

Supporting Information for

Non-covalent interactions in gold(III) tetrakis-(4-butoxyphenyl)-porphyrinate structures

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Table S1. Cartesian atomic coordinates for model structures.

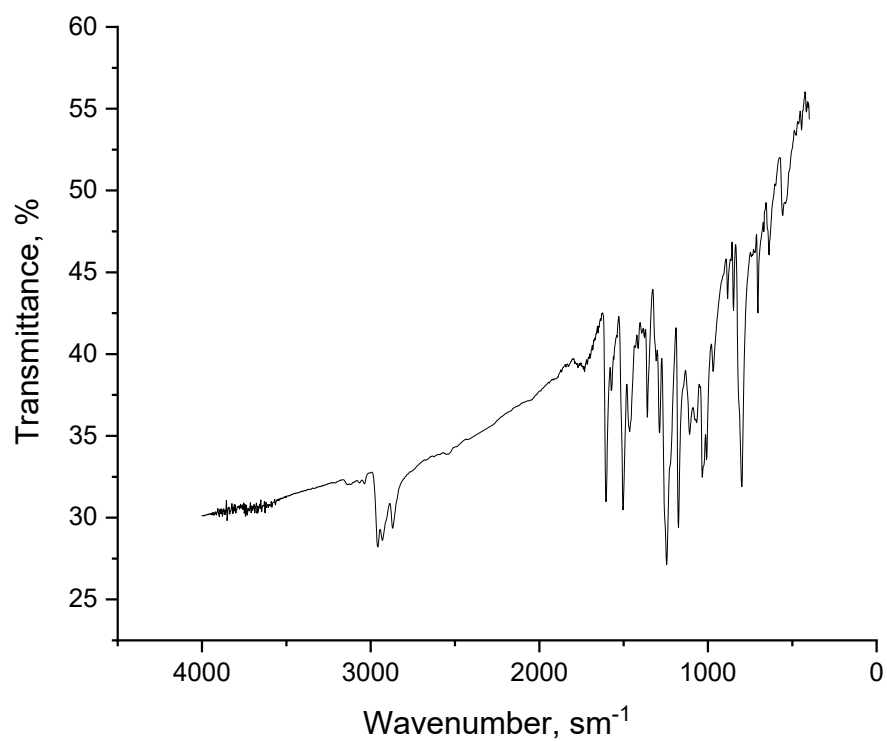


Fig. S1. FT-IR spectrum of [Au(TBPP)][AuCl₄] (**1**) in KBr.

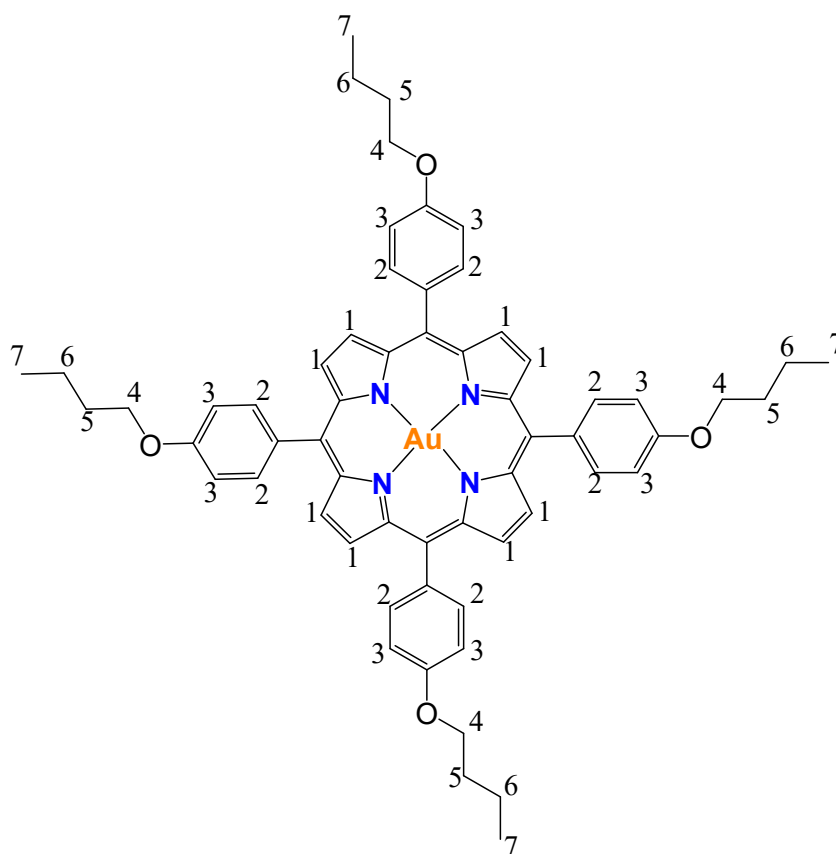
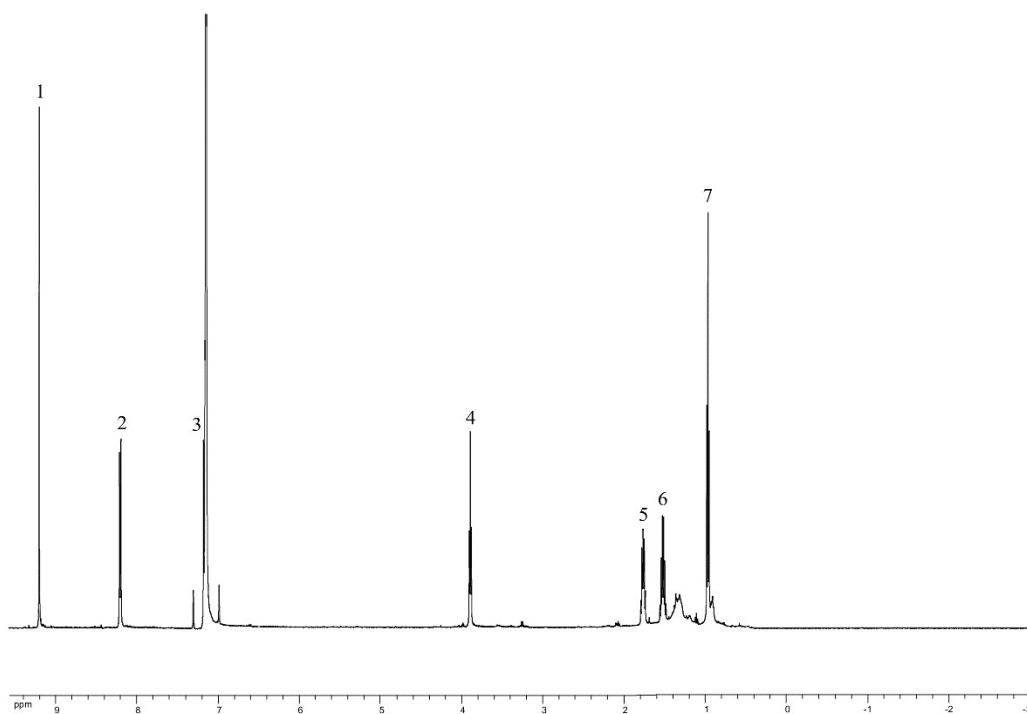


Fig. S2. ^1H NMR spectrum of $[\text{Au}(\text{TBPP})][\text{AuCl}_4]$ (**1**) in C_6D_6 (top) and numeration of protons in $[\text{Au}(\text{TBPP})]^+$ (bottom).

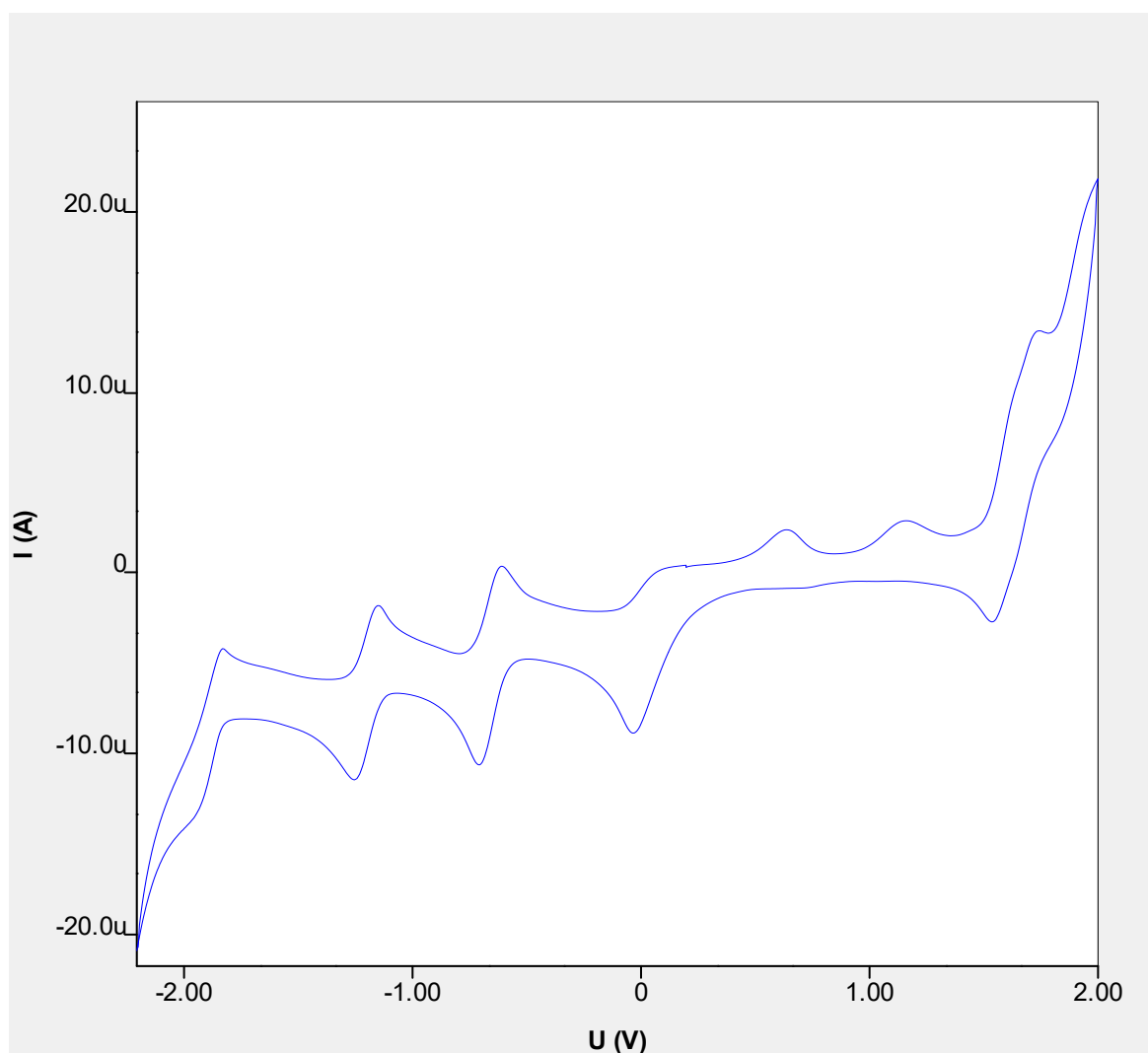


Fig. S3. CV of **1** in CH_2Cl_2 in the range from -2.2 to 2.0 V at potential scan rate of 100 mV/s.

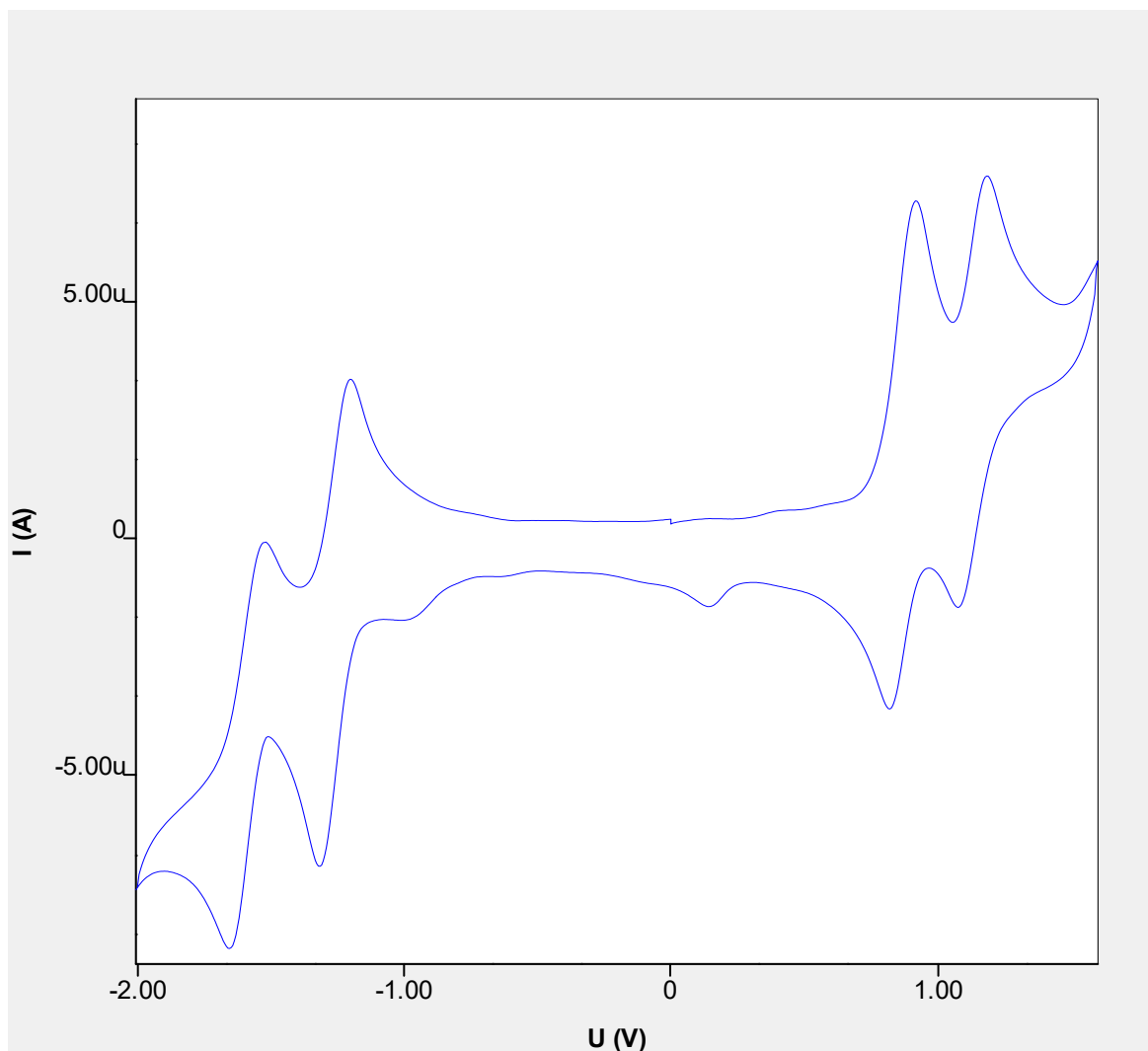


Fig. S4. CV of TBPPH₂ in CH₂Cl₂ in the range from -2.0 to 1.6 V at potential scan rate of 100 mV/s.

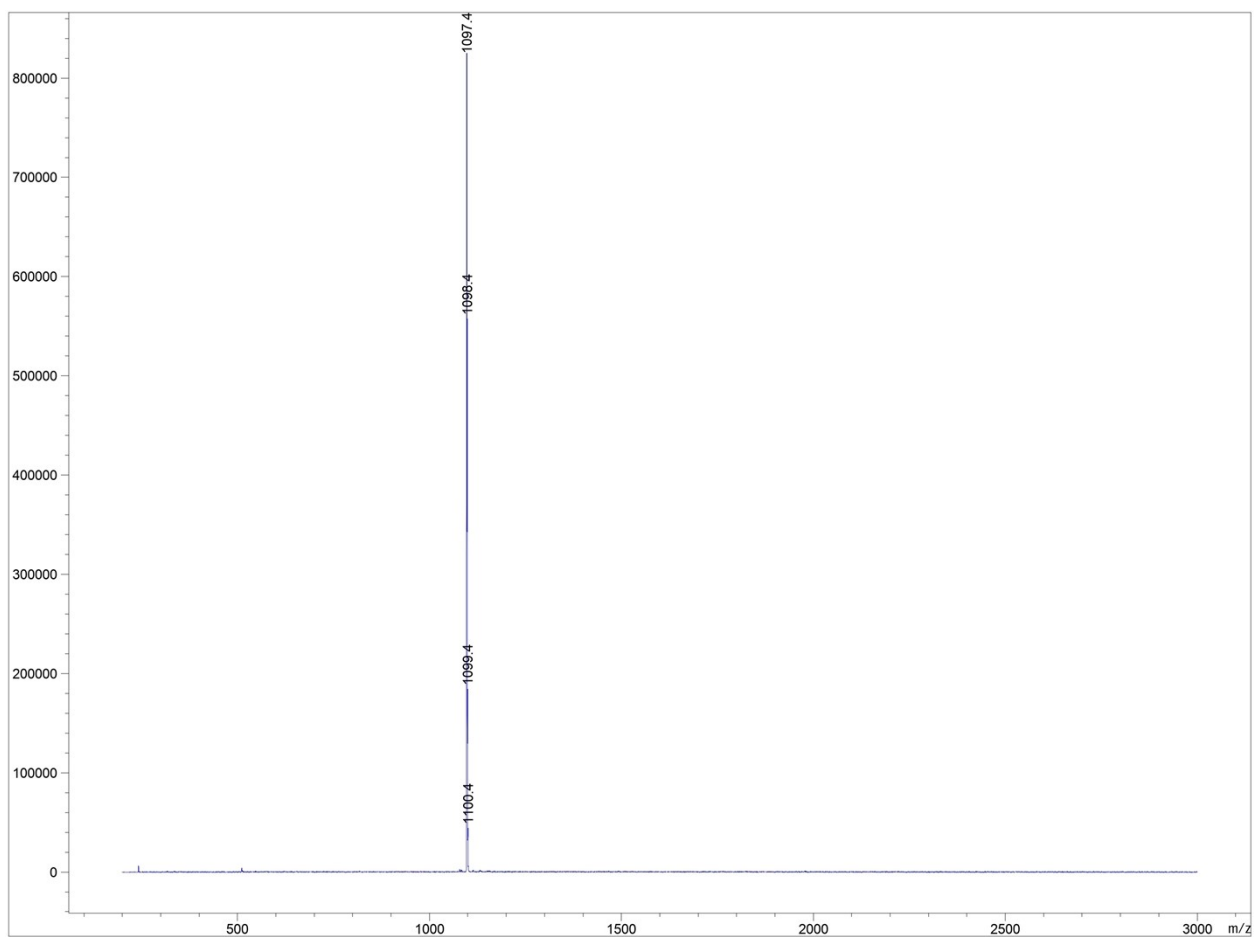


Fig. S5. ESI-MS of $[\text{Au}(\text{TBPP})][\text{AuCl}_4]$ (**1**) in CH_3CN .

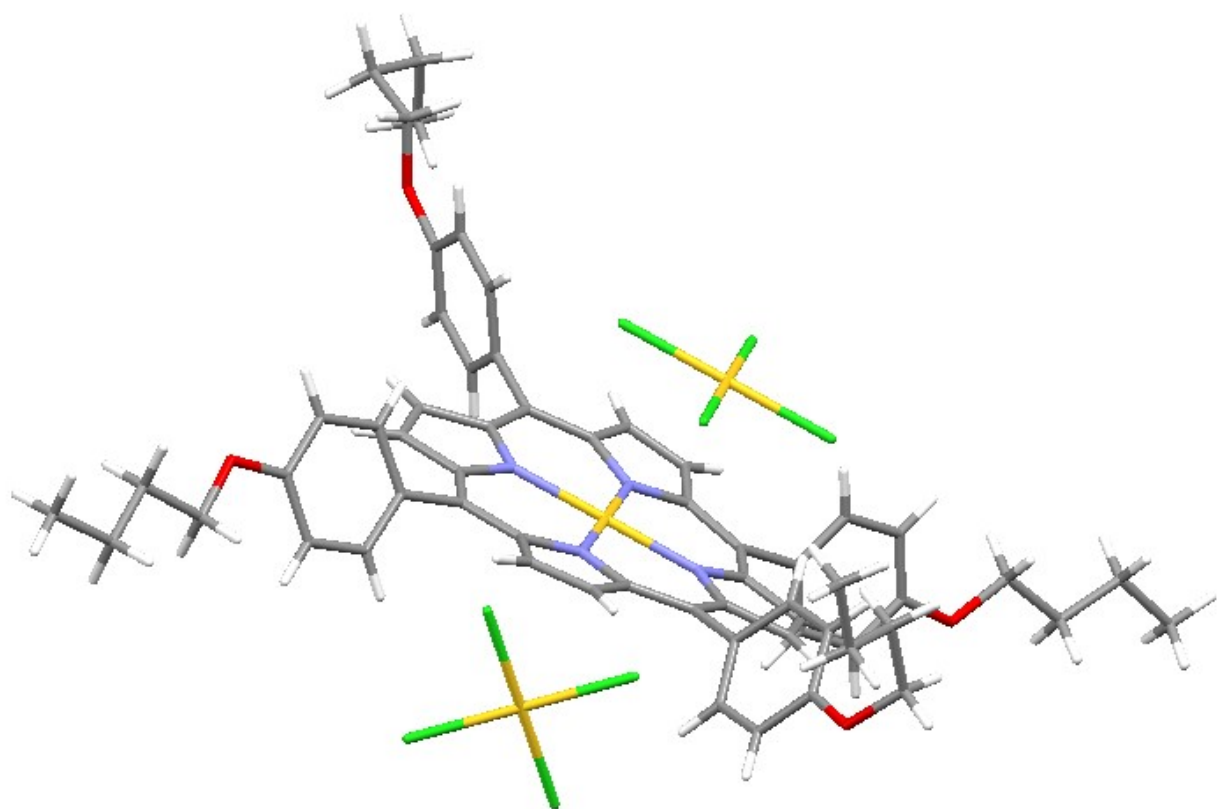


Fig. S6. Model structure 1 (part a).

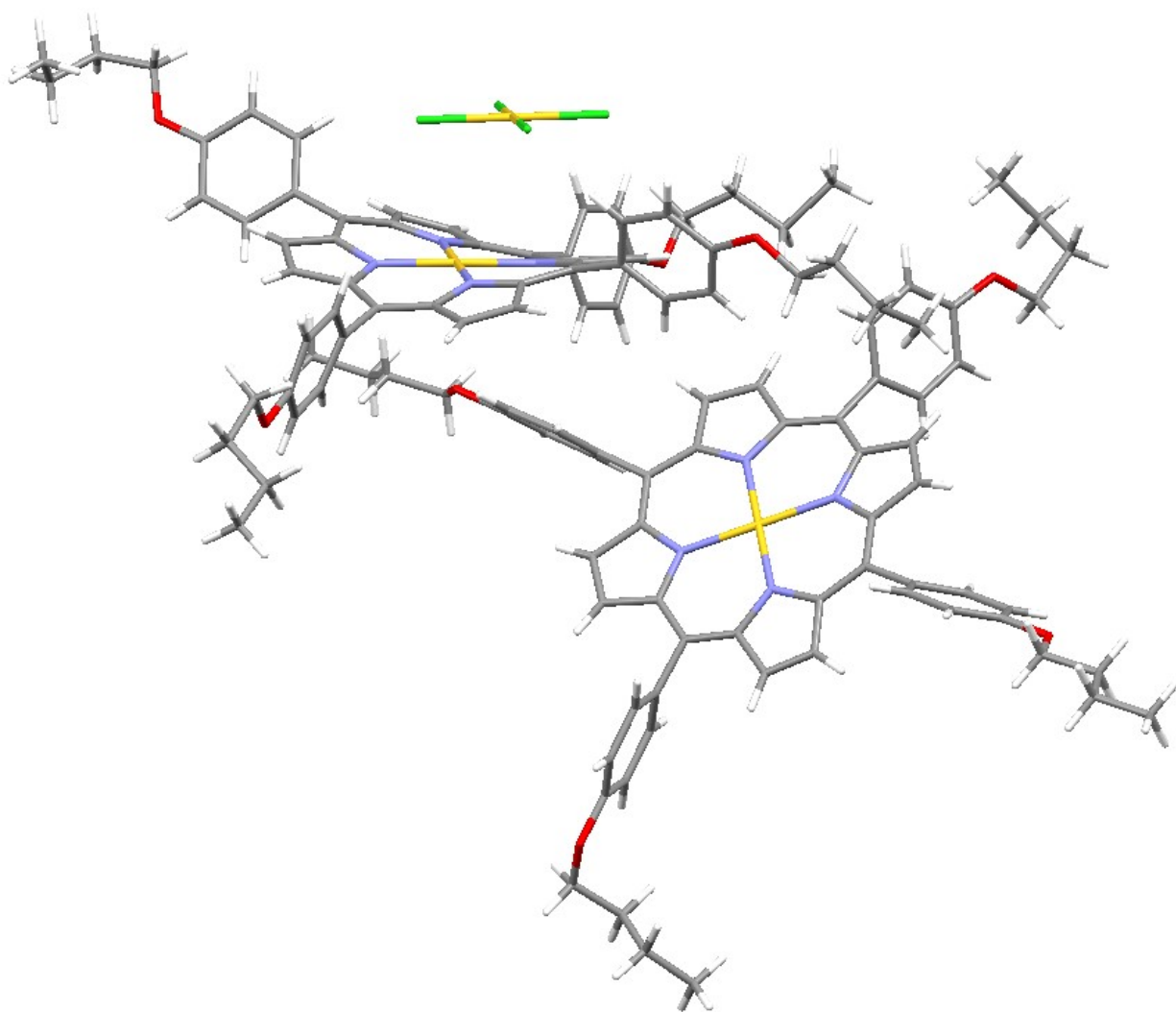


Fig. S7. Model structure 1 (part b).

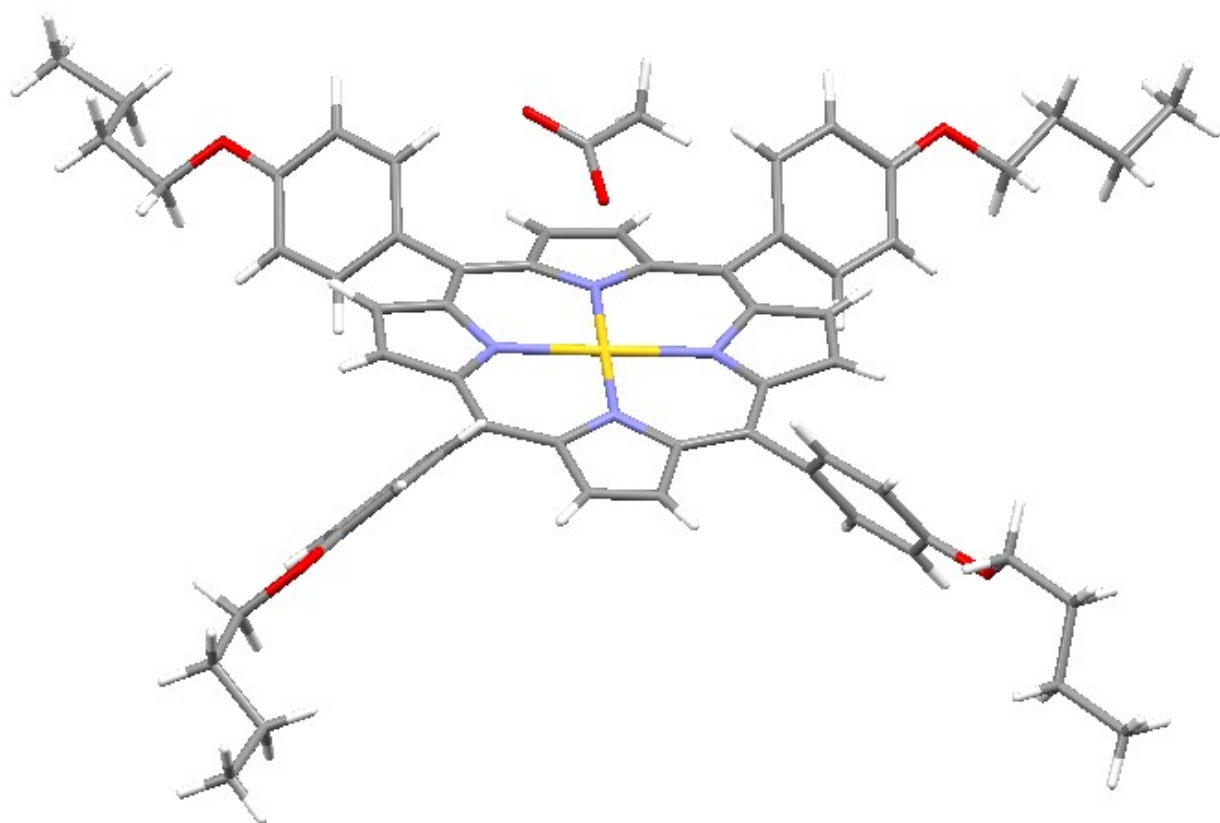


Fig. S8. Model structure **1a** (part a).

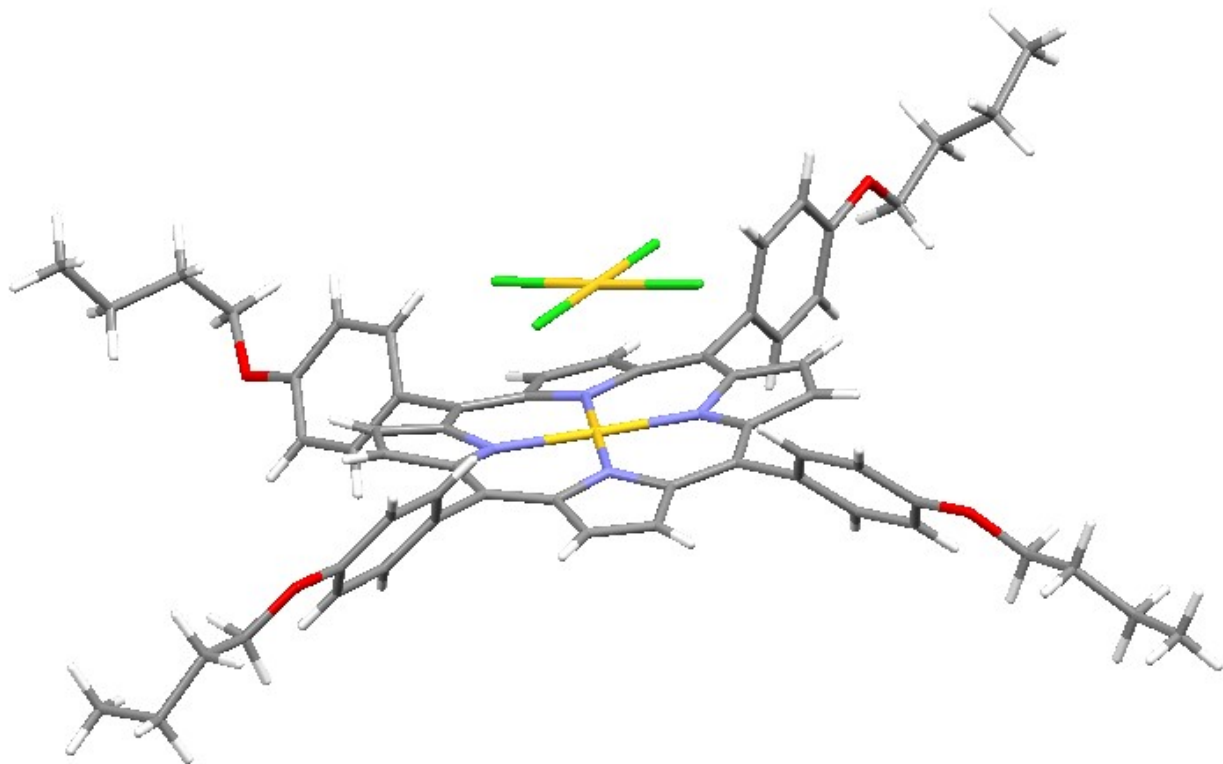


Fig. S9. Model structure **1a** (part b).

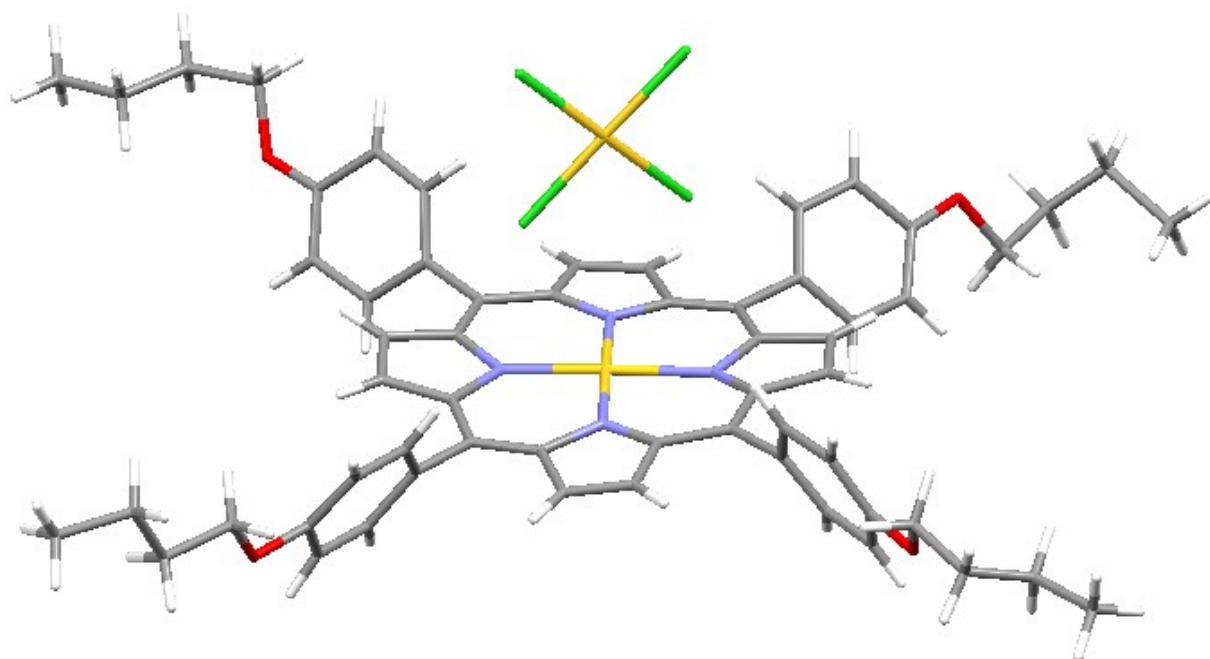


Fig. S10. Model structure **1b**.

Table S1. Cartesian atomic coordinates for model structures.

Atom	X	Y	Z
1 (part a)			
Au	6.177394	9.212468	1.131917
Cl	6.571315	8.948653	-1.092832
Cl	3.956893	8.812639	0.771445
Cl	5.813553	9.464046	3.355118
Cl	8.393470	9.630194	1.502257
Au	5.075128	12.261851	-0.351958
O	10.404439	15.121007	6.450959
O	-0.476323	10.446798	-7.356686
O	12.309407	11.055907	-5.704087
O	-2.062256	10.561412	5.009458
N	7.054233	12.587376	-0.104485
N	4.790884	12.523320	1.634991
N	3.096069	11.946129	-0.601754
N	5.359270	11.991049	-2.343165
C	7.089492	13.151817	2.300597
C	7.683703	12.991850	1.058391
C	8.030266	12.468784	-1.071935
C	10.950893	14.288349	7.451302
H	10.235944	13.976007	8.061860
H	11.380386	13.497460	7.041142
C	11.980121	15.102746	8.225263
H	11.546628	15.926798	8.560484
H	12.701722	15.373531	7.604256
C	12.580550	14.381954	9.366854
H	11.864702	14.099403	9.990821
H	13.038354	13.567702	9.038463

C	13.583787	15.266971	10.107921
H	14.263063	15.588587	9.479775
H	13.114660	16.033543	10.501654
H	14.014598	14.748920	10.819287
C	9.068149	13.144418	0.789439
H	9.727129	13.424695	1.414277
C	9.288850	12.825796	-0.506944
H	10.126941	12.837931	-0.954835
C	2.382411	12.019592	1.760760
C	5.765606	12.885883	2.565678
C	3.624891	12.319447	2.312206
C	5.148404	12.927190	3.848517
H	5.570627	13.166578	4.665607
C	3.862992	12.566770	3.701465
H	3.221410	12.491007	4.398532
C	3.005338	11.679688	-3.064883
C	2.141136	11.918645	0.396655
C	2.423709	11.816709	-1.799458
C	-0.368288	11.137284	-8.614178
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H	0.544460	11.042570	-8.983821
C	-1.390814	10.497881	-9.546800
H	-2.302422	10.636653	-9.188553
H	-1.225615	9.523053	-9.603260
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H	-1.436937	12.089840	-10.862861
H	-0.370829	10.971102	-11.280664
C	-2.297751	10.512548	-11.903509
H	-2.140349	9.548642	-11.985046
H	-3.205800	10.667569	-11.568055
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H	0.024791	11.805276	0.254672
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H	0.341592	11.738147	-2.172700
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C	6.582350	11.872303	-2.966203
C	13.150748	9.920183	-5.535751
H	13.960654	10.066459	-6.087217
H	13.443826	9.903606	-4.590939
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H	4.588261	11.168167	-5.321809
C	6.342448	11.486458	-4.320633
H	7.008687	11.320114	-4.977280
C	7.959062	13.641291	3.434449
C	8.396590	14.942594	3.447993
H	8.131994	15.538923	2.758491
C	9.230599	15.391960	4.477360
H	9.544623	16.288734	4.466176
C	9.598925	14.559524	5.497053
C	9.154617	13.253939	5.497053

H	9.401509	12.665418	6.200776
C	8.331567	12.800937	4.448337
H	8.029371	11.900638	4.446382
C	1.223518	11.725743	2.658554
C	0.631237	12.693849	3.442188
H	0.959368	13.584527	3.436442
C	-0.476535	12.338291	4.256781
H	-0.878763	12.997182	4.809544
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C	-0.372287	10.099208	3.484756
H	-0.690653	9.204260	3.489303
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H	11.690753	9.147842	-7.637285

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H	11.726766	7.028903	-8.708678
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Au	4.490680	17.066474	0.000000
Cl	6.230162	15.877043	0.840908
Cl	3.428411	15.119461	-0.530937
Cl	2.751197	18.255905	-0.840908
Cl	5.552948	19.013487	0.530937
1 (part b)			
Au	5.075128	12.261851	-0.351958
O	10.404439	15.121007	6.450959
O	-0.476323	10.446798	-7.356686
O	12.309407	11.055907	-5.704087
O	-2.062256	10.561412	5.009458
N	7.054233	12.587376	-0.104485
N	4.790884	12.523320	1.634991
N	3.096069	11.946129	-0.601754
N	5.359270	11.991049	-2.343165
C	7.089492	13.151817	2.300597
C	7.683703	12.991850	1.058391
C	8.030266	12.468784	-1.071935
C	10.950893	14.288349	7.451302
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H	11.380386	13.497460	7.041142
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H	12.701722	15.373531	7.604256
C	12.580550	14.381954	9.366854
H	11.864702	14.099403	9.990821
H	13.038354	13.567702	9.038463
C	13.583787	15.266971	10.107921
H	14.263063	15.588587	9.479775
H	13.114660	16.033543	10.501654
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H	9.727129	13.424695	1.414277
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H	10.126941	12.837931	-0.954835
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C	3.624891	12.319447	2.312206
C	5.148404	12.927190	3.848517
H	5.570627	13.166578	4.665607
C	3.862992	12.566770	3.701465
H	3.221410	12.491007	4.398532
C	3.005338	11.679688	-3.064883
C	2.141136	11.918645	0.396655
C	2.423709	11.816709	-1.799458
C	-0.368288	11.137284	-8.614178
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C	-2.297751	10.512548	-11.903509
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C	6.342448	11.486458	-4.320633
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C	9.154617	13.253939	5.497053
H	9.401509	12.665418	6.200776
C	8.331567	12.800937	4.448337
H	8.029371	11.900638	4.446382
C	1.223518	11.725743	2.658554
C	0.631237	12.693849	3.442188
H	0.959368	13.584527	3.436442
C	-0.476535	12.338291	4.256781
H	-0.878763	12.997182	4.809544
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C	0.703899	10.447907	2.697252
H	1.107439	9.778561	2.158150
C	2.102878	11.400020	-4.208409
C	2.054624	12.219766	-5.322912
H	2.608831	12.990454	-5.352438
C	1.212985	11.947337	-6.400651
H	1.202215	12.519440	-7.159249
C	0.387114	10.824553	-6.354214
C	0.409068	9.996527	-5.247451
H	-0.160407	9.236715	-5.218446

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H	1.260320	9.680209	-3.433578
C	9.033923	11.816660	-3.235154
C	9.402290	12.660094	-4.278065
H	8.895980	13.447135	-4.441487
C	10.495535	12.376133	-5.081049
H	10.725370	12.960232	-5.794137
C	11.245263	11.250333	-4.850796
C	10.905292	10.404576	-3.802080
H	11.424205	9.627385	-3.627745
C	9.809649	10.696233	-3.012640
H	9.585536	10.112278	-2.297965
C	-2.485295	9.174825	5.059765
H	-2.750578	8.859953	4.160191
H	-1.749589	8.600806	5.392433
C	-3.676205	9.124349	6.017541
H	-4.143516	8.258090	5.918706
H	-4.314852	9.845837	5.787346
C	-3.231594	9.289611	7.424214
H	-3.918586	8.913998	8.030476
H	-2.391809	8.785595	7.563353
C	-3.009405	10.729756	7.758952
H	-2.717247	10.806051	8.690568
H	-3.844328	11.226379	7.635060
H	-2.318934	11.098087	7.168343
C	12.615991	8.543183	-5.870489
H	13.271688	7.850360	-5.603530
H	11.771488	8.378759	-5.382197
C	12.370871	8.476779	-7.377776
H	13.209200	8.680698	-7.864230
H	11.690753	9.147842	-7.637285
C	11.886441	7.076897	-7.743472
H	11.726766	7.028903	-8.708678
H	11.052873	6.885565	-7.264236
H	12.567073	6.419715	-7.490562
Au	8.622024	17.655005	7.545532
O	1.156108	17.803981	2.436040
O	13.225343	21.945365	1.097089
O	13.752959	20.654956	14.351158
O	5.902513	10.304112	12.052496
N	7.058136	16.426114	7.393255
N	8.203275	18.407006	5.736980
N	10.226383	18.858612	7.677686
N	9.035453	16.916689	9.368789
C	5.951235	17.392431	5.396438
C	6.005646	16.527001	6.485787
C	6.772922	15.355330	8.225263
C	0.720040	16.759059	1.561465
H	1.472180	16.454961	0.993881
H	0.392072	15.988270	2.087584
C	-0.397697	17.314720	0.694629
H	-1.191755	17.492602	1.258072

H	-0.107373	18.174295	0.296640
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H	0.022852	16.279875	-1.002104
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C	5.035924	15.506556	6.795371
H	4.205330	15.367511	6.356903
C	5.524745	14.792605	7.818934
H	5.108368	14.034785	8.210403
C	10.305679	19.630161	5.334521
C	7.054458	18.176836	5.011393
C	9.081847	19.101933	4.930127
C	12.876452	23.257866	0.597884
H	11.923128	23.279429	0.333190
H	13.020272	23.939801	1.302846
C	13.763802	23.555724	-0.605624
H	14.703926	23.369509	-0.360433
H	13.694858	24.519876	-0.819585
C	13.430036	22.777920	-1.820742
H	13.557532	21.814080	-1.633830
H	12.474788	22.918634	-2.043410
C	14.285183	23.170987	-3.026185
H	14.084793	22.574602	-3.778048
H	14.086885	24.095701	-3.280740
H	15.234143	23.092565	-2.792255
C	7.229056	18.753588	3.720814
H	6.582747	18.766215	3.025159
C	8.448213	19.269311	3.658897
H	8.837179	19.681037	2.896740
C	10.743190	18.568274	10.075028
C	10.761252	19.602555	6.650254
C	10.895195	19.196163	8.838626
C	11.793498	20.446720	7.192026
H	12.342476	21.051021	6.705127
C	11.836923	20.221617	8.519368
H	12.399240	20.668924	9.140935
C	7.501509	14.998560	9.351375
C	9.936129	17.447515	10.268518
C	8.534992	15.749949	9.898952
C	5.037395	10.304173	13.161194
H	5.171894	9.463441	13.666939
H	5.285225	11.054472	13.756292
C	3.579595	10.426842	12.814847
H	3.449453	11.259313	12.294107
H	3.063407	10.518034	13.654517
C	3.013169	9.292212	12.035082
H	3.324153	9.301514	11.095514
H	3.233067	8.419180	12.447197
C	9.966200	16.588264	11.390760
H	10.480572	16.726689	12.178884
C	9.156440	15.550761	11.164377
H	9.018793	14.810122	11.743609
C	4.714622	17.452264	4.570235

C	4.251466	16.387544	3.844648
H	4.754839	15.582711	3.840313
C	3.072484	16.445435	3.117125
H	2.771445	15.683944	2.632974
C	2.339147	17.614630	3.099711
C	2.820705	18.725461	3.798210
H	2.342429	19.546466	3.764717
C	3.970668	18.640264	4.525733
H	4.272729	19.399717	5.010483
C	11.118143	20.328894	4.293545
C	10.756542	21.561182	3.794340
H	10.010608	22.016970	4.168337
C	11.466120	22.150326	2.751429
H	11.214442	23.008732	2.433525
C	12.528876	21.496610	2.178698
C	12.940393	20.294504	2.720470
H	13.697645	19.850308	2.357212
C	12.265709	19.731798	3.776926
H	12.587763	18.924754	4.161197
C	11.529174	19.075511	11.239838
C	10.883146	19.568177	12.354341
H	9.934877	19.528330	12.399056
C	11.601009	20.126848	13.420471
H	11.140943	20.482825	14.171735
C	12.976073	20.158721	13.372098
C	13.637559	19.590204	12.280815
H	14.586977	19.573901	12.261349
C	12.934459	19.068542	11.257252
H	13.403063	18.683026	10.525898
C	7.078612	13.769403	10.094377
C	7.451985	12.523324	9.657089
H	7.987932	12.434748	8.877769
C	7.042919	11.386137	10.353653
H	7.319572	10.527997	10.055737
C	6.240473	11.493827	11.472026
C	5.845596	12.714449	11.891899
H	5.282883	12.802192	12.652064
C	6.276944	13.853343	11.195335
H	6.001852	14.710386	11.500314
C	-1.255558	14.976001	-0.253472
H	-0.530149	14.416220	0.094752
H	-2.006424	14.966988	0.374655
H	-1.549973	14.625381	-1.120675
C	13.220887	21.383217	15.293455
H	12.775152	22.176347	14.904888
H	12.547950	20.857238	15.794730
C	14.361330	21.818550	16.229947
H	14.717577	21.017307	16.690705
H	13.990637	22.421267	16.923028
C	15.484353	22.512483	15.544992
H	16.164788	22.752160	16.222072
H	15.904262	21.878507	14.911544

C	15.095549	23.794829	14.767162
H	15.896007	24.179536	14.351584
H	14.704007	24.446133	15.385556
H	14.442836	23.570345	14.071836
C	1.335568	9.647180	12.153111
H	0.822481	8.963527	11.673217
H	1.158589	10.525837	11.758585
H	1.068432	9.652467	13.096569
Au	5.729344	18.883857	9.674503
Cl	6.316029	17.802105	11.591022
Cl	7.588889	20.195814	9.846516
Cl	5.142659	19.965609	7.757984
Cl	3.869799	17.571900	9.502491
1a (part a)			
Au	3.311404	8.264257	9.299897
N	4.329607	7.284385	10.743442
N	2.292596	9.284373	10.726465
N	4.339035	7.254787	7.893137
N	2.273167	9.225379	7.854393
C	3.239436	8.239897	12.761620
C	4.027789	7.301791	12.110805
C	5.245438	6.267914	10.543627
C	5.524903	5.642505	11.793017
H	6.132770	4.926360	11.938677
C	4.771000	6.247434	12.724617
H	4.736897	6.011915	13.643593
C	0.814977	10.648402	9.268118
C	2.495767	9.218454	12.097746
C	1.395894	10.319526	10.497918
C	1.755202	10.252858	12.709381
H	1.726959	10.441804	13.639588
C	1.093889	10.929248	11.742954
H	0.527135	11.680816	11.875729
C	3.317789	8.218925	5.855152
C	1.195502	10.072210	8.068792
C	2.367033	8.999279	6.492907
C	0.600774	10.346700	6.784576
H	-0.170062	10.881262	6.631384
C	1.318317	9.722524	5.842092
H	1.158225	9.753597	4.905703
C	5.817779	5.889855	9.342124
C	4.238776	7.418485	6.516850
C	5.380013	6.387539	8.107971
C	5.264237	6.659409	5.892155
H	5.429336	6.610583	4.958813
C	5.966710	6.024241	6.852052
H	6.709021	5.446135	6.720539
C	3.183404	8.159853	14.250439
C	1.974629	7.997628	14.944786
H	1.151793	8.045980	14.473936
C	1.970457	7.771506	16.296477
H	1.142853	7.666732	16.750611

C	3.168753	7.691659	17.014768
C	4.364601	7.900078	16.346540
H	5.184911	7.885421	16.827141
C	4.365875	8.127809	14.992672
H	5.193143	8.268419	14.547267
C	-0.250616	11.695615	9.239822
C	-1.428916	11.566846	9.960289
H	-1.575730	10.784055	10.478938
C	-2.400934	12.565138	9.934169
H	-3.201266	12.463171	10.436972
C	-2.197051	13.710953	9.174523
C	-1.029584	13.854489	8.456233
H	-0.883703	14.637388	7.937562
C	-0.069728	12.855008	8.488882
H	0.731359	12.964626	7.989366
C	3.301243	8.183838	4.342390
C	3.510095	9.350168	3.663279
H	3.571830	10.160251	4.155896
C	3.634141	9.400690	2.283292
H	3.738995	10.232068	1.834186
C	3.604280	8.244080	1.593298
C	3.376406	7.058779	2.226699
H	3.307300	6.259162	1.718476
C	3.246175	7.008047	3.604510
H	3.121602	6.173742	4.043472
C	6.921980	4.895340	9.350830
C	8.129374	5.188025	9.988585
H	8.242336	6.032692	10.407827
C	9.159571	4.272249	10.021234
H	9.973833	4.486720	10.461089
C	9.001776	3.033833	9.407423
C	7.809371	2.722321	8.763139
H	7.699947	1.877096	8.343592
C	6.782810	3.648036	8.739196
H	5.970072	3.433166	8.297839
O	3.068026	7.436960	18.353181
C	4.301075	7.261952	19.084749
H	4.877949	8.058478	18.977963
H	4.789843	6.471475	18.744279
C	3.948077	7.067335	20.536565
H	3.441869	6.223816	20.644570
H	3.372544	7.813023	20.840402
C	5.213737	7.017317	21.394160
H	5.704325	7.872341	21.307682
H	5.803442	6.291658	21.068405
C	4.877187	6.770843	22.874273
H	4.350366	7.523364	23.218726
H	5.706527	6.691153	23.389940
H	4.358372	5.944270	22.958966
O	-3.197235	14.646761	9.217403
C	-3.015778	15.831410	8.445350
H	-2.836402	15.590634	7.501517

H	-2.237860	16.338392	8.787974
C	-4.273160	16.698068	8.525885
H	-4.176885	17.452599	7.890960
H	-5.048221	16.158009	8.231169
C	-4.559006	17.236270	9.840574
H	-3.785483	17.761375	10.167744
H	-4.727976	16.499308	10.479177
C	-5.828039	18.157847	9.736095
H	-5.691274	18.822253	9.027709
H	-5.970371	18.616490	10.590033
H	-6.612213	17.610923	9.523285
O	3.764686	8.200400	0.217664
C	3.983466	9.449941	-0.485390
H	4.676547	9.986989	-0.025314
H	3.146183	9.977785	-0.517082
C	4.447092	9.091033	-1.921970
H	3.918175	8.325178	-2.261286
H	4.295536	9.861235	-2.524637
C	5.925801	8.727521	-1.917617
H	6.455485	9.450970	-1.496786
H	6.073193	7.892330	-1.407000
C	6.345110	8.536790	-3.365080
H	7.297030	8.306108	-3.400537
H	5.816366	7.822925	-3.768258
H	6.196985	9.374761	-3.857653
O	10.074333	2.176111	9.513643
C	9.917289	0.839974	8.980802
H	9.712408	0.876983	8.013178
H	9.178528	0.369951	9.442597
C	11.209267	0.130751	9.211526
H	11.120449	-0.807199	8.907537
H	11.399464	0.116033	10.183481
C	12.385055	0.777702	8.486706
H	12.493292	1.705734	8.813484
H	12.182282	0.819708	7.518821
C	13.714329	0.018225	8.686956
H	13.936933	-0.003480	9.641020
H	14.428148	0.474967	8.195036
H	13.620419	-0.897616	8.352059
O	-1.229895	7.178548	9.553258
C	-0.151919	6.834135	10.132243
C	-0.111396	6.891406	11.629769
H	-0.889179	6.421460	11.996271
H	-0.127444	7.826929	11.922200
H	0.709972	6.463509	11.951389
O	0.830687	6.440738	9.487959
1a (part b)			
Au	-2.642132	19.871009	1.625512
N	-1.767472	18.874013	3.151770
N	-3.529163	20.893652	0.134951
N	-1.030646	21.075554	1.490996
N	-4.228811	18.620465	1.732167

C	0.267700	20.256914	3.415143
C	-0.620760	19.284699	3.824350
C	-2.309816	17.819385	3.857000
C	-0.468194	18.446798	4.964908
H	0.233199	18.508177	5.602575
C	-1.472365	17.558107	4.995381
H	-1.605401	16.882374	5.649221
C	-1.762547	22.557122	-0.333025
C	0.111213	21.009502	2.276762
C	-0.790692	22.038262	0.531099
C	1.073771	21.897507	1.730426
H	1.949014	22.043450	2.070221
C	0.540529	22.497039	0.646461
H	0.977032	23.114303	0.070784
C	-5.684629	19.678736	0.028296
C	-3.047129	22.065801	-0.446210
C	-4.852261	20.756504	-0.267726
C	-4.110449	22.675308	-1.181914
H	-4.057111	23.488542	-1.669676
C	-5.200420	21.895106	-1.064375
H	-6.053645	22.069252	-1.444960
C	-3.447308	17.109890	3.519621
C	-5.341629	18.649391	0.901128
C	-4.313146	17.468182	2.481366
C	-6.109390	17.483223	1.129674
H	-6.920379	17.255886	0.692257
C	-5.485369	16.745523	2.083041
H	-5.771698	15.907119	2.423968
C	1.426450	20.556626	4.314094
C	2.740713	20.251450	4.018071
H	2.930969	19.793539	3.207883
C	3.785195	20.585099	4.853899
H	4.682372	20.376986	4.621587
C	3.480633	21.237717	6.053226
C	2.178302	21.574109	6.371015
H	1.986537	22.040127	7.176392
C	1.159300	21.226810	5.506890
H	0.262941	21.448826	5.729038
C	-1.354704	23.738063	-1.162324
C	-0.896447	24.896762	-0.563749
H	-0.916892	24.973274	0.381934
C	-0.400344	25.961461	-1.334278
H	-0.074252	26.747654	-0.911358
C	-0.389828	25.854861	-2.720796
C	-0.898018	24.726748	-3.304134
H	-0.933368	24.667257	-4.252190
C	-1.358359	23.680384	-2.551018
H	-1.684741	22.901615	-2.984299
C	-7.013783	19.627502	-0.652991
C	-7.095430	19.688101	-2.041685
H	-6.293436	19.752886	-2.546621
C	-8.304489	19.656114	-2.712089

H	-8.330194	19.705254	-3.660928
C	-9.471238	19.555271	-1.985092
C	-9.427413	19.504822	-0.585515
H	-10.233802	19.454082	-0.085498
C	-8.207984	19.529878	0.069652
H	-8.181156	19.479674	1.018405
C	-3.763340	15.896754	4.335860
C	-4.972342	15.766442	5.021500
H	-5.620169	16.459363	4.963014
C	-5.244642	14.641064	5.785500
H	-6.075168	14.568665	6.239677
C	-4.305478	13.617586	5.889978
C	-3.096114	13.724734	5.228281
H	-2.447776	13.033516	5.298739
C	-2.837117	14.865228	4.451222
H	-2.006901	14.935604	3.994563
O	4.414785	21.620647	6.984827
C	5.793782	21.317573	6.710570
H	6.090465	21.770056	5.880401
H	5.922178	20.341971	6.603262
C	6.575662	21.833927	7.912074
H	7.536360	21.632457	7.780387
H	6.479765	22.818947	7.957870
C	6.128906	21.237501	9.235469
H	6.292553	20.261761	9.222648
H	5.154538	21.380888	9.342102
C	6.855840	21.852255	10.419559
H	7.811238	21.641331	10.360137
H	6.491607	21.484697	11.251818
H	6.733910	22.823715	10.409546
O	0.142806	26.778947	-3.571860
C	0.669956	28.028480	-3.069057
H	1.064819	27.898305	-2.171521
H	1.373208	28.372233	-3.676165
C	-0.406424	28.935518	-3.003758
H	-0.103834	29.747352	-2.524659
H	-1.130914	28.525847	-2.469481
C	-0.979907	29.356554	-4.353273
H	-0.277913	29.810161	-4.885569
H	-1.274673	28.555234	-4.853703
C	-2.145212	30.288521	-4.161729
H	-2.845682	29.832931	-3.649588
H	-2.499771	30.552067	-5.036759
H	-1.849825	31.085400	-3.675077
O	-10.727663	19.516901	-2.533170
C	-10.809983	19.576683	-3.968008
H	-10.274995	18.846079	-4.368901
H	-10.452032	20.439970	-4.292458
C	-12.250410	19.436106	-4.368509
H	-12.740686	20.257889	-4.117652
H	-12.653675	18.677675	-3.875153
C	-12.402639	19.197079	-5.863859

H	-11.875774	18.397399	-6.115717
H	-13.352878	19.006895	-6.062956
C	-11.950352	20.365210	-6.712747
H	-12.434609	21.173225	-6.440711
H	-12.135130	20.175600	-7.655666
H	-10.987879	20.505548	-6.589832
O	-4.691875	12.545074	6.636129
C	-3.810929	11.402722	6.677921
H	-2.985696	11.626947	7.177698
H	-3.557363	11.133019	5.760142
C	-4.538407	10.282515	7.363561
H	-5.380224	10.092770	6.876757
H	-4.772818	10.557255	8.284126
C	-3.690275	9.017225	7.413624
H	-2.882516	9.190377	7.959437
H	-3.393839	8.788118	6.497347
C	-4.448157	7.829750	8.005669
H	-4.703659	8.031892	8.930261
H	-3.874470	7.034966	7.992370
H	-5.254608	7.658309	7.474940
Au	-4.925927	21.128121	4.275785
Cl	-5.218382	19.521461	5.857764
Cl	-2.834959	21.508098	5.080705
Cl	-6.993051	20.761271	3.439086
Cl	-4.594912	22.772761	2.734726
1b			
Au	14.213292	1.264276	2.111820
N	13.240106	2.215975	0.699938
N	15.894451	1.371417	1.023456
N	15.178106	0.241267	3.585149
N	12.532858	1.112095	3.214833
C	17.322879	1.749366	-0.726389
H	17.643120	2.070427	-1.560618
C	18.030616	1.004719	0.136325
H	18.925165	0.700415	0.036319
C	17.092877	0.752261	1.318488
C	16.006507	1.987038	-0.195332
C	13.732187	2.830477	-0.463913
C	16.555860	-0.010809	3.570906
C	11.827948	2.591825	0.710112
C	12.733423	3.657076	-1.074324
H	12.859072	4.251015	-1.804437
C	11.561716	3.424782	-0.398802
H	10.709325	3.769414	-0.638470
C	14.741114	-0.065703	4.816145
C	16.983665	-0.504381	4.867013
H	17.864565	-0.736134	5.137038
C	15.842735	-0.565493	5.609680
H	15.781317	-0.882639	6.502589
C	12.427128	0.576942	4.411239
C	11.267611	1.508850	2.775337
C	11.028861	0.590914	4.848700

H	10.696457	0.291606	5.685920
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C	17.430683	0.206729	2.480305
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C	19.177860	-1.580207	2.997119
H	18.456661	-2.186721	3.111388
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C	21.565433	-1.177145	3.062230
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C	25.238236	-4.189198	5.111177

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C	11.054356	-1.264287	11.127798
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C	10.567413	-2.160453	12.248920
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C	8.700979	2.037751	0.392698
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C	3.630424	5.126463	0.966485
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