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The nature of Au—N bond in gold(III) complexes with aromatic nitrogen-containing heterocycles. The influence of Au(III) ion on the ligand aromaticity

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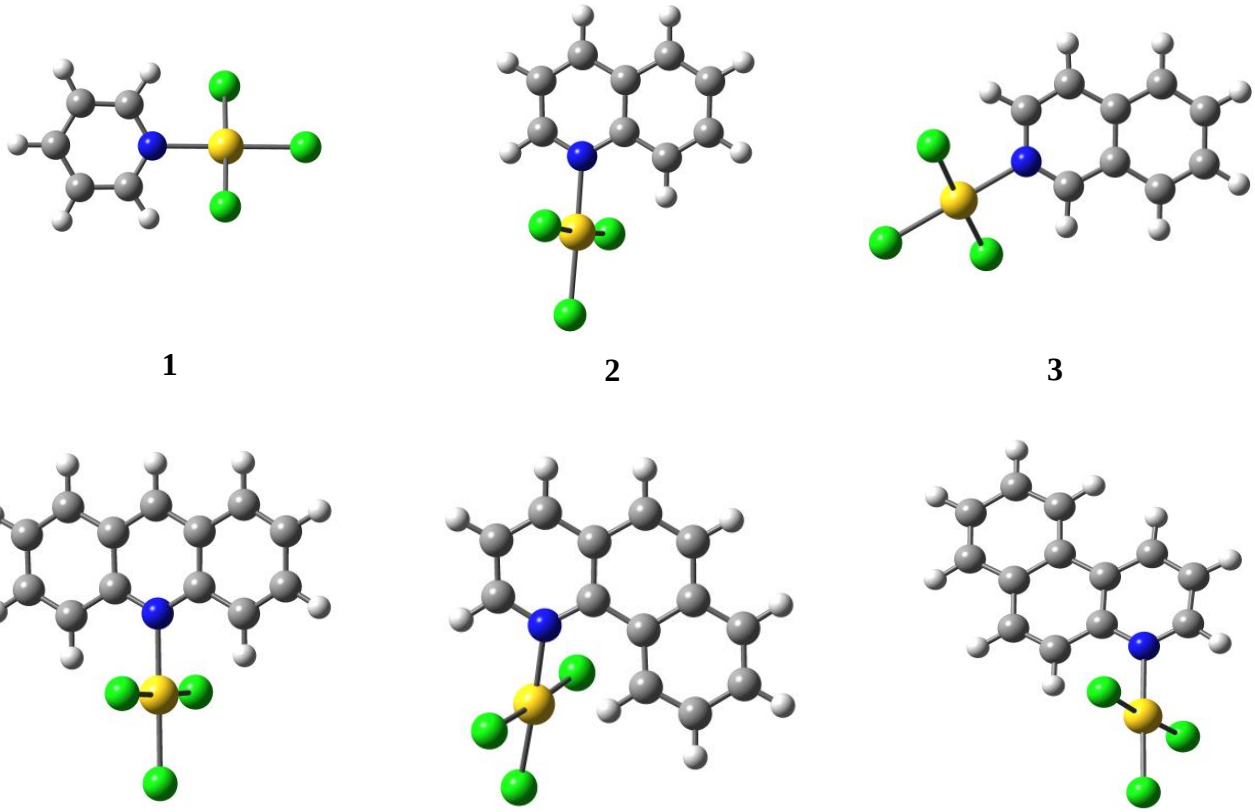
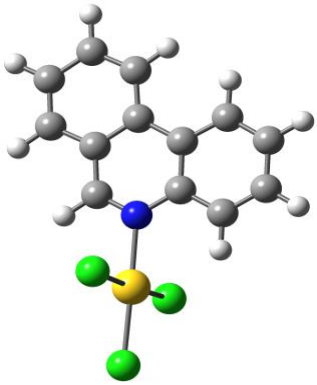


1 **2** **3**

4 **5** **6**

Fig. S1 Optimized geometries of the studied gold(III) complexes obtained at the B3LYP/cc-pVTZ+LanL2TZ(f) level of theory.



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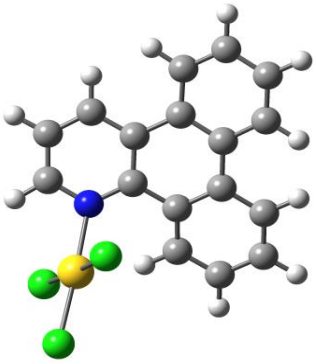

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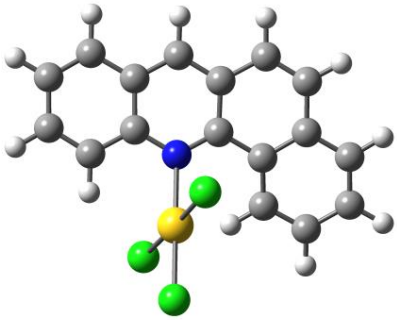

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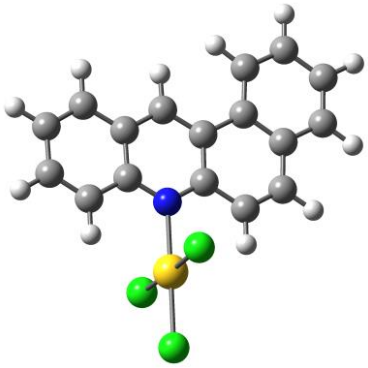

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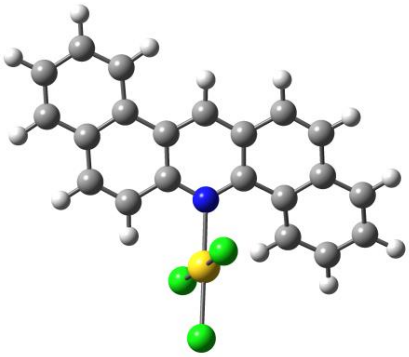

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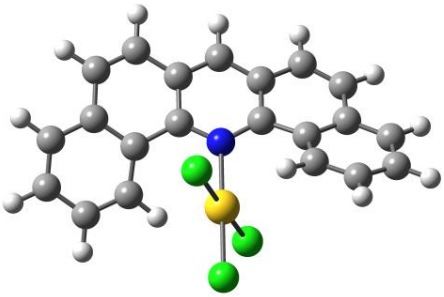

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Fig. S1 Continued.

Table S1 Results of the NBO, AIM, EDA and CDA methods obtained for the experimental X-ray structure of **1**.

NBO		AIM			EDA		CDA	
atom	charge (a.u.)	bond	$\rho(r_c)$ (a.u.)	$\nabla^2\rho(r_c)$ (a.u.)		(kcal/mol)		(a.u.)
Au	0.5518	Au-N	0.1387	0.4278	ΔE_{int}	-45.23	*d*	0.1024
N	-0.4378	Au-Cl1	0.1075	0.1817	ΔE_{es}	-123.71	*b*	0.0342
Cl1	-0.3128	Au-Cl2	0.1144	0.1715	ΔE_{Pauli}	175.5	*d-b*	0.0682
Cl2	-0.2547	N-C1	0.3022	-0.8184	ΔE_{pol}	-83.02	*r*	-0.4369
C1	0.0881	C1-C2	0.3217	-1.0651	ΔE_{disp}	-14.01		
C2	-0.2275	C2-C3	0.3208	-1.0654				
C3	-0.1269							

Table S2 Cartesian coordinates of the optimized geometries of the studied ligands and their gold(III) complexes obtained at the B3LYP/cc-pVTZ+LanL2TZ(f) level of theory.

L1			
C	1.13904	0.71949	0.00000
C	1.19341	-0.66977	0.00000
C	0.00000	-1.37903	0.00000
C	-1.19341	-0.66977	0.00000
C	-1.13904	0.71949	0.00000
N	0.00000	1.41272	0.00000
H	0.00000	-2.46106	0.00000
H	2.05342	1.30256	0.00000
H	2.14805	-1.17781	0.00000
H	-2.14805	-1.17781	0.00000
H	-2.05342	1.30256	0.00000
L2			
C	2.41363	0.65058	0.00000
C	1.26143	1.38820	0.00000
C	0.01424	0.72437	0.00000
C	0.02854	-0.70231	0.00000
C	2.31836	-0.75899	0.00000
H	-1.23466	2.48492	0.00000
H	3.38611	1.12322	0.00000
H	1.28982	2.47091	0.00000
C	-1.22794	1.40197	0.00000
C	-1.20254	-1.39959	0.00000
H	3.22513	-1.35562	0.00000
C	-2.38921	-0.71428	0.00000
C	-2.40348	0.69795	0.00000
H	-1.16716	-2.48003	0.00000
H	-3.32622	-1.25516	0.00000
H	-3.34967	1.22227	0.00000
N	1.18550	-1.41969	0.00000
L3			
C	-2.41186	0.61571	0.00000
C	-1.26884	1.37012	0.00000
C	-0.01016	0.72649	0.00000
C	-0.00859	-0.69622	0.00000
H	1.23513	2.49241	0.00000
H	-3.38586	1.08973	0.00000
H	-1.32703	2.45089	0.00000
C	1.22942	1.40993	0.00000
C	1.22120	-1.39346	0.00000

C	2.40593	-0.70501	0.00000
C	2.40682	0.70770	0.00000
H	1.21150	-2.47620	0.00000
H	3.34655	-1.23901	0.00000
H	3.35062	1.23680	0.00000
N	-2.42145	-0.74176	0.00000
C	-1.26335	-1.35533	0.00000
H	-1.28417	-2.44184	0.00000
L4			
C	3.57408	-0.76588	0.00000
C	2.37797	-1.42041	0.00000
C	1.15145	-0.69418	0.00000
C	1.20713	0.74492	0.00000
C	2.47774	1.38819	0.00000
C	3.62704	0.65492	0.00000
C	0.00000	1.43816	0.00000
C	-1.20713	0.74492	0.00000
C	-1.15145	-0.69418	0.00000
C	-2.37797	-1.42041	0.00000
H	-2.31750	-2.49971	0.00000
C	-3.57408	-0.76588	0.00000
C	-3.62704	0.65492	0.00000
C	-2.47774	1.38819	0.00000
H	4.49819	-1.32868	0.00000
H	2.31750	-2.49971	0.00000
H	2.51286	2.47054	0.00000
H	4.58854	1.15045	0.00000
H	0.00000	2.52228	0.00000
H	-4.49819	-1.32868	0.00000
H	-4.58854	1.15045	0.00000
H	-2.51286	2.47054	0.00000
N	0.00000	-1.37530	0.00000
L5			
C	3.48459	-0.38259	0.00000
C	2.84049	0.83086	0.00000
C	1.43506	0.87098	0.00000
C	0.73987	-0.36565	0.00000
H	1.25130	3.03031	0.00000
H	4.56356	-0.44990	0.00000
H	3.39933	1.75863	0.00000
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C	-0.70881	-0.36569	0.00000
C	-1.39847	0.87379	0.00000
C	-0.65422	2.09705	0.00000

H	-1.20157	3.03123	0.00000
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C	-2.82564	-1.53475	0.00000
H	-3.38285	-2.46212	0.00000
C	-2.80792	0.87240	0.00000
C	-3.51118	-0.30989	0.00000
H	-4.59302	-0.29721	0.00000
H	-0.90907	-2.49668	0.00000
H	-3.33168	1.82005	0.00000
N	1.38761	-1.55006	0.00000
C	2.70543	-1.54977	0.00000
H	3.18727	-2.52204	0.00000
L6			
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C	1.50681	-1.56873	0.00000
C	0.73049	-0.39596	0.00000
C	1.43780	0.83564	0.00000
H	3.49376	-2.37267	0.00000
H	1.03339	-2.53999	0.00000
C	-0.71997	-0.38615	0.00000
C	0.71344	2.06876	0.00000
C	-0.63989	2.07820	0.00000
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H	-1.18051	3.01640	0.00000
C	-2.80523	0.88862	0.00000
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C	-3.53606	-0.27586	0.00000
H	-4.61716	-0.24177	0.00000
C	-2.87259	-1.51107	0.00000
H	-3.44398	-2.42961	0.00000
H	-1.01256	-2.52779	0.00000
H	-3.30674	1.84818	0.00000
N	2.78971	0.90961	0.00000
C	3.47540	-0.21425	0.00000
H	4.55655	-0.12172	0.00000
L7			
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C	0.72038	-0.39605	0.00007
C	-0.72638	-0.40332	-0.00001
C	-1.38560	0.84855	-0.00015
H	-1.04694	-2.54198	0.00015
C	-1.51709	-1.56933	0.00005
C	-2.79121	0.90999	-0.00023

C	-3.53949	-0.24327	-0.00018
C	-2.89205	-1.48901	-0.00004
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H	-3.48076	-2.39679	0.00000
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H	-1.10180	2.99857	-0.00031
C	1.51030	-1.56235	0.00021
C	2.78575	0.91169	0.00008
C	3.53038	-0.24387	0.00022
H	4.61103	-0.19519	0.00027
C	2.88534	-1.48994	0.00029
H	3.47126	-2.39933	0.00039
H	1.03574	-2.53337	0.00027
H	3.24983	1.88807	0.00003
	L8		
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C	0.27009	1.42230	0.00028
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C	-1.34375	-0.47129	-0.00054
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C	1.10295	-0.92287	0.00034
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C	2.71472	0.89534	-0.00051
C	3.49588	-1.37054	-0.00045
H	4.30893	-2.08399	-0.00075
C	3.76146	-0.00009	-0.00076
H	4.78155	0.35954	-0.00133
H	2.94127	1.95071	-0.00103
H	2.01298	-2.87860	-0.00002
N	-2.11981	1.79684	-0.00087
C	-1.90651	3.09817	-0.00025
H	-2.78641	3.73284	-0.00064
C	-0.60237	-2.77075	0.00132
C	-2.67218	-0.92891	-0.00115
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H	-3.98460	-2.61439	-0.00109
H	0.18199	-3.51173	0.00251
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	L9		
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C	-0.29612	-0.00885	0.00000
C	0.07012	1.38055	0.00000
C	-0.95630	2.38402	0.00000
C	-2.26364	2.04455	0.00000
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C	1.91434	-0.67154	0.00000
C	2.86987	-1.72283	0.00000
H	2.49931	-2.73833	0.00000
C	4.20831	-1.44557	0.00000
C	4.67079	-0.10559	0.00000
C	3.78129	0.93152	0.00000
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C	-4.04575	0.32362	0.00000
C	-4.43953	-0.99730	0.00000
H	-5.49172	-1.24915	0.00000
C	-3.47644	-2.01405	0.00000
H	-3.78753	-3.05020	0.00000
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H	-3.48002	-1.81204	0.00000
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N	1.10338	-1.82833	0.00000
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C	1.66557	3.72571	0.00000
C	-0.70995	4.05961	0.00000
H	-1.56163	4.72655	0.00000
H	-1.92353	2.32031	0.00000
H	2.67454	4.11832	0.00000
C	0.58729	4.58308	0.00000
H	0.74090	5.65369	0.00000
L11			
C	-3.64417	0.85128	-0.00002
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C	-1.36458	-0.11439	0.00015
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C	-1.71540	2.33326	0.00014
C	-3.05702	2.16148	0.00006
C	0.55687	1.34963	0.00015
C	1.39155	0.23699	0.00014
C	0.74979	-1.04109	0.00019
C	1.55129	-2.23000	0.00020
H	1.02902	-3.17624	0.00027
C	2.90085	-2.15922	0.00010
C	3.58914	-0.90020	-0.00001
C	2.84457	0.30776	0.00003
H	-1.28718	3.32790	0.00018
H	-3.71805	3.01891	0.00004
H	0.96875	2.34968	0.00012
H	3.49535	-3.06429	0.00009
N	-0.57970	-1.19061	0.00019
C	3.55287	1.52340	-0.00007
C	4.99538	-0.84863	-0.00017
C	5.66203	0.35573	-0.00029
H	6.74334	0.38111	-0.00042
C	4.93138	1.55022	-0.00023
H	5.44954	2.49981	-0.00031
H	3.01625	2.46107	-0.00002
H	5.54935	-1.77889	-0.00020
C	-3.39310	-1.56919	-0.00003

C	-5.04069	0.67661	-0.00016
C	-4.76389	-1.71424	-0.00018
H	-5.20155	-2.70362	-0.00024
H	-2.74116	-2.42992	0.00002
H	-5.67753	1.55226	-0.00021
C	-5.59412	-0.58480	-0.00025
H	-6.66937	-0.70474	-0.00037
	L12		
C	0.00000	3.63252	-0.25093
C	0.00000	2.40193	0.45241
C	0.00000	1.15587	-0.29794
C	0.00000	1.20853	-1.72530
C	0.00000	2.47752	-2.39052
C	0.00000	3.63195	-1.68630
C	0.00000	0.00000	-2.41369
C	0.00000	-1.20853	-1.72530
C	0.00000	-1.15587	-0.29794
C	0.00000	-2.40193	0.45241
C	0.00000	-3.63252	-0.25093
C	0.00000	-3.63195	-1.68630
C	0.00000	-2.47752	-2.39052
H	0.00000	2.49153	-3.47324
H	0.00000	4.58547	-2.19906
H	0.00000	0.00000	-3.49769
H	0.00000	-4.58547	-2.19906
H	0.00000	-2.49153	-3.47324
N	0.00000	0.00000	0.36817
C	0.00000	2.41930	1.85704
C	0.00000	4.83711	0.47718
C	0.00000	4.83013	1.85430
H	0.00000	5.76343	2.40150
H	0.00000	1.47536	2.38068
H	0.00000	5.77492	-0.06393
C	0.00000	-2.41930	1.85704
C	0.00000	-4.83711	0.47718
C	0.00000	-4.83013	1.85430
H	0.00000	-5.76343	2.40150
H	0.00000	-1.47536	2.38068
H	0.00000	-5.77492	-0.06393
C	0.00000	3.61197	2.54769
C	0.00000	-3.61197	2.54769
H	0.00000	-3.60880	3.62954
H	0.00000	3.60880	3.62954
	1		
C	-3.51972	0.93092	0.74880
C	-3.51973	-0.93091	-0.74878

C	-2.13708	0.91108	0.72019
N	-1.46504	0.00001	-0.00001
C	-2.13710	-0.91106	-0.72020
H	-4.02394	1.67401	1.34835
H	-1.54405	1.63337	1.25755
H	-4.02397	-1.67400	-1.34831
H	-1.54407	-1.63336	-1.25757
Au	0.63159	0.00000	0.00000
Cl	0.60534	-2.29910	0.31802
Cl	0.60538	2.29910	-0.31805
Cl	2.90904	-0.00001	0.00003
C	-4.22528	0.00001	0.00002
H	-5.30648	0.00000	0.00003
	2		
C	-2.36192	2.40125	0.92853
C	-3.27169	0.33197	0.10610
C	-1.08167	1.87121	0.72946
N	-0.88265	0.65487	0.25482
C	-1.94242	-0.15189	-0.07109
H	-2.46085	3.40191	1.32096
H	-0.20201	2.45345	0.95983
Au	1.09989	0.03380	0.02151
Cl	0.96573	-0.97917	2.10629
Cl	1.11879	1.09562	-2.04261
Cl	3.27468	-0.60482	-0.21876
C	-3.45128	1.63304	0.61680
H	-4.45533	2.01187	0.75673
C	-4.35795	-0.50750	-0.23582
C	-1.74095	-1.45064	-0.57940
C	-2.81832	-2.23485	-0.89928
H	-2.65331	-3.22995	-1.28822
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H	-4.97010	-2.40241	-0.98798
H	-0.73508	-1.82022	-0.71047
H	-5.36427	-0.13437	-0.09951
	3		
C	-2.92351	-0.41916	-0.29197
C	-2.49424	1.61205	0.95696
C	-1.52843	-0.58720	-0.36311
N	-0.68526	0.27947	0.16737
C	-1.15781	1.37999	0.82445
H	-1.10301	-1.45416	-0.84594
H	-2.82785	2.49027	1.49139
H	-0.41338	2.05458	1.21267
Au	1.37920	-0.02896	0.00383
Cl	1.62473	2.17454	-0.67878

Cl	1.07609	-2.22885	0.67928
Cl	3.62683	-0.36153	-0.17887
C	-3.43319	0.71834	0.39418
C	-4.83239	0.89564	0.47466
C	-5.67423	-0.01903	-0.10446
C	-5.16583	-1.14835	-0.78433
H	-5.85179	-1.85508	-1.23017
H	-5.22754	1.75805	0.99444
H	-6.74487	0.12208	-0.04186
C	-3.81471	-1.34940	-0.87783
H	-3.41561	-2.21250	-1.39355
	4		
C	-2.89877	1.20902	0.00611
C	-2.89905	-1.20851	-0.00562
C	-1.46359	1.18146	0.00681
N	-0.80242	0.00000	0.00049
C	-1.46387	-1.18129	-0.00600
Au	1.29621	-0.00012	-0.00002
Cl	1.24038	-0.03898	2.32184
Cl	3.58082	0.00009	-0.00067
Cl	1.23914	0.03849	-2.32178
C	-3.58286	0.00034	0.00022
H	-4.66609	0.00046	0.00008
C	-3.57378	-2.46121	-0.01160
C	-0.76846	-2.41728	-0.01329
C	-1.45547	-3.59718	-0.01913
H	-0.90505	-4.52783	-0.02454
C	-2.87232	-3.62811	-0.01808
H	-3.38696	-4.57854	-0.02255
H	0.31075	-2.41926	-0.01388
H	-4.65571	-2.46097	-0.01088
C	-0.76791	2.41730	0.01400
C	-3.57321	2.46188	0.01145
C	-2.87148	3.62862	0.01756
H	-3.38590	4.57917	0.02133
C	-1.45464	3.59737	0.01911
H	-0.90400	4.52788	0.02430
H	0.31131	2.41905	0.01503
H	-4.65513	2.46189	0.01042
	5		
C	-1.02504	3.47369	-0.23237
C	-2.66486	1.73452	0.03216
C	-0.06138	2.47893	-0.33329
N	-0.35618	1.18029	-0.27799
C	-1.65305	0.75760	-0.18464
Au	1.37187	0.02243	0.08514

Cl	0.68764	-0.17776	2.29467
Cl	3.28588	-1.13388	0.53071
Cl	2.00547	0.32833	-2.13405
C	-2.32466	3.09378	-0.00532
H	-3.10022	3.83299	0.14653
C	-4.00529	1.32620	0.30948
C	-2.03523	-0.63515	-0.29972
C	-3.37383	-0.99250	0.03054
C	-4.33159	0.01639	0.35548
H	-5.33979	-0.29121	0.59943
H	-4.74314	2.09338	0.50184
H	-0.72867	4.51004	-0.28762
H	0.98232	2.73028	-0.44141
C	-3.76520	-2.34360	-0.02125
C	-1.18519	-1.64981	-0.78125
C	-1.59939	-2.96091	-0.84357
H	-0.92142	-3.71364	-1.22076
C	-2.89004	-3.31909	-0.43562
H	-3.20351	-4.35333	-0.47315
H	-4.77969	-2.59886	0.25542
H	-0.20443	-1.40797	-1.15654
	6		
C	-1.17324	2.90714	0.70632
C	-2.44411	0.91732	0.20716
C	-0.00601	2.17496	0.52724
N	-0.03096	0.88598	0.21358
C	-1.21277	0.22587	0.04333
Au	1.82749	-0.05416	0.00331
Cl	1.56696	-0.93811	2.13535
Cl	3.87397	-1.03620	-0.21554
Cl	1.99705	0.90223	-2.10535
C	-2.38516	2.27668	0.54643
H	-3.29459	2.84176	0.68292
C	-3.69113	0.20006	0.01733
C	-1.20934	-1.15498	-0.30252
C	-2.37706	-1.81705	-0.47904
C	-3.64310	-1.17491	-0.32752
H	-1.10913	3.95328	0.96427
H	0.96547	2.63310	0.63208
H	-2.36210	-2.86660	-0.74179
H	-0.26572	-1.66600	-0.41498
C	-4.84205	-1.88955	-0.51678
C	-4.95402	0.80702	0.15911
C	-6.06047	-1.27059	-0.37171
H	-6.97593	-1.82679	-0.51895
C	-6.11308	0.08837	-0.03119

H	-7.07064	0.57760	0.08349
H	-5.03152	1.85162	0.42127
H	-4.78729	-2.93784	-0.77958
	7		
C	2.54660	-1.31393	0.06843
C	2.58515	1.13113	-0.05943
C	1.13224	-1.22582	0.05812
N	0.48410	-0.09635	-0.00100
C	1.16671	1.11275	-0.06464
H	0.54502	-2.13276	0.09959
Au	-1.60429	-0.20186	0.01011
Cl	-1.54716	0.09692	2.31188
Cl	-1.53676	-0.52064	-2.28835
Cl	-3.87799	-0.37154	0.02838
C	3.30408	-0.12062	0.01081
C	4.70676	-0.23286	0.02424
C	5.31158	-1.46851	0.09104
C	4.55091	-2.64791	0.14729
H	5.04499	-3.60776	0.19917
H	5.32412	0.65138	-0.01787
H	6.39134	-1.53146	0.10014
C	3.18065	-2.57079	0.13604
H	2.57460	-3.46605	0.17862
C	3.22592	2.38295	-0.12551
C	0.44470	2.31396	-0.13620
C	1.10485	3.51732	-0.20087
H	0.53915	4.43657	-0.25581
C	2.50514	3.55192	-0.19469
H	3.02171	4.50037	-0.24492
H	4.30432	2.43006	-0.12269
H	-0.63448	2.28308	-0.13812
	8		
C	-0.71772	-3.28285	-0.66093
C	-2.19095	-1.39410	-0.35623
C	0.35418	-2.41039	-0.60180
N	0.18401	-1.09349	-0.47374
C	-1.06424	-0.54409	-0.46153
Au	1.94797	-0.13080	0.18544
Cl	0.96124	0.09861	2.27396
Cl	3.87691	0.80870	0.95699
Cl	2.89052	-0.46420	-1.91884
C	-1.98478	-2.77246	-0.48801
H	-2.82175	-3.45206	-0.45568

C	-3.50309	-0.82380	-0.06544
C	-1.25426	0.89137	-0.58433
C	-2.51818	1.44638	-0.26962
C	-3.64090	0.57579	0.06959
H	-0.54242	-4.34071	-0.78389
H	1.37260	-2.76435	-0.64062
C	-4.88599	1.08985	0.47351
C	-4.62435	-1.64296	0.15813
C	-5.96721	0.26715	0.70180
H	-6.91143	0.69215	1.01361
C	-5.83962	-1.11216	0.53037
H	-6.68408	-1.76504	0.70257
H	-4.54435	-2.71455	0.05953
H	-5.00821	2.15192	0.61653
C	-2.67207	2.83973	-0.36640
C	-0.24821	1.73048	-1.09627
C	-1.64728	3.65289	-0.80086
H	-1.80033	4.72144	-0.86674
C	-0.43378	3.09123	-1.19735
H	0.35528	3.71237	-1.59697
H	-3.62042	3.29349	-0.12596
H	0.67052	1.30763	-1.46939
9			
C	1.34397	2.68169	0.12622
C	-1.01629	3.14950	-0.10333
C	1.08822	1.30662	-0.19556
N	-0.18820	0.87538	-0.29018
C	-1.23972	1.75196	-0.29352
Au	-0.69970	-1.13997	0.15491
Cl	-1.25399	-1.57066	-2.07745
Cl	-1.25829	-3.27885	0.73194
Cl	-0.19060	-0.64742	2.36515
C	0.28663	3.56994	0.15405
H	0.47327	4.60995	0.39234
C	-2.11500	4.04709	-0.11261
C	-2.57166	1.30856	-0.47443
C	-3.60697	2.20435	-0.48238
H	-4.61366	1.84199	-0.63847
C	-3.38599	3.58726	-0.29928
H	-4.22257	4.27174	-0.30720
H	-2.76894	0.26254	-0.64506
H	-1.91932	5.10089	0.03570
C	2.23438	0.42891	-0.38894
C	2.66961	3.10607	0.47171
C	3.69454	2.23265	0.48353
H	4.68479	2.54538	0.78688

C	3.51603	0.88602	0.02487
H	2.81143	4.14072	0.75369
C	2.15849	-0.81785	-1.03619
C	4.62551	0.03271	-0.09182
C	3.26816	-1.62664	-1.16516
C	4.50484	-1.21613	-0.66059
H	1.23780	-1.13820	-1.49451
H	3.17438	-2.57751	-1.67069
H	5.36851	-1.86137	-0.74629
H	5.58843	0.38498	0.25406
	10		
C	2.46724	0.55583	0.00023
C	1.21510	2.63338	-0.00010
C	1.21381	-0.14373	0.00043
N	0.04542	0.52670	0.00039
C	-0.00030	1.88556	0.00018
Au	-1.76775	-0.53698	-0.00002
Cl	-1.71959	-0.50950	2.32227
Cl	-3.74361	-1.68483	-0.00068
Cl	-1.71781	-0.51005	-2.32227
C	2.42469	1.93682	-0.00008
H	3.33863	2.51312	-0.00038
C	1.16085	4.05135	-0.00041
C	-1.22830	2.58807	0.00022
C	-1.24053	3.95594	-0.00008
H	-2.18871	4.47544	-0.00005
C	-0.03925	4.70099	-0.00042
H	-0.07816	5.78119	-0.00066
H	-2.15759	2.03928	0.00051
H	2.09169	4.60300	-0.00064
C	1.21785	-1.57304	0.00061
C	3.71395	-0.20055	0.00021
C	3.65672	-1.61446	0.00021
C	2.38034	-2.26206	0.00045
H	2.35630	-3.34402	0.00053
H	0.27669	-2.10025	0.00087
C	4.84565	-2.36472	0.00004
C	4.97916	0.41101	0.00018
C	6.13503	-0.34231	0.00004
H	7.09574	0.15422	0.00002
C	6.07248	-1.74008	-0.00007
H	5.06697	1.48731	0.00031
H	4.78051	-3.44492	0.00000
H	6.98256	-2.32381	-0.00022
	11		
C	-3.20403	-1.77228	-0.38227

C	-1.90116	-1.40496	-0.39489
C	-1.52366	-0.03474	-0.24999
C	-2.54760	0.94106	-0.06620
C	-3.94586	0.54335	-0.08267
C	-4.26466	-0.82782	-0.23061
C	-2.13523	2.23716	0.19848
C	-0.79686	2.60218	0.15624
C	0.17829	1.61881	-0.18083
C	1.54783	2.05595	-0.39681
C	1.90626	3.37505	0.00118
C	0.90854	4.28593	0.47384
C	-0.39285	3.93365	0.49234
H	-3.46052	-2.81630	-0.50639
H	-1.13871	-2.15016	-0.55073
H	-2.85718	2.99801	0.45776
H	1.21637	5.28086	0.76665
H	-1.15929	4.63779	0.78738
C	2.52445	1.27995	-1.04937
C	3.81729	1.73393	-1.19960
C	4.18858	2.99158	-0.71383
C	3.23757	3.80414	-0.13995
H	2.26068	0.33654	-1.49709
H	4.54051	1.11224	-1.70857
H	5.20849	3.33565	-0.81838
H	3.49769	4.80038	0.19304
C	-5.00360	1.46297	0.03603
C	-6.31619	1.04201	0.02429
C	-6.62600	-0.31744	-0.11019
C	-5.61096	-1.23704	-0.23879
H	-4.80047	2.51969	0.12763
H	-7.11167	1.76886	0.11623
H	-7.65827	-0.63925	-0.11784
H	-5.83523	-2.28976	-0.35113
N	-0.20952	0.32085	-0.26655
Au	1.16437	-1.24816	0.15609
Cl	1.08500	-0.55682	2.37002
Cl	2.60250	-2.93623	0.70681
Cl	1.16767	-1.94322	-2.07932
	12		
C	-3.65043	1.59454	0.21971
C	-2.48979	0.89367	-0.22114
C	-1.19102	1.52775	-0.01715
C	-1.19195	2.94049	0.18327

C	-2.39557	3.62924	0.53459
C	-3.56054	2.95971	0.64036
C	0.00008	3.62084	-0.00006
C	1.19209	2.94043	-0.18333
C	1.19112	1.52772	0.01720
C	2.48984	0.89359	0.22125
C	3.65051	1.59437	-0.21962
C	3.56069	2.95952	-0.64034
C	2.39575	3.62911	-0.53465
H	0.00011	4.70390	-0.00009
H	4.46318	3.46053	-0.96401
H	2.33192	4.68805	-0.74604
C	2.69420	-0.32059	0.90311
C	3.94560	-0.89013	1.00808
C	5.05902	-0.26269	0.44396
C	4.90995	0.97526	-0.13854
H	1.88140	-0.79719	1.42483
H	4.05796	-1.82172	1.54456
H	6.03505	-0.72412	0.50539
H	5.77217	1.51058	-0.51411
N	0.00004	0.86133	0.00005
Au	-0.00004	-1.26065	0.00000
Cl	-0.70830	-1.22628	2.22399
Cl	-0.00028	-3.55170	-0.00025
Cl	0.70845	-1.22600	-2.22395
H	-4.46300	3.46077	0.96402
H	-2.33170	4.68820	0.74589
C	-4.90990	0.97551	0.13862
C	-2.69421	-0.32051	-0.90297
C	-3.94565	-0.88997	-1.00794
C	-5.05904	-0.26245	-0.44386
H	-4.05806	-1.82156	-1.54441
H	-1.88143	-0.79711	-1.42471
H	-6.03510	-0.72380	-0.50531
H	-5.77211	1.51090	0.51411

Table S3 Complete reference 39.

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