0.05159014	-0.77581401	-0.25036728
N	2.12838484	-0.77578661	-0.25037168
C	3.27294174	-0.77582221	-0.25037318
Br	-2.33082436	-0.77583931	-0.25036618
N	4.69692944	-0.77583081	-0.25037778
O	5.20621894	-1.86456681	-0.25038408
O	5.20622604	0.31289459	-0.25037508
Ag	0.05159690	-0.80403926	2.76200049
N	0.05156955	1.27266428	2.78145875
C	0.05160516	2.41717093	2.79218393
Br	0.05162219	-3.18634915	2.73967476
N	0.05161380	3.84109614	2.80552447
O	1.14030210	4.35026776	2.82048892
O	-1.03706386	4.35046592	2.80010232

12.

Ag	-0.11177952	-0.35541299	-0.05513012
N	1.97166468	-0.35541669	-0.05513342

C	3.11632978	-0.35541919	-0.05513672
Br	-2.50553312	-0.35541289	-0.05513092
C	4.55978828	-0.35542509	-0.05514322
H	4.92819968	0.64861881	-0.27060102
H	4.92819768	-0.67085659	0.92211448
H	4.92818958	-1.04404109	-0.81694192
Ag	-0.11177524	2.60348825	-0.68404065
N	-0.11177924	2.17033122	-2.72195986
C	-0.11178299	1.93235026	-3.84161305
Br	-0.11177600	3.10115691	1.65740809
C	-0.11179057	1.63224668	-5.25353028
H	-0.11379394	2.56011388	-5.82738708
H	0.77853295	1.05511816	-5.50750239
H	-1.00011030	1.05172539	-5.50677299

13.

Ag	-0.18056846	-0.59293706	-0.44774720
N	1.90270254	-0.59294176	-0.44775160
C	3.05406314	-0.59293986	-0.44775350
Br	-2.57664126	-0.59293596	-0.44774640
N	4.36284624	-0.59298246	-0.44775530
H	4.87053964	0.27433314	-0.44775640
H	4.87051584	-1.46020056	-0.44776350
Ag	-0.18056199	-0.56629854	2.57713551
N	-0.18055733	1.51689169	2.55878998
C	-0.18055925	2.66820765	2.54865154
Br	-0.18056309	-2.96227847	2.59823131
N	-0.18051667	3.97694001	2.53712685
H	-1.04779863	4.48468098	2.54029526
H	0.68666772	4.48452261	2.52501076

14.

Ag	-0.07751117	-0.09962542	0.28030044
N	2.01692093	-0.09238952	0.28702554
C	3.16389573	-0.06300852	0.31422024
Br	-2.47130607	-0.08896022	0.29015284
O	4.43807633	-0.09614892	0.28348024
H	4.83294823	0.55301448	0.88483134
Ag	-0.07646137	1.78258873	-2.07181033
N	-0.06660985	0.14728804	-3.38041187
C	-0.02667922	-0.74980774	-4.09509969
Br	-0.06197902	3.65045715	-0.57470555
O	-0.07175979	-1.74232020	-4.89414049
H	0.81079914	-2.09069493	-5.09082513

15.

Ag	1.14979197	-2.59573824	0.00000045
N	3.26054507	-2.59574174	-0.00000285
C	4.40150237	-2.59574334	-0.00000435
H	5.47154867	-2.59574684	-0.00000765
I	-1.40209083	-2.59573794	0.00000065
Ag	1.14979697	0.41676176	-0.00000011
N	1.14979367	0.41676136	-2.11075321
C	1.14979217	0.41676143	-3.25171051
H	1.14978887	0.41675950	-4.32175681
I	1.14979717	0.41675832	2.55188269

16.

Ag	0.22355935	-1.34948151	0.00000004
N	2.35339425	-1.34948571	-0.00000396
C	3.49768205	-1.34948741	-0.00000566
I	-2.32916335	-1.34948101	0.00000044
F	4.74334985	-1.34949031	-0.00000826
Ag	0.22356521	1.63801849	-0.00000093
N	0.22356121	1.63801777	-2.12983583
C	0.22355951	1.63801794	-3.27412363
I	0.22356561	1.63801481	2.55272177
F	0.22355691	1.63801708	-4.51979143

17.

Ag	0.34394513	0.78359864	-0.07795274
N	2.45279953	0.78352584	-0.07800794
C	3.59507913	0.78324544	-0.07811744
I	-2.20478307	0.78357524	-0.07792954
C	5.08701263	0.78337594	-0.07804654
F	5.52757713	-0.11413136	-0.94143054
F	5.52699763	0.48451264	1.13118046
F	5.52673633	1.98015494	-0.42369904
Ag	0.34402247	3.67224500	-0.93286704
N	0.34394888	3.07377535	-2.95501959
C	0.34376430	2.74940909	-4.05027722
I	0.34403807	4.39545541	1.51110148
C	0.34386932	2.32615221	-5.48091316
F	-0.73873665	1.61087774	-5.72869350
F	1.41855080	1.59741845	-5.72410617

F 0.35209240 3.39583763 -6.25603770

18.

Ag -0.37833232 -0.07149832 -0.19697620
N 1.72232948 -0.07148782 -0.19698080
C 2.86712738 -0.07152462 -0.19698230
I -2.92268472 -0.07150402 -0.19697500
N 4.29025138 -0.07154682 -0.19698660
O 4.80010558 -1.16054522 -0.19699290
O 4.80003988 1.01751658 -0.19698390
Ag -0.37832563 -0.09569131 2.80292625
N -0.37833609 2.00490218 2.81986669
C -0.37829928 3.14966284 2.82910007
I -0.37831994 -2.63996094 2.78240332
N -0.37827705 4.57274057 2.84057567
O 0.71068601 5.08250742 2.85346148
O -1.46730508 5.08258329 2.83591076

19.

Ag 0.11177002 -0.28049487 0.08357388
N 2.21689772 -0.28049777 0.08357088
C 3.36166062 -0.28050237 0.08356718
I -2.44381358 -0.28049657 0.08357268
C 4.80518222 -0.28050667 0.08356258
H 5.17359102 0.70603973 -0.20142372
H 5.17359162 -0.52697967 1.08043038
H 5.17358352 -1.02058957 -0.62832542
Ag 0.11177283 2.61923555 -0.73295519
N 0.11176916 2.04864703 -2.75927978
C 0.11176435 1.73836023 -3.86118913
I 0.11177122 3.31191522 1.72696400
C 0.11175876 1.34709657 -5.25067369
H 0.10484200 2.23566250 -5.88361822
H 1.00450368 0.75879075 -5.46775110
H -0.77407824 0.74726392 -5.46449688

20.

Ag 0.01719569 -0.47647672 -0.54663323
N 2.12089709 -0.47648152 -0.54663783
C 3.27243609 -0.47647922 -0.54663953
I -2.54042401 -0.47647602 -0.54663243
N 4.58127789 -0.47650682 -0.54664123
H 5.08900209 0.39077018 -0.54664243
H 5.08898609 -1.34373272 -0.54664953
Ag 0.01720229 -0.48054046 2.46586403
N 0.01720709 1.62315903 2.46870185
C 0.01720480 2.77469698 2.47025604
I 0.01720159 -3.03815782 2.46240911
N 0.01723240 4.08353759 2.47202281
H -0.85004381 4.59126290 2.47153959
H 0.88445752 4.59124376 2.47386846

21.

Ag -0.31856891 -0.76259561 0.45921488
N 1.79766789 -0.75418451 0.46703608
C 2.94486169 -0.72584621 0.49326648
I -2.87426961 -0.75097191 0.46995098
O 4.21899489 -0.75840931 0.46304288
H 4.61204139 -0.10885871 1.06497068
Ag -0.31628399 0.95175867 -2.00269173
N -0.30491211 -0.78490641 -3.21201186
C -0.26667069 -1.72890185 -3.86389752
I -0.30061314 3.04669803 -0.53884748
O -0.31065899 -2.77038350 -4.59790722
H 0.56626454 -3.16337974 -4.72151020

22.

Ag 0.70834879 -0.57045602 -0.01676630
C -1.29652421 -0.57045542 -0.01676580
N -2.45269311 -0.57045542 -0.01676570
N 2.79171459 -0.57045922 -0.01676930
C 3.93187499 -0.57046072 -0.01677070
H 5.00224239 -0.57046372 -0.01677350
Ag 0.70835359 2.50418293 0.03035373
C 0.70835408 2.47345855 2.03499130
N 0.70835418 2.45574008 3.19102442
N 0.70835064 2.53610759 -2.05276745
C 0.70834926 2.55357921 -3.19279398
H 0.70834650 2.56997971 -4.26303572

23.

Ag 0.72568512 0.28324311 0.00000014
C -1.27871278 0.28324381 0.00000074
N -2.43486328 0.28324381 0.00000074
N 2.82399172 0.28323911 -0.00000356

C	3.96746152	0.28323751	-0.00000506
F	5.21137422	0.28323521	-0.00000726
Ag	0.72569103	3.38324311	-0.00000174
C	0.72569177	3.45265677	2.00319388
N	0.72569184	3.49269466	3.15865090
N	0.72568719	3.31057404	-2.09704962
C	0.72568562	3.27097370	-3.23983350
F	0.72568334	3.22789429	-4.48300001

24.

Ag	4.03570393	0.01753695	0.05480566
C	2.03104923	0.01752384	0.05470377
N	0.87501273	0.01751377	0.05465870
N	6.11840363	0.01769725	0.05484446
C	7.25974343	0.01811795	0.05481346
C	8.75411023	0.01779005	0.05475436
F	9.19176883	1.15364355	-0.45588884
F	9.19113363	-0.10821145	1.29392176
F	9.19056343	-0.99272175	-0.67380394
Ag	4.03551235	2.81074277	-1.20094411
C	4.03541404	3.63273286	0.62743571
N	4.03536881	4.10674771	1.68182193
N	4.03559894	1.95692502	-3.10058442
C	4.03559410	1.48932813	-4.14174237
C	4.03556932	0.87629772	-5.50457983
F	3.52487446	1.73279712	-6.36948689
F	5.27475359	0.58225661	-5.85151476
F	3.30707593	-0.22436374	-5.48831859

25.

Ag	0.74580695	0.33244808	0.16117131
C	-1.25853165	0.33245358	0.16117761
N	-2.41456455	0.33245388	0.16117791
N	2.82796255	0.33243238	0.16115341
C	3.97109595	0.33244278	0.16116621
N	5.40033795	0.33244338	0.16116791
O	5.90589175	-0.36890542	-0.67137939
O	5.90591235	1.03379158	0.99371561
Ag	0.74580762	2.66398909	-1.80514924
C	0.74581598	3.95617646	-0.27295310
N	0.74581641	4.70146523	0.61076445
N	0.74578382	1.32163323	-3.39683159
C	0.74580031	0.58466050	-4.27068808
N	0.74580199	-0.33676529	-5.36325716
O	-0.34278645	-0.66223415	-5.75010988
O	1.83439035	-0.66316637	-5.74935064

26.

Ag	0.75032791	0.14087902	-0.00000027
C	-1.25479879	0.14088312	0.00000123
N	-2.41121569	0.14088372	0.00000133
N	2.82903331	0.14087342	-0.00000417
C	3.97328981	0.14087362	-0.00000607
C	5.41620271	0.14087132	-0.00001117
H	5.78385061	1.07776882	-0.42113717
H	5.78385151	0.03712642	1.02193063
H	5.78384401	-0.69228698	-0.60082597
Ag	0.75033617	3.21587902	-0.00000191
C	0.75033728	3.07539410	2.00019736
N	0.75033715	2.99437046	3.15377233
N	0.75033267	3.36151772	-2.07359914
C	0.75033099	3.44169014	-3.21504355
C	0.75032617	3.54278540	-4.65441055
H	0.32920337	4.50314103	-4.95551128
H	1.77226770	3.46505131	-5.02842475
H	0.14950866	2.73743540	-5.07952347

27.

Ag	0.78082690	0.59446709	0.57560100
C	-1.22409446	0.59408435	0.57562365
N	-2.38063454	0.59386275	0.57563613
N	2.85777417	0.59486069	0.57557452
C	4.00887365	0.59508083	0.57556080
N	5.31637492	0.59531674	0.57554570
H	5.82398248	1.46286159	0.56352339
H	5.82430375	-0.27201016	0.58754720
Ag	0.73805693	0.40128941	-2.50555290
C	0.73767349	2.40228197	-2.63100595
N	0.73745151	3.55655567	-2.70337424
N	0.73845142	-1.67158810	-2.37559615
C	0.73867200	-2.82043195	-2.30356961
N	0.73890840	-4.12537113	-2.22175691
H	1.60600817	-4.63008941	-2.15977720
H	-0.12797263	-4.63419971	-2.22020004

28.

Ag	0.74939081	-0.30585694	0.68663808
C	-1.25529899	-0.30946714	0.68331118
N	-2.41145589	-0.31016854	0.68266978
N	2.82444521	-0.30915824	0.68354818
C	3.96957871	-0.30283464	0.68942898
C	5.44811151	-0.30580684	0.68671738
O	6.06144761	0.44220436	1.38108018
H	5.89865451	-1.04214624	0.00323628
Ag	0.74939843	2.06983065	-1.26572804
C	0.74453595	3.34263998	0.28305796
N	0.74359507	4.07689995	1.17612072
N	0.74491349	0.75234576	-2.86887640
C	0.75347091	0.02642338	-3.75452235
C	0.74948768	-0.91244041	-4.89671076
O	1.76086340	-1.19582785	-5.45764957
H	-0.24607128	-1.30266412	-5.15923490

29.

Ag	0.74939081	-0.30585694	0.68663808
C	-1.25529899	-0.30946714	0.68331118
N	-2.41145589	-0.31016854	0.68266978
N	2.82444521	-0.30915824	0.68354818
C	3.96957871	-0.30283464	0.68942898
C	5.44811151	-0.30580684	0.68671738
O	6.06144761	0.44220436	1.38108018
H	5.89865451	-1.04214624	0.00323628
Ag	0.74939843	2.06983065	-1.26572804
C	0.74453595	3.34263998	0.28305796
N	0.74359507	4.07689995	1.17612072
N	0.74491349	0.75234576	-2.86887640
C	0.75347091	0.02642338	-3.75452235
C	0.74948768	-0.91244041	-4.89671076
O	1.76086340	-1.19582785	-5.45764957
H	-0.24607128	-1.30266412	-5.15923490

30.

Ag	0.70594776	0.48272433	-1.50854761
N	2.83557766	0.48278343	-1.50849081
C	3.52122886	-0.66332007	-1.46829451
C	3.52118366	1.62895113	-1.54865891
C	4.90033516	-0.71674777	-1.46651081
H	2.93800946	-1.57518247	-1.43629911
C	4.90028416	1.68238983	-1.55060351
H	2.93793276	2.54078413	-1.58062011
C	5.58298606	0.48285253	-1.50873301
H	5.42814126	-1.66005167	-1.43338521
H	5.42802966	2.62575403	-1.58363371
F	6.90596616	0.48283953	-1.50911091
Cl	-1.56009714	0.48266573	-1.50853511
Ag	0.70586760	0.56196668	1.41537880
N	0.70581006	2.69081492	1.35768413
C	1.85258162	3.37646245	1.34825014
C	-0.44102491	3.37592108	1.32996117
C	1.90603802	4.75507068	1.31118737
H	2.76497593	2.79365565	1.37136870
C	-0.49449667	4.75450087	1.29206416
H	-1.35338891	2.79268749	1.33850927
C	0.70573443	5.43720636	1.28293753
H	2.84989290	5.28288833	1.30445499
H	-1.43840924	5.28184924	1.27026820
F	0.70573720	6.75968963	1.24668191
Cl	0.70592651	-1.70324451	1.47684215

31.

Ag	0.70710770	0.51954190	-0.08337466
N	2.84052190	0.52014990	-0.08756946
C	3.52407510	-0.62583160	-0.04093926
C	3.52321350	1.66700430	-0.12068976
C	4.90470310	-0.67100730	-0.02324746
H	2.93976210	-1.53700240	-0.01428496
C	4.90412020	1.71443470	-0.10628556
H	2.93825560	2.57732340	-0.15737476
C	5.60508670	0.52231880	-0.05482566
H	5.41656480	-1.62291800	0.02296094
H	5.41506950	2.66764670	-0.12652866
C	7.11240480	0.51998370	-0.07402366
F	7.61028400	1.62758820	0.47678814
F	7.56645710	0.45424860	-1.33019546
F	7.60685750	-0.52701820	0.58793634
Cl	-1.55829510	0.51949950	-0.07250806
Ag	0.71281765	0.64560870	2.83890177
N	0.71202942	2.77704459	2.74695333
C	1.85895074	3.45980691	2.71378627
C	-0.43515008	3.45992685	2.73742422

C	1.90488285	4.83990887	2.67259962
H	2.77039500	2.87539194	2.72342172
C	-0.48187816	4.84034415	2.69711298
H	-1.34619986	2.87564737	2.76585325
C	0.71134837	5.54061786	2.66597350
H	2.85791075	5.35146828	2.65481202
H	-1.43503240	5.35179921	2.69878802
C	0.71282197	7.04586575	2.58468082
F	-0.36884201	7.56802321	3.16383510
F	0.72190145	7.44777328	1.30920441
F	1.78858410	7.56516627	3.17793481
Cl	0.71334091	-1.61742869	2.94296630

32.

Ag	0.71085702	0.57700564	1.31418573
N	2.84520202	0.57708874	1.31426543
C	3.52541702	-0.57178066	1.35459413
C	3.52544272	1.72587064	1.27397073
C	4.90683712	-0.62335276	1.35623963
H	2.93956622	-1.48165196	1.38656953
C	4.90687952	1.77750114	1.27204833
H	2.93959302	2.63578044	1.24204813
C	5.58288122	0.57700134	1.31392913
H	5.44107242	-1.56225616	1.38915363
H	5.44107842	2.71637224	1.23909653
N	7.05875112	0.57684874	1.31317213
O	7.60491492	1.65368024	1.27603403
O	7.60467182	-0.50003636	1.34961713
Cl	-1.55263538	0.57692144	1.31418973
Ag	0.71097080	0.45831134	-1.60840501
N	0.71105060	-1.67427565	-1.52179489
C	-0.43850876	-2.35418967	-1.50058295
C	1.86052116	-2.35369767	-1.48782303
C	-0.49010514	-3.73449237	-1.44502989
H	-1.34892797	-1.76902353	-1.52933770
C	1.91218713	-3.73399164	-1.43164286
H	2.77097668	-1.76812436	-1.50651521
C	0.71097693	-4.40971797	-1.41114760
H	-1.42957061	-4.26850130	-1.42861711
H	2.85162186	-4.26754014	-1.40477995
N	0.71085521	-5.88440547	-1.35207720
O	1.78830653	-6.42985143	-1.32330956
O	-0.36662151	-6.43017438	-1.33726545
Cl	0.71088650	2.71994295	-1.70016730

33.

Ag	0.69989848	0.45250729	-1.09296624
N	2.82856288	0.45255359	-1.09639934
C	3.51938888	-0.68994171	-1.05083294
C	3.51912218	1.59546029	-1.13095344
C	4.89860748	-0.72998581	-1.03695894
H	2.93792468	-1.60329601	-1.02153454
C	4.89844828	1.63663989	-1.11993004
H	2.93752428	2.50856709	-1.16568354
C	5.62772408	0.45365149	-1.07283724
H	5.40040088	-1.68921381	-0.99419104
H	5.40007688	2.59659059	-1.14445854
C	7.12037168	0.45301219	-1.08330904
H	7.48938428	0.40079489	-2.11209974
H	7.52190298	1.36291659	-0.63616424
H	7.52129078	-0.40796961	-0.54726234
Cl	-1.57011222	0.45277509	-1.08498524
Ag	0.70462189	0.64348568	1.83831525
N	0.70435249	2.76764935	1.69992248
C	1.84734711	3.45513893	1.62553336
C	-0.43831542	3.45946364	1.69771191
C	1.88823008	4.83229051	1.54923100
H	2.76062273	2.87283795	1.63085443
C	-0.47866562	4.83688547	1.62396429
H	-1.35170895	2.88069836	1.76071469
C	0.70483394	5.56267289	1.54596488
H	2.84817761	5.33172548	1.49622604
H	-1.43811656	5.34001025	1.63155319
C	0.70477806	7.05165145	1.44084702
H	0.68834383	7.35461087	0.38953700
H	-0.17331585	7.48451081	1.92113415
H	1.59955887	7.48203932	1.89196279
Cl	0.70488050	-1.62145078	1.99022024

34.

Ag	0.71523378	0.56722092	1.07019322
N	2.84051298	0.56727092	1.07023822
C	3.54135388	-0.57261788	1.11018362
C	3.54134508	1.70722932	1.03030522
C	4.91350328	-0.62439748	1.11185462

H	2.96497928	-1.48927648	1.14240692
C	4.91354108	1.75895562	1.02838722
H	2.96497608	2.62380682	0.99822262
C	5.64887858	0.56730032	1.06988552
H	5.41237008	-1.58537148	1.14562602
H	5.41233638	2.71996702	0.99473702
N	6.99901538	0.56718372	1.06955142
H	7.51496968	-0.29163718	1.09846682
H	7.51521618	1.42563092	1.03901042
Cl	-1.55790392	0.56714562	1.07018892
Ag	0.71529877	0.44765142	-1.86487226
N	0.71534690	-1.67586641	-1.77836383
C	-0.42522301	-2.37639201	-1.75635808
C	1.85598584	-2.37585279	-1.74333094
C	-0.47702770	-3.74742331	-1.70097457
H	-1.34243343	-1.80070351	-1.78493795
C	1.90774734	-3.74690505	-1.68731664
H	2.77310950	-1.79974642	-1.76151029
C	0.71539064	-4.48192133	-1.66446369
H	-1.43857980	-4.24609655	-1.68606882
H	2.86933187	-4.24506298	-1.66151258
N	0.71528774	-5.83095417	-1.60987517
H	-0.14399824	-6.34672889	-1.59496531
H	1.57426654	-6.34654675	-1.58443259
Cl	0.71522371	2.71890695	-1.95735632

35.

Ag	0.70742531	0.48335542	-1.18211006
N	2.83677091	0.47702042	-1.18180556
C	3.52237091	-0.66805098	-1.14171056
C	3.53773731	1.61704912	-1.22178086
C	4.89935521	-0.72544518	-1.13989886
H	2.93869751	-1.57975648	-1.10964406
C	4.91270221	1.66186892	-1.22352166
H	2.96140381	2.53329532	-1.25381776
C	5.61869951	0.46426752	-1.18181306
H	5.39906471	-1.68670278	-1.10618396
H	5.44012241	2.60563662	-1.25663096
O	6.95508281	0.51832372	-1.18417526
H	7.32661591	-0.36915498	-1.15369306
Cl	-1.56245479	0.47860802	-1.18200156
Ag	0.70733133	0.59225588	1.74086200
N	0.71367327	2.72012519	1.66158471
C	1.85944364	3.40515483	1.63351089
C	-0.42705343	3.42069643	1.63792294
C	1.91686551	4.78117071	1.58187595
H	2.77171097	2.82181711	1.65339158
C	-0.47190696	4.79470371	1.58661527
H	-1.34385722	2.84484028	1.66146597
C	0.72641707	5.50010376	1.55744006
H	2.87871196	5.28045617	1.56119063
H	-1.41625309	5.32183291	1.56898124
O	0.67231041	6.83554590	1.50729286
H	1.56030878	7.20672587	1.49089814
Cl	0.71207947	-1.67605031	1.82537649

36.

Ag	0.69462153	0.52344678	-0.01247469
C	-1.30807747	0.52339640	-0.01250547
N	-2.46466407	0.52337552	-0.01249749
N	2.82946783	0.52350368	-0.01243599
C	3.51333563	-0.62346782	0.02775031
C	3.51327273	1.67051998	-0.05267119
C	4.89457533	-0.66715152	0.02918561
H	2.92650793	-1.53326012	0.05971531
C	4.89450563	1.71424798	-0.05429059
H	2.92640343	2.58027938	-0.08451259
C	5.60014153	0.52357438	-0.01262139
H	5.39989483	-1.62347192	0.06270291
H	5.39979453	2.67060468	-0.08784239
H	6.68363833	0.52361408	-0.01271649
Ag	0.69456678	0.56300623	2.94976117
C	0.69461674	-1.43951414	2.97650866
N	0.69463155	-2.59599727	2.99197881
N	0.69450902	2.69766219	2.92125371
C	1.84191398	3.38180239	2.93699483
C	-0.45294227	3.38107177	2.88717594
C	1.88561205	4.76293002	2.91937764
H	2.75205202	2.79529291	2.96467020
C	-0.49668886	4.76216729	2.86767021
H	-1.36304500	2.79399083	2.87531825
C	0.69443407	5.46808571	2.88402017
H	2.84229404	5.26848258	2.93338057
H	-1.45340826	5.26713232	2.84011953
H	0.69439241	6.55148437	2.86943723

37.

Ag	0.69312673	0.49002569	-1.06344413
C	-1.30875247	0.48997179	-1.06348023
N	-2.46526007	0.48995609	-1.06347393
N	2.82972853	0.49007609	-1.06339703
C	3.51546753	-0.65620151	-1.02323903
C	3.51544183	1.63639649	-1.10361173
C	4.89453333	-0.70982991	-1.02148693
H	2.93200563	-1.56798311	-0.99118203
C	4.89445583	1.69007359	-1.10560873
H	2.93191233	2.54815939	-1.13550243
C	5.57693713	0.49012709	-1.06365023
H	5.42302123	-1.65280871	-0.98843593
H	5.42294933	2.63306299	-1.13869353
F	6.89892253	0.49016839	-1.06383823
Ag	0.69305927	0.58355678	1.89757903
C	0.69311200	-1.41732422	1.96078952
N	0.69312789	-2.57325427	1.99733452
N	0.69301038	2.71909346	1.83012294
C	1.83998432	3.40461569	1.81242963
C	-0.45400812	3.40433713	1.80443070
C	1.89364130	4.78299489	1.76891810
H	2.75232340	2.82154855	1.83413748
C	-0.50772150	4.78265312	1.76055913
H	-1.36632327	2.82100069	1.81975883
C	0.69295142	5.46492263	1.74307509
H	2.83719341	5.31132273	1.75550378
H	-1.45128528	5.31077795	1.74054528
F	0.69290421	6.78624216	1.70112120

38.

Ag	0.69799328	0.51033510	-0.18384499
C	-1.30326402	0.51012990	-0.17563989
N	-2.45965622	0.51013730	-0.17246219
N	2.83591088	0.51097590	-0.18768609
C	3.51856368	-0.63555390	-0.14025949
C	3.51790188	1.65821120	-0.21990459
C	4.89909368	-0.68075510	-0.12190169
H	2.93406708	-1.54670970	-0.11393849
C	4.89864558	1.70550110	-0.20482789
H	2.93286818	2.56868510	-0.25683089
C	5.59900638	0.51295240	-0.15379779
H	5.41093698	-1.63262030	-0.07537419
H	5.40980358	2.65863900	-0.22463679
C	7.10703068	0.51049590	-0.17412289
F	7.60450178	1.61818910	0.37591841
F	7.55798308	0.44436670	-1.43091549
F	7.60103978	-0.53627730	0.48769591
Ag	0.70326011	0.72487491	2.78340457
C	0.70406467	-1.27084966	2.93233724
N	0.70428843	-2.42415390	3.01684937
N	0.70234398	2.85722963	2.62923145
C	1.84924649	3.53555592	2.54389221
C	-0.44413425	3.54123681	2.63375104
C	1.89568476	4.91371846	2.46170513
H	2.75985499	2.94961557	2.54404550
C	-0.49017672	4.91986334	2.55510119
H	-1.35484991	2.95979683	2.70527204
C	0.70288521	5.61586724	2.46870952
H	2.84838770	5.42260771	2.40183379
H	-1.44217171	5.43332197	2.56967930
C	0.70383810	7.11871667	2.34222195
F	-0.36018934	7.65930448	2.93603807
F	0.67693620	7.48003640	1.05537187
F	1.79664732	7.65248870	2.88870039

39.

Ag	0.70033775	0.47635814	-1.15076380
C	-1.30093365	0.47626694	-1.15081580
N	-2.45728095	0.47624634	-1.15080760
N	2.84108875	0.47639904	-1.15067870
C	3.51990935	-0.67317346	-1.11035510
C	3.51995335	1.62595354	-1.19107530
C	4.90138735	-0.72443466	-1.10880710
H	2.93263275	-1.58225576	-1.07831870
C	4.90146495	1.67710304	-1.19304740
H	2.93272625	2.53504794	-1.22292730
C	5.57636965	0.47634174	-1.15113460
H	5.43684725	-1.66247776	-1.07597030
H	5.43694105	2.61514794	-1.22602720
N	7.05323645	0.47624464	-1.15177670
O	7.59831105	1.55318274	-1.18869990
O	7.59821445	-0.60078446	-1.11542920
Ag	0.70021774	0.59801818	1.80923706
C	0.70030673	-1.40156392	1.89144799

N	0.70032765	-2.55693351	1.93898947
N	0.70018037	2.73696326	1.72132352
C	1.85043934	3.41492755	1.68655198
C	-0.45006360	3.41553355	1.70021086
C	1.90172089	4.79521498	1.62920747
H	2.76007059	2.82793003	1.70541094
C	-0.50125094	4.79588268	1.64354877
H	-1.35969937	2.82902773	1.72981699
C	0.70021893	5.46991333	1.60842642
H	2.84032140	5.32998899	1.60152583
H	-1.43985911	5.33113359	1.62706460
N	0.70028960	6.94550526	1.54707164
O	-0.37725661	7.49041883	1.53194959
O	1.77790312	7.48969912	1.51680626

40.

Ag	0.69334153	0.47416075	-0.89303432
C	-1.30886537	0.47425465	-0.89022872
N	-2.46544767	0.47424975	-0.89073062
N	2.82364593	0.47412765	-0.89809432
C	3.51362603	-0.66920085	-0.85513692
C	3.51335613	1.61763425	-0.93530642
C	4.89256583	-0.70920905	-0.84479092
H	2.93144403	-1.58228185	-0.82369622
C	4.89241543	1.65854905	-0.92779312
H	2.93106723	2.53063055	-0.96788892
C	5.62124273	0.47498195	-0.88020752
H	5.39487903	-1.66815455	-0.80412212
H	5.39459223	2.61800525	-0.95438472
C	7.11353623	0.47456795	-0.88600612
H	7.48582473	0.42239305	-1.91356832
H	7.51256073	1.38473565	-0.43711522
H	7.51192173	-0.38649205	-0.34819612
Ag	0.70039964	0.63859034	2.07740977
C	0.70045634	-1.36066447	2.18613216
N	0.70042579	-2.51565376	2.24681659
N	0.70015302	2.76564440	1.95966681
C	1.84406063	3.45343440	1.90018366
C	-0.44359346	3.45591673	1.95190008
C	1.88460641	4.83086750	1.83524705
H	2.75743255	2.87093880	1.90977114
C	-0.48399942	4.83356677	1.88879091
H	-1.35695319	2.87551145	2.00277181
C	0.70034687	5.56027108	1.82955065
H	2.84430459	5.33169577	1.79402296
H	-1.44339039	5.33656696	1.89093937
C	0.70043436	7.05016745	1.74480124
H	0.69329666	7.36750627	0.69768608
H	-0.18234417	7.47512104	2.22359697
H	1.59106405	7.47376826	2.21032893

41.

Ag	0.70766928	0.52031906	-1.30023924
C	-1.29565142	0.52024406	-1.30027734
N	-2.45243552	0.52022266	-1.30027414
N	2.83411718	0.52036826	-1.30018544
C	3.53463128	-0.62046474	-1.26025664
C	3.53465608	1.66116456	-1.34018594
C	4.90622608	-0.67180444	-1.25864644
H	2.95793678	-1.53717984	-1.22800224
C	4.90626998	1.71249476	-1.34213944
H	2.95797668	2.57790676	-1.37221824
C	5.64144328	0.52030476	-1.30057864
H	5.40681918	-1.63169714	-1.22498274
H	5.40686058	2.67236776	-1.37577964
N	6.99036928	0.52022786	-1.30075514
H	7.50667288	-0.33848624	-1.27185984
H	7.50681168	1.37882936	-1.33155664
Ag	0.70759414	0.52789269	1.66225108
C	0.70766904	-1.47542144	1.66738507
N	0.70769045	-2.63220167	1.67037486
N	0.70754508	2.65433364	1.65681483
C	1.84847549	3.35494104	1.69204715
C	-0.43334881	3.35477438	1.61789340
C	1.89981910	4.72653509	1.68998614
H	2.76526929	2.77832574	1.72346996
C	-0.48468379	4.72637900	1.61252853
H	-1.35016916	2.77802019	1.58967060
C	0.70760758	5.46164937	1.64917337
H	2.85979393	5.22720716	1.71992756
H	-1.44463887	5.22688736	1.58002566
N	0.70768404	6.81057041	1.64551395
H	1.56646853	7.32694128	1.67090253
H	-0.15099267	7.32693718	1.61555250

42.			
Ag	0.69864547	0.50460512	-1.01362811
C	-1.30383253	0.50185642	-1.01358921
N	-2.46046143	0.49977792	-1.01351561
N	2.83048277	0.49838612	-1.01332791
C	3.51588197	-0.64725968	-0.97322131
C	3.53125517	1.63891892	-1.05332801
C	4.89242737	-0.70496058	-0.97140851
H	2.93211527	-1.55918988	-0.94114351
C	4.90578607	1.68338712	-1.05506731
H	2.95544057	2.55576112	-1.08538031
C	5.61170947	0.48526792	-1.01334191
H	5.39176037	-1.66639758	-0.93769231
H	5.43356067	2.62697982	-1.08817111
O	6.94678037	0.54094052	-1.01575841
H	7.32182847	-0.34526178	-0.98528581
Ag	0.69842026	0.57037214	1.94814178
C	0.70116914	-1.43160946	1.99272674
N	0.70324875	-2.58795074	2.01851921
N	0.70464439	2.70168407	1.90081581
C	1.85089710	3.38724178	1.90029502
C	-0.43649420	3.40195386	1.87045183
C	1.90862399	4.76345754	1.87016697
H	2.76331377	2.80388489	1.92519051
C	-0.48098999	4.77612686	1.83907812
H	-1.35382112	2.82602017	1.87152111
C	0.71775909	5.48221387	1.83855751
H	2.87057160	5.26294368	1.87147810
H	-1.42508411	5.30349830	1.81510472
O	0.66204666	6.81692711	1.80763376
H	1.54870622	7.19212403	1.81013550

43.			
Cl	-0.98180985	-3.14134800	0.00000065
Au	1.24014035	-3.14134860	0.00000015
N	3.20334965	-3.14135110	-0.00000225
C	4.34536045	-3.14135310	-0.00000405
H	5.41425065	-3.14135720	-0.00000785
Cl	1.24014504	0.12114961	2.22194972
Au	1.24014454	0.12115140	-0.00000048
N	1.24014214	0.12115102	-1.96320978
C	1.24014034	0.12115025	-3.10522058
H	1.24013654	0.12114730	-4.17411078

44.			
Cl	-0.97565964	-2.36638890	0.00000072
Au	1.24679626	-2.36638960	0.00000012
N	3.23273986	-2.36639280	-0.00000288
C	4.37577366	-2.36639490	-0.00000478
F	5.62264616	-2.36639860	-0.00000828
Cl	1.24680205	0.85860844	2.22245468
Au	1.24680145	0.85861040	-0.00000122
N	1.24679845	0.85860958	-1.98594482
C	1.24679655	0.85860884	-3.12897862
F	1.24679305	0.85860664	-4.37585112

45.			
Cl	-0.92106328	-2.25722743	-0.24855706
Au	1.29693892	-2.25727653	-0.24856626
N	3.25163292	-2.25730423	-0.24866526
C	4.39550612	-2.25729363	-0.24887886
C	5.88291932	-2.25727053	-0.24873736
F	6.32749072	-3.09239713	-1.17252006
F	6.32687672	-2.63982773	0.93658144
F	6.32728152	-1.03957003	-0.50994726
Cl	1.29703027	-5.39733739	2.11203597
Au	1.29708060	-3.30284455	2.84185341
N	1.29713933	-1.45696763	3.48494520
C	1.29719818	-0.37672208	3.86113063
C	1.29713154	1.02782446	4.35066823
F	2.38423785	1.64751940	3.92331277
F	1.27969302	1.03727381	5.67280115
F	0.22734392	1.65725068	3.89475160

46.			
Cl	-0.87842450	-3.15533593	0.81576075
Au	1.33505540	-3.15533423	0.81576235
N	3.28421250	-3.15534093	0.81575615
C	4.43042740	-3.15535943	0.81573915
N	5.84720580	-3.15533333	0.81576315
O	6.36035820	-2.35691253	1.55585725
O	6.36037900	-3.95377413	0.07565055
Cl	1.33505364	0.71593877	0.06967793
Au	1.33505597	-0.85097118	-1.49374348
N	1.33504685	-2.23076879	-2.87046857

C	1.33502175	-3.04216861	-3.68006039
N	1.33505717	-4.04509706	-4.68075793
O	2.42299680	-4.38008057	-5.07154414
O	0.24709033	-4.43664440	-5.01488354

47.

Cl	-0.91913753	-2.62499572	0.05975897
Au	1.30719387	-2.62499732	0.05975807
N	3.27835537	-2.62499972	0.05975547
C	4.42319357	-2.62500192	0.05975287
C	5.86596127	-2.62500792	0.05974717
H	6.23551367	-1.62111682	-0.15567893
H	6.23551117	-2.94039182	1.03685487
H	6.23550327	-3.31351992	-0.70193703
Cl	1.22941765	1.07652900	1.55440832
Au	1.23064221	0.56652566	-0.61272033
N	1.23172447	0.11497549	-2.53146443
C	1.23235181	-0.14728258	-3.64585880
C	1.23313945	-0.47779262	-5.05025943
H	1.20544432	0.43662102	-5.64511688
H	2.13615015	-1.03835506	-5.29747395
H	0.35843082	-1.08561320	-5.28734981

48.

Cl	-0.91731660	-2.65388450	0.34095942
Au	1.31103740	-2.65388600	0.34095792
N	3.28824020	-2.65388950	0.34095462
C	4.43888740	-2.65389130	0.34095292
N	5.74730530	-2.65389740	0.34094742
H	6.25552510	-3.28985720	-0.24855398
H	6.25553630	-2.01793840	0.93044782
Cl	1.31103942	1.19323568	-0.55855448
Au	1.31103730	-0.44952238	-2.06417977
N	1.31103249	-1.90713003	-3.40011047
C	1.31103002	-2.75539515	-4.17756482
N	1.31102181	-3.71997000	-5.06161955
H	0.44388117	-4.09133090	-5.40860995
H	2.17816117	-4.09794359	-5.40141154

49.

Cl	-0.95192426	-2.96807171	0.77220375
Au	1.27416444	-2.96843971	0.77190365
N	3.25803694	-2.96206731	0.77782925
C	4.40399704	-2.93718831	0.80084755
O	5.67864044	-2.97659231	0.76429885
H	6.07650904	-2.32835131	1.36478275
Cl	1.27560731	0.79875099	-0.34202133
Au	1.27513266	-0.93058540	-1.74375831
N	1.28381415	-2.47213237	-2.99251104
C	1.31763447	-3.36377971	-3.71236836
O	1.26401154	-4.35171176	-4.51779938
H	2.14567868	-4.69783754	-4.72263283

50.

N	2.76351490	-1.85525006	-0.00000244
C	3.90546800	-1.85525196	-0.00000414
H	4.97451060	-1.85525596	-0.00000784
Br	-1.56382740	-1.85524686	0.00000066
Au	0.78498290	-1.85524746	0.00000006
N	0.78498040	1.38224976	-1.97853223
C	0.78497870	1.38224775	-3.12048533
H	0.78497500	1.38224365	-4.18952793
Br	0.78498350	1.38225336	2.34881007
Au	0.78498290	1.38225254	-0.00000023

51.

N	1.70973589	-1.22660620	-0.00000309
C	2.85296069	-1.22660810	-0.00000489
Br	-2.64125681	-1.22660200	0.00000081
F	4.09961919	-1.22661150	-0.00000799
Au	-0.29234801	-1.22660280	0.00000011
N	-0.29234577	1.97339665	-2.00208467
C	-0.29234757	1.97339638	-3.14530947
Br	-0.29234187	1.97339465	2.34890803
F	-0.29235067	1.97339476	-4.39196797
Au	-0.29234257	1.97339720	-0.00000077

52.

N	-0.11177999	-0.21814160	0.00707053
C	1.03205921	-0.21812940	0.00685343
Br	-4.42715189	-0.21806380	0.00716603
C	2.51994371	-0.21810670	0.00699243
F	2.96411121	-1.05324490	-0.91680677
F	2.96349681	-0.60066940	1.19232423

F	2.96390181	0.99961130	-0.25422507
Au	-2.08203729	-0.21811360	0.00716093
N	-2.08211749	2.52694096	-2.59037910
C	-2.08232732	2.28925650	-3.70925096
Br	-2.08200791	3.42392071	1.63074183
C	-2.08218663	1.98000190	-5.16464158
F	-3.15939590	1.27644578	-5.46923070
F	-1.00225899	1.28078232	-5.46952403
F	-2.08459324	3.10594829	-5.85775732
Au	-2.08202325	2.93645579	-0.66315015

53.

N	1.63746502	-0.95129477	-0.42906997
C	2.78377052	-0.95130057	-0.42907157
Br	-2.66707168	-0.95128867	-0.42906507
N	4.20063062	-0.95129277	-0.42907657
O	4.71375982	-2.04013927	-0.42908297
O	4.71376752	0.13752003	-0.42907397
Au	-0.32674188	-0.95129097	-0.42906667
N	-0.32673263	1.02171060	2.81560180
C	-0.32672683	2.16801190	2.81249760
Br	-0.32673871	-3.28281032	2.82725734
N	-0.32673464	3.58486679	2.80865776
O	0.76210784	4.09798611	2.80431180
O	-1.41554344	4.09800981	2.81022214
Au	-0.32673642	-0.94248910	2.82092141

54.

N	1.67606255	-1.04497790	0.04208236
C	2.82091295	-1.04497990	0.04207946
Br	-2.66244115	-1.04497380	0.04208556
C	4.26369465	-1.04498550	0.04207396
H	4.63297575	-0.04102250	-0.17336774
H	4.63297315	-1.36039260	1.01925206
H	4.63296505	-1.73354770	-0.71966534
Au	-0.30954445	-1.04497530	0.04208486
N	-0.30954416	1.70903849	-2.57314928
C	-0.30954741	1.47104985	-3.69299027
Br	-0.30954018	2.61091405	1.67057960
C	-0.30955396	1.17112543	-5.10425367
H	-0.31158711	2.09874670	-5.67891878
H	0.58071108	0.59388703	-5.35910516
H	-1.19778999	0.59044546	-5.35836548
Au	-0.30954117	2.12180119	-0.63091806

55.

N	1.99106916	-0.76473805	-0.75488378
C	3.14184596	-0.76473965	-0.75488588
Br	-2.35463724	-0.76473295	-0.75487898
N	4.45011666	-0.76474705	-0.75488818
H	4.95826126	0.10247105	-0.75488888
H	4.95825246	-1.63196235	-0.75489608
Au	-0.00000134	-0.76473445	-0.75488028
N	0.00000797	1.24248577	2.47263192
C	0.00000956	2.39324820	2.46688256
Br	0.00000289	-3.10316641	2.49434023
N	0.00001695	3.70150258	2.46034641
H	-0.86719033	4.20966248	2.46214202
H	0.86722138	4.20961035	2.45346667
Au	0.00000439	-0.74855988	2.48257932

56.

N	1.59444907	0.11614457	0.39864530
C	2.74064717	0.14105427	0.42168830
Br	-2.75659293	0.11098217	0.39379130
O	4.01503087	0.10242697	0.38585240
H	4.41256307	0.75080347	0.98648570
Au	-0.40425363	0.11005177	0.39297640
N	-0.39514916	0.61248337	-3.35702594
C	-0.36127082	-0.27275172	-4.08512803
Br	-0.40222043	3.96851600	-0.58780012
O	-0.41387124	-1.25366096	-4.89868833
H	0.46848654	-1.59269710	-5.11242540
Au	-0.40345655	2.15429888	-2.08516996

57.

N	3.14698086	-0.49914512	-0.00000259
C	4.28890216	-0.49914702	-0.00000439
H	5.35813716	-0.49915082	-0.00000789
I	-1.36686724	-0.49914182	0.00000051
Au	1.14334446	-0.49914232	0.00000001
N	1.14334638	2.71335755	-2.00363660
C	1.14334458	2.71335717	-3.14555790
H	1.14334108	2.71335480	-4.21479290
I	1.14334948	2.71335483	2.51021150

Au 1.14334898 2.71335768 -0.00000020

58.

N 1.39268054 -2.29269498 -0.00000330
C 2.53622684 -2.29269698 -0.00000510
I -3.14561136 -2.29269088 0.00000060
F 3.78281384 -2.29270028 -0.00000820
Au -0.63628556 -2.29269148 0.00000000
N -0.63628340 0.88230803 -2.02896685
C -0.63628520 0.88230773 -3.17251315
I -0.63627950 0.88230540 2.50932505
F -0.63628830 0.88230628 -4.41910015
Au -0.63628010 0.88230852 -0.00000075

59.

N 1.79780228 -0.21665782 0.18511559
C 2.94161418 -0.21689292 0.18502279
I -2.70489052 -0.21655482 0.18521169
C 4.42994388 -0.21673592 0.18510769
F 4.87401508 -1.11418702 -0.67821381
F 4.87350538 -0.51559392 1.39420239
F 4.87326868 0.97989958 -0.16052471
Au -0.19779072 -0.21655542 0.18517759
N -0.19775005 2.28468314 -2.63726765
C -0.19790582 1.95959656 -3.73390999
I -0.19762866 3.56372563 1.67994125
C -0.19777981 1.53696296 -5.16097206
F -1.28050904 0.82099013 -5.41201400
F 0.87657247 0.80684929 -5.40729319
F -0.18917513 2.60525740 -5.93982258
Au -0.19766152 2.85160153 -0.72389498

60.

N 1.96254182 -1.82751901 -0.02540899
C 3.10906922 -1.82752511 -0.02541059
I -2.52771198 -1.82750481 -0.02540389
N 4.52534772 -1.82749601 -0.02541529
O 5.03885792 -2.91665861 -0.02542169
O 5.03883932 -0.73836391 -0.02541269
Au -0.02579538 -1.82750801 -0.02540549
N -0.02577854 0.20342027 3.17294411
C -0.02577246 1.34984686 3.15774072
I -0.02579267 -4.28643875 3.23248528
N -0.02580162 2.76600081 3.13895810
O 1.06326510 3.27927426 3.11769928
O -1.11483789 3.27963883 3.14659579
Au -0.02578949 -1.78474210 3.19931094

61.

N 0.03439366 0.69339398 0.05826098
C 1.17930266 0.69338998 0.05825828
I -4.48835974 0.69339558 0.05826348
C 2.62220036 0.69338318 0.05825218
H 2.99142006 1.67983558 -0.22670552
H 2.99142076 0.44693658 1.05502328
H 2.99141196 -0.04662412 -0.65356432
Au -1.97492254 0.69339608 0.05826328
N -1.97492318 3.12652944 -2.72152335
C -1.97492687 2.81374245 -3.82287748
I -1.97492034 4.36212618 1.62917763
C -1.97493460 2.41954459 -5.21088390
H -1.97955630 3.30639085 -5.84656838
H -1.08341094 1.82866699 -5.42689663
H -2.86183994 1.82096988 -5.42470151
Au -1.97492039 3.67546694 -0.78864487

62.

N 1.75605721 -0.82034579 -0.08629612
C 2.90702831 -0.82034789 -0.08629802
I -2.77250119 -0.82034069 -0.08629112
N 4.21531871 -0.82035159 -0.08630022
H 4.72339581 0.04689701 -0.08630102
H 4.72338871 -1.68760669 -0.08630812
Au -0.25795369 -0.82034209 -0.08629242
N -0.25794413 1.16342284 3.14497250
C -0.25794201 2.31434322 3.15577742
I -0.25794928 -3.36493599 3.10245751
N -0.25793829 3.62257597 3.16805917
H -1.12514869 4.13070711 3.16468952
H 0.60927868 4.13054722 3.18096108
Au -0.25794787 -0.85049932 3.12606603

63.

N 2.29840673 0.17734839 0.22967992
C 3.44487763 0.20244709 0.25290202

I	-2.23719767	0.17374669	0.22626222
O	4.71921523	0.16512729	0.21825852
H	5.11578303	0.81371169	0.81930052
Au	0.27510723	0.17129879	0.22404762
N	0.28383235	0.72953080	-3.50988680
C	0.31800777	-0.13754326	-4.25993969
I	0.27887218	4.15704847	-0.53939358
O	0.26711698	-1.09936152	-5.09590921
H	1.15087864	-1.41844488	-5.33324938
Au	0.27557199	2.25864929	-2.18491978

64.

Au	1.17755111	-2.76696743	-0.00000027
N	3.18005811	-2.76697003	-0.00000267
C	4.32042041	-2.76697173	-0.00000427
H	5.39021461	-2.76697513	-0.00000747
C	-0.76660729	-2.76696673	0.00000043
N	-1.92188469	-2.76696663	0.00000043
Au	1.17755537	0.48303257	-0.00000054
N	1.17755297	0.48303240	-2.00250754
C	1.17755137	0.48303209	-3.14286984
H	1.17754817	0.48302999	-4.21266404
C	1.17755607	0.48303090	1.94415786
N	1.17755607	0.48302960	3.09943526

65.

Au	1.18369720	-3.23992148	0.00000014
N	3.20607050	-3.23992488	-0.00000296
C	4.34830270	-3.23992658	-0.00000456
C	-0.75711930	-3.23992058	0.00000094
N	-1.91236920	-3.23992058	0.00000104
F	5.59216490	-3.23992928	-0.00000706
Au	1.18370261	-0.01492148	-0.00000127
N	1.18369951	-0.01492232	-2.02237457
C	1.18369791	-0.01492258	-3.16460677
C	1.18370341	-0.01492304	1.94081523
N	1.18370351	-0.01492450	3.09606513
F	1.18369541	-0.01492370	-4.40846897

66.

Au	1.23505366	-2.47279273	0.02850938
N	3.23173266	-2.47282553	0.02839768
C	4.37359746	-2.47280563	0.02813848
C	-0.70931264	-2.47274323	0.02850378
N	-1.86444424	-2.47272013	0.02849228
C	5.86604486	-2.47276593	0.02833588
F	6.30455636	-1.25493573	-0.23287372
F	6.30406576	-2.85535443	1.21380348
F	6.30483446	-3.30797223	-0.89551762
Au	1.23506731	0.69147421	-0.65619566
N	1.23495120	0.26919278	-2.60770928
C	1.23470207	0.02777493	-3.72376154
C	1.23507230	1.10273236	1.24417984
N	1.23506595	1.34705301	2.37317782
C	1.23490340	-0.28786233	-5.18245012
F	1.23716891	0.83675113	-5.87445635
F	2.31263842	-0.99102469	-5.47845625
F	0.15530571	-0.98753775	-5.47999725

67.

Au	1.26416596	-2.75580057	0.43440303
N	3.25668146	-2.75580797	0.43439613
C	4.40045306	-2.75579637	0.43440703
C	-0.67953924	-2.75580127	0.43440243
N	-1.83474754	-2.75580157	0.43440213
N	5.82526676	-2.75585257	0.43435483
O	6.33268066	-1.95732597	1.17454693
O	6.33271306	-3.55426827	-0.30573457
Au	1.26416615	-0.52107868	-1.90812218
N	1.26415604	-1.96278302	-3.28347909
C	1.26417195	-2.79037017	-4.07298082
C	1.26416523	0.88530837	-0.56645704
N	1.26416481	1.72117075	0.23093892
N	1.26409526	-3.82130889	-5.05647430
O	2.35280327	-4.17767214	-5.41802381
O	0.17553838	-4.19925621	-5.39544546

68.

Au	1.24175423	-2.65560036	0.06056692
N	3.24870383	-2.65560366	0.06056372
C	4.39264493	-2.65560526	0.06056142
C	-0.70199007	-2.65559896	0.06056762
N	-1.85756377	-2.65559876	0.06056762
C	5.83482103	-2.65561046	0.06055622
H	6.20259043	-1.65117286	-0.15498698

H	6.20258823	-2.97116606	1.03819622
H	6.20258033	-3.34449736	-0.70154268
Au	1.24175853	0.52337856	-0.55221305
N	1.24175476	0.14351186	-2.52288501
C	1.24175220	-0.07300798	-3.64614829
C	1.24175948	0.89128075	1.35639636
N	1.24175952	1.11000143	2.49108215
C	1.24174611	-0.34597900	-5.06225518
H	1.22021601	0.59292495	-5.61777650
H	2.14198664	-0.90153852	-5.32970354
H	0.36303270	-0.93815338	-5.32263766

69.

Au	1.24890151	-3.01052888	0.72087166
N	3.25911011	-3.01053248	0.72086826
C	4.40935701	-3.01053398	0.72086686
C	-0.69368479	-3.01052728	0.72087316
N	-1.84945789	-3.01052718	0.72087326
N	5.71584231	-3.01053958	0.72086186
H	6.22379791	-3.64688118	0.13100656
H	6.22380851	-2.37419838	1.31071646
Au	1.24890145	-0.79949435	-1.66110783
N	1.24889650	-2.27280994	-3.02868957
C	1.24889445	-3.11584519	-3.81122359
C	1.24890364	0.62425974	-0.33953081
N	1.24890379	1.47134524	0.44676278
N	1.24888694	-4.07339029	-4.70004934
H	0.38121215	-4.44608768	-5.04518106
H	2.11656097	-4.44527887	-5.04606799

70.

Au	1.21339808	-1.73559285	-0.59608879
N	3.23108851	-1.72998660	-0.58442434
C	4.37680573	-1.70996886	-0.56224681
C	-0.72810682	-1.73811995	-0.59845839
N	-1.88351612	-1.73446185	-0.59508609
O	5.64819216	-1.75386094	-0.59889288
H	6.05421413	-1.10865171	0.00010457
Au	1.20667743	-4.04262110	1.67525041
N	1.19444208	-2.62366831	3.10970691
C	1.16460245	-1.81713284	3.92344559
C	1.21013029	-5.40770197	0.29467243
N	1.20515630	-6.21983526	-0.52716100
O	1.22150982	-0.92519656	4.82948318
H	0.34209259	-0.60970651	5.08840032

71.

Cl	-1.00691151	-2.34964325	-0.31596895
N	3.27108939	-2.34951385	-0.31591485
C	3.95423629	-3.50016265	-0.27557435
C	3.95417859	-1.19884995	-0.35625175
C	5.33430489	-3.53935465	-0.27428485
H	3.36329689	-4.40555325	-0.24377775
C	5.33424189	-1.15957805	-0.35770285
H	3.36319409	-0.29347395	-0.38796125
C	6.04106609	-2.34945735	-0.31609725
H	5.83837499	-4.49637555	-0.24070555
H	5.83826549	-0.20253755	-0.39123745
H	7.12427459	-2.34942575	-0.31626835
Au	1.22556679	-2.34957495	-0.31594535
Cl	1.22558560	-4.50012704	2.85372362
N	1.22545766	-0.22358126	2.74215369
C	2.37676697	0.45960281	2.73466318
C	0.07413334	0.45900570	2.71399852
C	2.41597926	1.83920849	2.69892012
H	3.28267871	-0.13092169	2.75826950
C	0.03483696	1.83858795	2.67756109
H	-0.83176154	-0.13198901	2.72131921
C	1.22539642	2.54544758	2.66969492
H	3.37355023	2.34333205	2.69439034
H	-0.92275243	2.34221604	2.65583152
H	1.22536037	3.62828282	2.64126023
Au	1.22551794	-2.26840821	2.79549615

72.

Cl	-1.00797692	-2.37692544	-0.64379895
N	3.27179538	-2.37679864	-0.64373415
C	3.95644498	-3.52674984	-0.60342225
C	3.95638968	-1.22682894	-0.68405075
C	5.33451038	-3.57594334	-0.60180685
H	3.36799098	-4.43378504	-0.57155375
C	5.33446308	-1.17756974	-0.68587355
H	3.36790978	-0.31981084	-0.71580335
C	6.01778598	-2.37675804	-0.64397965
H	5.86144588	-4.51976654	-0.56868905

H	5.86135488	-0.23373624	-0.71894875
Au	1.22339108	-2.37685454	-0.64376655
F	7.34048928	-2.37672714	-0.64425125
Cl	1.22340601	-4.43265056	2.59943333
N	1.22328297	-0.15937964	2.36362273
C	2.37370884	0.52295667	2.30283314
C	0.07283837	0.52544647	2.34894196
C	2.42291663	1.89886694	2.22578523
H	3.28112240	-0.06560269	2.31715337
C	0.02355355	1.90147440	2.27388049
H	-0.83455174	-0.06113279	2.39960375
C	1.22322891	2.58242361	2.21203331
H	3.36713117	2.42395874	2.17785238
H	-0.92066892	2.42861044	2.26377406
Au	1.22333700	-2.20467228	2.47648637
F	1.22318310	3.90310152	2.13886266

73.

Cl	-0.99502541	-2.34263603	-0.01959045
N	3.27857069	-2.34177963	-0.03477645
C	3.96138579	-3.49210323	0.01215235
C	3.96060669	-1.19065763	-0.06784005
C	5.34051009	-3.53243243	0.03008785
H	3.37210029	-4.39849023	0.03850965
C	5.33991119	-1.14807153	-0.05284915
H	3.37062129	-0.28503683	-0.10444935
C	6.04183939	-2.33963473	-0.00118145
H	5.85153219	-4.48469463	0.07595475
H	5.85009919	-0.19452103	-0.07341365
Au	1.23424409	-2.34239423	-0.03159875
C	7.54836439	-2.34199893	-0.02124595
F	8.04334399	-3.38892803	0.64060175
F	8.00193919	-2.40789963	-1.27771015
F	8.04669269	-1.23432613	0.52919005
Cl	1.22904952	-0.14921806	-3.16116522
N	1.23006854	-4.42264479	-3.12020330
C	0.07933359	-5.10493895	-3.07585337
C	2.38146600	-5.10490174	-3.13275346
C	0.03882976	-6.48371409	-3.04020902
H	-0.82727368	-4.51547974	-3.06633469
C	2.42390284	-6.48388461	-3.09921900
H	3.28740714	-4.51532657	-3.16802113
C	1.23188287	-7.18523352	-3.05029353
H	-0.91384351	-6.99421744	-2.99719023
H	3.37761292	-6.99417073	-3.10351147
Au	1.22941716	-2.37845292	-3.14388613
C	1.22972375	-8.69189240	-3.05058955
F	0.17620728	-9.17827634	-2.39283469
F	1.17643535	-9.16194076	-4.30158522
F	2.33181867	-9.18279898	-2.48256893

74.

Cl	-0.95802098	-2.38935541	-1.17786860
N	3.31062642	-2.38924301	-1.17775340
C	3.99047102	-3.54271421	-1.13728430
C	3.99044462	-1.23568041	-1.21826900
C	5.36991222	-3.58923031	-1.13589330
H	3.39883432	-4.44733661	-1.10542060
C	5.37001952	-1.18928051	-1.22007110
H	3.39892312	-0.33111951	-1.24996400
C	6.04749152	-2.38927691	-1.17820600
H	5.90333782	-4.52848161	-1.10298510
H	5.90338632	-0.25003671	-1.25306840
Au	1.26887602	-2.38925361	-1.17780400
N	7.52102282	-2.38948831	-1.17889070
O	8.06749932	-3.46639391	-1.14252250
O	8.06775602	-1.31242601	-1.21587540
Cl	1.26889709	-4.48717713	2.03519000
N	1.26878946	-0.22206298	1.86154698
C	2.42295229	0.45695512	1.82741728
C	0.11453343	0.45745300	1.84028657
C	2.46948648	1.83523255	1.77076384
H	3.32812219	-0.13439235	1.84656326
C	0.06809863	1.83588792	1.78421440
H	-0.79056817	-0.13337029	1.86946899
C	1.26880494	2.51251517	1.74968498
H	3.40929912	2.36800002	1.74374827
H	-0.87171014	2.36902499	1.76771511
Au	1.26879800	-2.26212313	1.94460898
N	1.26898833	3.98479692	1.68901021
O	2.34648212	4.53051739	1.65932571
O	0.19131289	4.53135522	1.67358462

75.

Cl	-1.00904268	-2.33659765	0.15536216
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N	3.26986522	-2.33677135	0.14364586
C	3.95906092	-3.48343435	0.18925736
C	3.95881232	-1.18967355	0.10884376
C	5.33700552	-3.51884705	0.20292996
H	3.37274662	-4.39211225	0.21874136
C	5.33685292	-1.15316485	0.11999986
H	3.37236022	-0.28123295	0.07462476
C	6.06671602	-2.33568905	0.16729806
H	5.83797252	-4.47837695	0.24532426
H	5.83768932	-0.19296195	0.09507706
Au	1.22467972	-2.33680735	0.14689366
C	7.55893682	-2.33632225	0.15689236
H	7.95957652	-3.19728505	0.69315276
H	7.92780522	-2.38853645	-0.87194534
H	7.96014422	-1.42639295	0.60424146
Cl	1.21969237	-0.20187521	-3.02936435
N	1.21987928	-4.47883611	-2.89976687
C	0.07236745	-5.16728360	-2.86565230
C	2.36750650	-5.16742247	-2.87755777
C	0.03656584	-6.54406029	-2.80754436
H	-0.83678712	-4.58121396	-2.88267137
C	2.40366936	-6.54430708	-2.81981482
H	3.27656226	-4.58152193	-2.90400572
C	1.22026206	-7.27337956	-2.78374217
H	-0.92380073	-7.04430299	-2.77727659
H	3.36418958	-7.04474396	-2.79952460
Au	1.21974119	-2.43465898	-2.96406390
C	1.21994353	-8.76513055	-2.74487711
H	0.34335681	-9.14870105	-2.22160498
H	1.19846678	-9.16781064	-3.76207164
H	2.11611388	-9.15045306	-2.25757308

76.

Cl	-0.98775387	-2.37549337	-1.13571454
N	3.29457923	-2.37537017	-1.13564354
C	3.99238993	-3.51968167	-1.09556954
C	3.99241493	-1.23103937	-1.17574924
C	5.36344163	-3.56678247	-1.09409614
H	3.41021813	-4.43110637	-1.06350114
C	5.36346483	-1.18398827	-1.17754084
H	3.41023433	-0.31962747	-1.20761274
C	6.09912243	-2.37537577	-1.13603654
H	5.86214013	-4.52753197	-1.06035994
H	5.86215373	-0.22319157	-1.21119694
Au	1.24868513	-2.37540417	-1.13567374
N	7.44897023	-2.37552317	-1.13629794
H	7.96505843	-3.23418207	-1.10738824
H	7.96527943	-1.51700017	-1.16693974
Cl	1.24872540	-4.51706096	2.05502089
N	1.24860439	-0.23665611	1.92652552
C	2.39360301	0.46101220	1.91130712
C	0.10358552	0.46069190	1.89981085
C	2.44072681	1.83144763	1.87020357
H	3.30557949	-0.12075552	1.93350148
C	0.05650185	1.83111233	1.85826791
H	-0.80837202	-0.12136176	1.91277858
C	1.24859820	2.56661100	1.84193092
H	3.40205593	2.33006859	1.86013415
H	-0.90487204	2.32943159	1.83847385
Au	1.24863746	-2.28162885	1.98791893
N	1.24873769	3.91584231	1.80113838
H	2.10787738	4.43179222	1.78878532
H	0.38968189	4.43177229	1.78076079

77.

Cl	-1.00560140	-2.37590470	-1.26075499
N	3.27504830	-2.37941090	-1.26051599
C	3.95882190	-3.52839250	-1.22026339
C	3.97337370	-1.23501510	-1.30062529
C	5.33455590	-3.58097490	-1.21859159
H	3.36986960	-4.43522050	-1.18838009
C	5.34717680	-1.19417270	-1.30220009
H	3.39119860	-0.32384140	-1.33250649
C	6.05403320	-2.39141940	-1.26050699
H	5.83363320	-4.54245700	-1.18483649
H	5.87231390	-0.24924760	-1.33532999
Au	1.22797820	-2.37456080	-1.26074119
O	7.39010400	-2.33758070	-1.26288269
H	7.76149240	-3.22522290	-1.23246509
Cl	1.22918397	-4.52072901	1.91270976
N	1.23269547	-0.24173579	1.79363455
C	2.38235170	0.44200482	1.78292717
C	0.08762725	0.45608694	1.76586619
C	2.43496025	1.81721108	1.74482405
H	3.28971532	-0.14653255	1.80602263

C	0.04675687	1.82934489	1.72716542
H	-0.82408034	-0.12604539	1.77550950
C	1.24469959	2.53616213	1.71591515
H	3.39700886	2.31629111	1.73797136
H	-0.89872377	2.35408657	1.70565883
Au	1.22784098	-2.28801437	1.85055532
O	1.19081569	3.87169017	1.67782561
H	2.07896022	4.24309502	1.67324330

78.

N	3.26019736	-2.36305329	-0.59598258
C	3.94176376	-3.51364829	-0.55566398
C	3.94169756	-1.21248489	-0.63633558
C	5.32191966	-3.55362629	-0.55435518
H	3.34995206	-4.41905009	-0.52385488
C	5.32185376	-1.17238869	-0.63782418
H	3.34984336	-0.30708099	-0.66803128
C	6.02762586	-2.36302339	-0.59616438
H	5.82661406	-4.51007859	-0.52082298
H	5.82650566	-0.21594649	-0.67136888
H	7.11105706	-2.36297569	-0.59628008
Au	1.18606856	-2.36312619	-0.59601188
C	-0.75773934	-2.36317439	-0.59604458
N	-1.91365824	-2.36319709	-0.59604698
N	1.18594887	-0.17665207	2.43862114
C	2.33724876	0.50439543	2.41197424
C	0.03467430	0.50445470	2.41540544
C	2.37724789	1.88362331	2.36137010
H	3.24320825	-0.08706757	2.43232747
C	-0.00544951	1.88368760	2.36493034
H	-0.87128314	-0.08695293	2.43843477
C	1.18591235	2.58892016	2.33727655
H	3.33428675	2.38792833	2.34149769
H	-0.96247874	2.38805380	2.34789296
H	1.18586046	3.67162307	2.29755761
Au	1.18602065	-2.24939576	2.51440958
C	1.18606762	-4.19190574	2.58543161
N	1.18609022	-5.34705218	2.62768333

79.

N	3.26063797	-2.31481753	0.66615382
C	3.94399267	-3.46465443	0.70644062
C	3.94390397	-1.16487143	0.62581742
C	5.32182327	-3.51472153	0.70807272
H	3.35539167	-4.37209503	0.73833922
C	5.32181067	-1.11477753	0.62395102
H	3.35531627	-0.25750743	0.59406992
C	6.00451427	-2.31475373	0.66590092
H	5.84961897	-4.45797383	0.74114962
H	5.84952647	-0.17153663	0.59087342
Au	1.18442387	-2.31484773	0.66611722
C	-0.75846333	-2.31489903	0.66607852
N	-1.91430903	-2.31492413	0.66607822
F	7.32595107	-2.31471533	0.66569512
N	1.18450946	-4.51355740	-2.37394296
C	0.03397988	-5.19658927	-2.35224707
C	2.33515013	-5.19607038	-2.34142267
C	-0.01611253	-6.57334764	-2.29789925
H	-0.87401154	-4.60861875	-2.37980336
C	2.38527863	-6.57288554	-2.28658743
H	3.24305900	-4.60777460	-2.36045858
C	1.18458326	-7.25527996	-2.26524794
H	-0.95993418	-7.10090325	-2.28137489
H	3.32908892	-7.10000916	-2.26120410
Au	1.18448074	-2.43898199	-2.45641632
C	1.18443102	-0.49762846	-2.53359890
N	1.18440595	0.65730575	-2.57949279
F	1.18462981	-8.57568285	-2.21298454

80.

N	3.27044065	-2.33581200	0.12950776
C	3.95116355	-3.48604140	0.17659216
C	3.95044795	-1.18489900	0.09672666
C	5.33049145	-3.52739360	0.19473246
H	3.36161385	-4.39290760	0.20273046
C	5.33003735	-1.14142490	0.11185666
H	3.36035375	-0.27873040	0.05995116
C	6.03056285	-2.33382010	0.16328716
H	5.84239555	-4.47914870	0.24066876
H	5.84119925	-0.18842180	0.09149586
Au	1.19548345	-2.33644350	0.13154046
C	-0.74735675	-2.33669310	0.13960286
N	-1.90308255	-2.33666120	0.14545536
C	7.53827565	-2.33629130	0.14269376
F	7.98823155	-2.40255860	-1.11442594

F	8.03565525	-1.22856490	0.69249736
F	8.03216635	-3.38304810	0.80444946
N	1.19317155	-4.53145027	-2.91033672
C	0.04198451	-5.21149710	-2.87979216
C	2.34450013	-5.21047976	-2.87230112
C	-0.00002508	-6.58906708	-2.80823314
H	-0.86522090	-4.62274834	-2.91159783
C	2.38736998	-6.58830252	-2.80052062
H	3.25141105	-4.62094830	-2.89819297
C	1.19388259	-7.28802685	-2.76644574
H	-0.95283740	-7.10017458	-2.77804171
H	3.34045971	-7.09842571	-2.76432309
Au	1.19246142	-2.45806409	-2.99109053
C	1.19190420	-0.51644889	-3.06053983
N	1.19171288	0.63859058	-3.10079101
C	1.19219615	-8.79536445	-2.72696665
F	1.17368758	-9.29516662	-3.96674761
F	2.27825865	-9.26875740	-2.11615113
F	0.12107880	-9.26407260	-2.08621028

81.

N	3.28676164	-2.33377510	0.25108548
C	3.96401294	-3.48701910	0.29154528
C	3.96404824	-1.18064980	0.21057418
C	5.34411224	-3.53440150	0.29296208
H	3.37227944	-4.39214940	0.32343798
C	5.34415804	-1.13322210	0.20873348
H	3.37234274	-0.27545200	0.17885778
C	6.01954484	-2.33390990	0.25063178
H	5.87950594	-4.47228570	0.32581628
H	5.87956184	-0.19541070	0.17577958
Au	1.21215014	-2.33383650	0.25102568
C	-0.73051126	-2.33391270	0.25096858
N	-1.88613996	-2.33395090	0.25097298
N	7.49554634	-2.33400510	0.24997228
O	8.04046244	-3.41109440	0.28632608
O	8.04064284	-1.25690810	0.21303988
N	1.21230214	-4.49997065	-2.79848775
C	0.05836506	-5.17674111	-2.77223931
C	2.36612212	-5.17714341	-2.78460311
C	0.01096148	-6.55623263	-2.73128532
H	-0.84731331	-4.58512064	-2.78482737
C	2.41358358	-6.55665840	-2.74408611
H	3.27186271	-4.58584057	-2.80694859
C	1.21218089	-7.23156437	-2.71786557
H	-0.92748489	-7.09124354	-2.71044506
H	3.35196014	-7.09197662	-2.73325844
Au	1.21224255	-2.42627427	-2.86010137
C	1.21216808	-0.48446985	-2.91779789
N	1.21212976	0.67065021	-2.95208120
N	1.21210534	-8.70693574	-2.67473554
O	0.13441136	-9.25148386	-2.65425280
O	2.28982422	-9.25193752	-2.66345636

82.

N	3.26112581	-2.33610555	0.33178792
C	3.94890931	-3.48305195	0.37448662
C	3.94869201	-1.18907765	0.29406802
C	5.32687991	-3.51957895	0.38403652
H	3.36243841	-4.39212955	0.40627052
C	5.32669731	-1.15172785	0.30102992
H	3.36208471	-0.27998025	0.26210282
C	6.05543241	-2.33531645	0.34844802
H	5.83026671	-4.47798625	0.42435322
H	5.83002101	-0.19277915	0.27412212
Au	1.18868921	-2.33612655	0.33566302
C	-0.75488899	-2.33604535	0.33865512
N	-1.91081949	-2.33601065	0.33920272
C	7.54755471	-2.33570055	0.34342032
H	7.94571751	-3.19671135	0.88138962
H	7.92135391	-2.38784205	-0.68360858
H	7.94634431	-1.42554455	0.79248582
N	1.18295295	-4.45759475	-2.74362333
C	0.03552448	-5.14480217	-2.70477450
C	2.33039819	-5.14543330	-2.75314342
C	-0.00112752	-6.52239688	-2.67134061
H	-0.87391041	-4.55808848	-2.69607631
C	2.36765193	-6.52309000	-2.72126465
H	3.23985131	-4.55925585	-2.78279152
C	1.18351906	-7.25116824	-2.67748425
H	-0.96000265	-7.02523139	-2.63550509
H	3.32688466	-7.02657069	-2.72586367
Au	1.18287059	-2.38541439	-2.77644127
C	1.18290320	-0.44208783	-2.80785915
N	1.18292621	0.71367119	-2.82777655

C	1.18321043	-8.74314577	-2.65609854
H	0.31477158	-9.13193847	-2.12323985
H	1.14541908	-9.13508081	-3.67697643
H	2.08700729	-9.13369488	-2.18737736

83.

N	3.26942515	-2.32354503	0.52354042
C	3.96679355	-3.46799813	0.56361032
C	3.96684235	-1.17925953	0.48343012
C	5.33718835	-3.51610393	0.56511592
H	3.38479065	-4.38007623	0.59570332
C	5.33717875	-1.13106213	0.48159552
H	3.38480495	-0.26708413	0.45154872
C	6.07245375	-2.32364413	0.52315752
H	5.83639065	-4.47671533	0.59882752
H	5.83641475	-0.17049153	0.44794322
Au	1.19830525	-2.32362853	0.52350502
C	-0.74583835	-2.32369323	0.52346802
N	-1.90210145	-2.32372733	0.52346672
N	7.42084015	-2.32375403	0.52294032
H	7.93738185	-3.18228553	0.55186272
H	7.93757325	-1.46526893	0.49223902
N	1.19844513	-4.49904449	-2.52980923
C	0.05329163	-5.19596883	-2.50488710
C	2.34343249	-5.19611347	-2.50772575
C	0.00516242	-6.56558771	-2.45877804
H	-0.85935003	-4.61425423	-2.52324799
C	2.39166435	-6.56567688	-2.46170468
H	3.25616425	-4.61444304	-2.52841788
C	1.19835902	-7.30049077	-2.43563784
H	-0.95603952	-7.06446366	-2.44068694
H	3.35282351	-7.06466902	-2.44605667
Au	1.19836287	-2.42910466	-2.59971444
C	1.19829946	-0.48606890	-2.66533720
N	1.19826542	0.66953603	-2.70434496
N	1.19825651	-8.64811718	-2.39037212
H	0.33923798	-9.16436784	-2.37303448
H	2.05728874	-9.16461326	-2.37463177

84.

N	3.26351050	-2.33073444	0.34228520
C	3.94644380	-3.47973064	0.38252480
C	3.96116990	-1.18637494	0.30216590
C	5.32189400	-3.53401304	0.38423770
H	3.35780870	-4.38731604	0.41444580
C	5.33449200	-1.14530664	0.30056410
H	3.38011060	-0.27394634	0.27025540
C	6.04094390	-2.34340654	0.34228640
H	5.82047760	-4.49566004	0.41798490
H	5.86140970	-0.20139774	0.26746380
Au	1.18943730	-2.32537504	0.34203590
C	-0.75411830	-2.32607554	0.34200620
N	-1.91013010	-2.32842984	0.34208400
O	7.37541660	-2.28648574	0.33981510
H	7.75273360	-3.17169574	0.37021070
N	1.18412057	-4.52426092	-2.69643509
C	0.03443738	-5.20689083	-2.67511984
C	2.32916601	-5.22109548	-2.66194705
C	-0.01986986	-6.58123398	-2.61994368
H	-0.87369619	-4.61893470	-2.70379925
C	2.37026548	-6.59329002	-2.60630777
H	3.24213837	-4.64030706	-2.68039720
C	1.17145882	-7.29943979	-2.58454754
H	-0.98209463	-7.07962066	-2.60498922
H	3.31474051	-7.11956747	-2.57983347
Au	1.18948567	-2.45188809	-2.78040216
C	1.18878695	-0.50992699	-2.85911334
N	1.18643143	0.64513710	-2.90591324
O	1.22843301	-8.63282593	-2.53070702
H	0.34271827	-9.01005561	-2.52091304

8. Coordinates of the dimeric assemblies subtracted from the CSD

BIQWEF

Ag	-0.34403669	-0.82568806	0.00000000
Cl	1.53696331	-0.82568806	-1.50700000
N	-2.18303669	-0.82568806	1.19200000
C	-3.43003669	-0.82568806	0.41000000
N	-5.92203669	-0.82568806	0.50300000
C	-4.67503669	-0.82568806	1.28500000
H	-5.92603669	-0.09968806	-0.02900000
H	-5.92603669	-1.55168806	-0.02900000
H	-4.66003669	-0.04168806	1.85600000
H	-4.66003669	-1.60968806	1.85600000
H	-2.17903669	-0.09968806	1.72400000
H	-2.17903669	-1.55168806	1.72400000
H	-3.44503669	-0.04168806	-0.16200000
H	-3.44503669	-1.60968806	-0.16200000
Ag	-7.76103669	-0.82568806	1.69500000
Cl	-9.64203669	-0.82568806	3.20200000
Ag	7.70996331	1.85831194	0.00000000
Cl	9.59096331	1.85831194	-1.50700000
N	5.87196331	1.85831194	1.19200000
H	5.87496331	1.13231194	1.72400000
H	5.87496331	2.58331194	1.72400000
C	4.62496331	1.85831194	0.41000000
H	4.60996331	1.07431194	-0.16200000
H	4.60996331	2.64131194	-0.16200000
N	2.13196331	1.85831194	0.50300000
H	2.12896331	1.13231194	-0.02900000
H	2.12896331	2.58331194	-0.02900000
C	3.37896331	1.85831194	1.28500000
H	3.39396331	1.07431194	1.85600000
H	3.39396331	2.64131194	1.85600000
Ag	0.29396331	1.85831194	1.69500000
Cl	-1.58703669	1.85831194	3.20200000

YUXVUJ

Ag	-1.37614678	0.18348624	0.00000000
Cl	-3.05714678	1.77348624	-0.52300000
N	0.33485322	-0.97551376	0.64400000
H	0.12385322	-1.41351376	1.43200000
H	0.53485322	-1.54251376	0.01900000
C	2.66885322	-0.93951376	1.56400000
C	3.65185322	-1.59051376	0.83300000
H	3.62585322	-1.56151376	-0.11600000
C	4.67285322	-2.28451376	1.47100000
H	5.34385322	-2.71951376	0.95800000
C	4.71085322	-2.33951376	2.85900000
H	5.40385322	-2.81751376	3.29800000
C	3.73985322	-1.70051376	3.59300000
H	3.76485322	-1.73451376	4.54200000
C	2.71685322	-1.00351376	2.95400000
H	2.04985322	-0.56851376	3.47000000
C	1.56285322	-0.16851376	0.90000000
H	1.32585322	0.60348624	1.47100000
H	1.89685322	0.18648624	0.03800000
Ag	-2.23214678	0.18348624	2.99600000
Cl	-0.55014678	1.77348624	3.51900000
N	-3.94214678	-0.97551376	2.35200000
H	-3.73214678	-1.41351376	1.56400000
H	-4.14314678	-1.54251376	2.97700000
C	-6.27614678	-0.93951376	1.43200000
C	-7.26014678	-1.59051376	2.16300000
H	-7.23414678	-1.56151376	3.11200000
C	-8.28114678	-2.28451376	1.52500000
H	-8.95214678	-2.71951376	2.03800000
C	-8.31914678	-2.33951376	0.13700000
H	-9.01214678	-2.81751376	-0.30200000
C	-7.34714678	-1.70051376	-0.59800000
H	-7.37314678	-1.73451376	-1.54600000
C	-6.32514678	-1.00351376	0.04100000
H	-5.65814678	-0.56851376	-0.47400000
C	-5.17114678	-0.16851376	2.09600000
H	-4.93414678	0.60348624	1.52500000
H	-5.50514678	0.18648624	2.95800000

UJOQAN

N	-3.38272903	1.76716513	0.09723382
C	-3.02172903	3.04316513	0.04423382
H	-2.09872903	3.26116513	0.01323382
C	-4.69672903	1.45416513	0.14823382
H	-4.95572903	0.54016513	0.18323382
C	-5.28472903	3.75616513	0.10223382
H	-5.93472903	4.44916513	0.11623382

C	-5.66472903	2.43116513	0.15223382
H	-6.58472903	2.19416513	0.18723382
C	-3.94772903	4.05016513	0.03523382
H	-3.66172903	4.95516513	-0.01776618
N	-0.55472903	-1.10883487	-0.09876618
C	-0.84672903	-2.42783487	-0.10476618
H	-1.75172903	-2.69983487	-0.02276618
C	0.12627097	-3.38083487	-0.22576618
H	-0.10572903	-4.30283487	-0.22676618
C	0.72527097	-0.75083487	-0.22576618
H	0.94527097	0.17216513	-0.22376618
C	1.43627097	-2.99583487	-0.34376618
H	2.12727097	-3.64483487	-0.41376618
C	1.73127097	-1.66883487	-0.36076618
H	2.63127097	-1.37883487	-0.46676618
Au	-2.39272903	0.29816513	-2.97476618
N	-1.00472903	1.76716513	-3.01976618
C	-1.36572903	3.04316513	-2.96576618
H	-2.28872903	3.26116513	-2.93476618
C	0.30927097	1.45416513	-3.07076618
H	0.56827097	0.54016513	-3.10476618
C	0.89727097	3.75616513	-3.02476618
H	1.54727097	4.44916513	-3.03776618
C	1.27727097	2.43116513	-3.07376618
H	2.19727097	2.19416513	-3.10876618
C	-0.43972903	4.05016513	-2.95676618
H	-0.72572903	4.95516513	-2.90376618
N	-3.83272903	-1.10883487	-2.82276618
C	-3.54072903	-2.42783487	-2.81676618
H	-2.63572903	-2.69983487	-2.89876618
C	-4.51372903	-3.38083487	-2.69576618
H	-4.28172903	-4.30283487	-2.69476618
C	-5.11272903	-0.75083487	-2.69576618
H	-5.33272903	0.17216513	-2.69876618
C	-5.82372903	-2.99583487	-2.57776618
H	-6.51472903	-3.64483487	-2.50876618
C	-6.11872903	-1.66883487	-2.56076618
H	-7.01872903	-1.37883487	-2.45476618
Au	-1.99472903	0.29816513	0.05223382
F	-9.45572903	2.89216513	2.92223382
F	-8.36972903	3.89116513	1.21423382
F	-8.83572903	1.71616513	1.13723382
F	-10.49572903	3.26116513	0.99923382
B	-9.28672903	2.93516513	1.55223382
F	0.45127097	7.34516513	-3.29176618
F	1.53727097	6.34616513	-4.99876618
F	1.07127097	8.52116513	-5.07576618
F	-0.58872903	6.97516513	-5.21376618
B	0.62027097	7.30116513	-4.66076618

FAZGET

C	-3.08205854	-0.12467756	3.20600000
C	-1.75005854	-0.12467756	2.53000000
C	-0.56605854	-0.12467756	3.46600000
H	-0.37605854	0.77532244	3.73600000
H	0.19694146	-0.49167756	3.01100000
H	-0.76805854	-0.65767756	4.23500000
C	-5.23005854	-0.12467756	3.45800000
C	-6.66405854	-0.12467756	3.25000000
C	-7.59705854	-0.12467756	4.24800000
N	-3.25805854	-0.12467756	4.50400000
N	-4.61905854	-0.12467756	4.60100000
H	-5.03405854	-0.12467756	5.35400000
N	-4.28905854	-0.12467756	2.53800000
N	-4.38205854	-0.12467756	1.14200000
H	-5.15405854	-0.12467756	0.76200000
H	-3.66705854	-0.12467756	0.66200000
H	-1.69205854	-0.90667756	1.95800000
H	-1.69205854	0.65732244	1.95800000
H	-6.85505854	-0.90167756	2.70200000
H	-6.85505854	0.65232244	2.70200000
H	-8.45105854	-0.37767756	3.88900000
H	-7.33905854	-0.75167756	4.93000000
H	-7.66005854	0.75432244	4.63100000
Au	1.43594146	-0.12467756	0.00000000
Au	1.43594146	3.12232244	0.00000000
C	3.17094146	-0.12467756	0.90400000
C	-0.15305854	3.12232244	1.14500000
N	4.16994146	-0.12467756	1.41400000
N	-1.10005854	3.12232244	1.82200000
C	-0.30005854	-0.12467756	-0.90400000
C	3.02394146	3.12232244	-1.14500000
N	-1.29905854	-0.12467756	-1.41400000
N	3.97094146	3.12232244	-1.82200000
C	-3.98405854	3.12132244	-3.20600000

C	-5.31705854	3.12232244	-2.53000000
H	-5.37505854	3.90432244	-1.95800000
H	-5.37505854	2.33932244	-1.95800000
C	-6.50005854	3.12132244	-3.46600000
H	-6.69105854	4.02132244	-3.73600000
H	-7.26405854	2.75532244	-3.01100000
H	-6.29905854	2.58832244	-4.23500000
C	-1.83705854	3.12132244	-3.45800000
C	-0.40205854	3.12132244	-3.25000000
H	-0.21105854	3.89832244	-2.70200000
H	-0.21105854	2.34532244	-2.70200000
C	0.53094146	3.12132244	-4.24800000
N	-3.80905854	3.12132244	-4.50400000
N	-2.44705854	3.12132244	-4.60100000
H	-2.03205854	3.12132244	-5.35400000
N	-2.77805854	3.12232244	-2.53800000
N	-2.68505854	3.12232244	-1.14200000
H	-1.91205854	3.12232244	-0.76200000
H	-3.39905854	3.12232244	-0.66200000
H	1.38494146	2.86932244	-3.88900000
H	0.27294146	2.49532244	-4.93000000
H	0.59294146	4.00132244	-4.63100000