

Coordinates of the calculated structures.

5-(4-Nitrophenyl)-10,15,20-triphenylporphyrin platinum (II) (**1**) on Au(111) Surface

Pt	6.662405	14.555208	2.820676
C	3.171835	12.001115	2.425719
C	4.193215	11.000079	2.398447
C	5.440183	11.663332	2.751168
N	5.217552	13.066222	2.900600
C	3.807458	13.261942	2.736780
C	4.219972	17.898251	3.937184
C	3.247948	16.897004	3.928798
C	3.843260	15.725875	3.285554
N	5.200963	15.979651	2.972173
C	5.414180	17.346133	3.294532
C	3.114926	14.522322	2.988981
C	10.136487	17.116967	2.403059
C	9.116127	18.117132	2.412250
C	7.875570	17.446762	2.756652
N	8.101085	16.045454	2.894187
C	9.506108	15.850088	2.698640
C	6.594026	18.107412	2.990558
C	9.127411	11.189102	3.815185
C	10.097371	12.195554	3.814386
C	9.492444	13.372640	3.200823
N	8.132189	13.119217	2.885571
C	7.923371	11.749169	3.204620
C	6.719904	10.997683	2.966143
C	10.209502	14.590744	2.947709
C	6.451761	19.598535	2.958460
C	1.631100	14.635076	2.904128
C	6.827322	9.506063	2.947811
C	11.694059	14.519063	2.920017
C	1.024488	15.902402	2.523116
C	-0.401051	16.074636	2.544647

C	-1.264024	14.941847	2.648100
C	-0.672869	13.652695	2.869325
C	0.730740	13.521483	3.089091
C	5.163880	20.182568	2.641881
C	4.962707	21.593402	2.627635
C	6.079558	22.482438	2.736173
C	7.370475	21.926440	3.000275
C	7.540782	20.519927	3.184645
C	12.371537	13.291425	2.541865
C	13.802512	13.187541	2.520479
C	13.937611	15.623923	3.034227
C	12.531234	15.672117	3.189933
C	8.080462	8.861000	2.604202
C	8.208646	7.439722	2.596874
C	7.052823	6.605274	2.735520
C	5.802676	7.224391	3.053619
C	5.711893	8.636273	3.235572
C	14.584550	14.368728	2.769865
N	16.018023	14.350608	2.621586
O	16.595192	15.540550	2.313369
O	16.592184	13.158666	2.327095
H	2.072628	11.834186	2.196857
H	4.023119	9.884951	2.285987
H	4.167620	18.949201	4.382741
H	2.188505	16.911686	4.358352
H	11.233887	17.284114	2.154079
H	9.283129	19.228858	2.262621
H	9.184547	10.139665	4.261954
H	11.152893	12.192179	4.252672
H	1.687188	16.819003	2.373760
H	-0.842668	17.120352	2.342749
H	-2.403234	15.048020	2.514207
H	-1.342834	12.714538	2.913025
H	1.133810	12.533943	3.490517

H	4.286277	19.492077	2.407508
H	3.916747	22.012013	2.384088
H	5.944292	23.618465	2.604171
H	8.286354	22.625084	3.076902
H	8.536197	20.129770	3.581890
H	11.756664	12.356792	2.312696
H	14.355195	12.196607	2.323630
H	14.620545	16.543582	3.167964
H	12.052543	16.621568	3.597409
H	8.992347	9.504410	2.374020
H	9.232223	6.969952	2.351819
H	7.129867	5.462653	2.615236
H	4.859088	6.572795	3.191802
H	4.763762	9.087880	3.677777
Au	7.194811	10.800209	0.000000
Au	10.072736	15.784920	0.000000
Au	14.389623	23.261988	0.000000
Au	-5.755849	23.261988	0.000000
Au	-8.633774	23.261988	0.000000
Au	15.828585	20.769632	0.000000
Au	11.511698	13.292564	0.000000
Au	8.633774	8.307853	0.000000
Au	17.267548	18.277275	0.000000
Au	-10.072736	20.769632	0.000000
Au	12.950661	10.800209	0.000000
Au	18.706511	15.784920	0.000000
Au	-4.316887	20.769632	0.000000
Au	10.072736	5.815497	0.000000
Au	20.145472	13.292564	0.000000
Au	14.389623	8.307853	0.000000
Au	1.438962	5.815497	0.000000
Au	21.584435	10.800209	0.000000
Au	-7.194811	20.769632	0.000000
Au	15.828585	5.815497	0.000000

Au	23.023397	8.307853	0.000000
Au	11.511698	3.323141	0.000000
Au	-2.877925	18.277275	0.000000
Au	24.462359	5.815497	0.000000
Au	17.267548	3.323141	0.000000
Au	-5.755849	13.292564	0.000000
Au	25.901321	3.323141	0.000000
Au	12.950661	0.830785	0.000000
Au	18.706511	0.830785	0.000000
Au	27.340284	0.830785	0.000000
Au	-2.877925	8.307853	0.000000
Au	-1.438962	15.784920	0.000000
Au	11.511698	23.261988	0.000000
Au	2.877925	23.261988	0.000000
Au	-2.877925	23.261988	0.000000
Au	12.950661	20.769632	0.000000
Au	-5.755849	18.277275	0.000000
Au	4.316887	20.769632	0.000000
Au	14.389623	18.277275	0.000000
Au	2.877925	3.323141	0.000000
Au	-1.438962	20.769632	0.000000
Au	15.828585	15.784920	0.000000
Au	5.755849	18.277275	0.000000
Au	0.000000	13.292564	0.000000
Au	17.267548	13.292564	0.000000
Au	-8.633774	18.277275	0.000000
Au	7.194811	15.784920	0.000000
Au	18.706511	10.800209	0.000000
Au	0.000000	18.277275	0.000000
Au	-4.316887	15.784920	0.000000
Au	20.145472	8.307853	0.000000
Au	8.633774	13.292564	0.000000
Au	1.438962	10.800209	0.000000
Au	21.584435	5.815497	0.000000

Au	1.438962	15.784920	0.000000
Au	10.072736	10.800209	0.000000
Au	23.023397	3.323141	0.000000
Au	0.000000	3.323141	0.000000
Au	4.316887	0.830785	0.000000
Au	24.462359	0.830785	0.000000
Au	11.511698	8.307853	0.000000
Au	2.877925	13.292564	0.000000
Au	8.633774	23.261988	0.000000
Au	2.877925	8.307853	0.000000
Au	12.950661	5.815497	0.000000
Au	10.072736	20.769632	0.000000
Au	-2.877925	13.292564	0.000000
Au	4.316887	10.800209	0.000000
Au	11.511698	18.277275	0.000000
Au	14.389623	3.323141	0.000000
Au	-4.316887	10.800209	0.000000
Au	12.950661	15.784920	0.000000
Au	4.316887	5.815497	0.000000
Au	15.828585	0.830785	0.000000
Au	14.389623	13.292564	0.000000
Au	5.755849	8.307853	0.000000
Au	-7.194811	15.784920	0.000000
Au	15.828585	10.800209	0.000000
Au	0.000000	23.261988	0.000000
Au	-1.438962	10.800209	0.000000
Au	17.267548	8.307853	0.000000
Au	7.194811	5.815497	0.000000
Au	1.438962	20.769632	0.000000
Au	18.706511	5.815497	0.000000
Au	5.755849	3.323141	0.000000
Au	-11.511698	23.261988	0.000000
Au	20.145472	3.323141	0.000000
Au	2.877925	18.277275	0.000000

Au	8.633774	3.323141	0.000000
Au	21.584435	0.830785	0.000000
Au	1.438962	0.830785	0.000000
Au	4.316887	15.784920	0.000000
Au	5.755849	23.261988	0.000000
Au	7.194811	0.830785	0.000000
Au	10.072736	0.830785	0.000000
Au	7.194811	20.769632	0.000000
Au	5.755849	13.292564	0.000000
Au	0.000000	8.307853	0.000000
Au	8.633774	18.277275	0.000000
Au	-1.438962	5.815497	0.000000
Au	0.000000	6.646282	-2.349816
Au	12.950661	24.092773	-2.349816
Au	-1.438962	24.092773	-2.349816
Au	14.389623	21.600416	-2.349816
Au	0.000000	11.630994	-2.349816
Au	15.828585	19.108061	-2.349816
Au	0.000000	21.600416	-2.349816
Au	17.267548	16.615706	-2.349816
Au	-1.438962	4.153926	-2.349816
Au	18.706511	14.123350	-2.349816
Au	1.438962	19.108061	-2.349816
Au	20.145472	11.630994	-2.349816
Au	1.438962	9.138637	-2.349816
Au	21.584435	9.138637	-2.349816
Au	2.877925	16.615706	-2.349816
Au	23.023397	6.646282	-2.349816
Au	1.438962	4.153926	-2.349816
Au	24.462359	4.153926	-2.349816
Au	4.316887	14.123350	-2.349816
Au	25.901321	1.661571	-2.349816
Au	2.877925	6.646282	-2.349816
Au	10.072736	24.092773	-2.349816

Au	5.755849	11.630994	-2.349816
Au	11.511698	21.600416	-2.349816
Au	-7.194811	14.123350	-2.349816
Au	12.950661	19.108061	-2.349816
Au	7.194811	9.138637	-2.349816
Au	14.389623	16.615706	-2.349816
Au	4.316887	4.153926	-2.349816
Au	15.828585	14.123350	-2.349816
Au	8.633774	6.646282	-2.349816
Au	17.267548	11.630994	-2.349816
Au	2.877925	1.661571	-2.349816
Au	18.706511	9.138637	-2.349816
Au	10.072736	4.153926	-2.349816
Au	20.145472	6.646282	-2.349816
Au	5.755849	1.661571	-2.349816
Au	21.584435	4.153926	-2.349816
Au	11.511698	1.661571	-2.349816
Au	23.023397	1.661571	-2.349816
Au	-2.877925	6.646282	-2.349816
Au	7.194811	24.092773	-2.349816
Au	-4.316887	24.092773	-2.349816
Au	8.633774	21.600416	-2.349816
Au	-10.072736	24.092773	-2.349816
Au	10.072736	19.108061	-2.349816
Au	-2.877925	21.600416	-2.349816
Au	11.511698	16.615706	-2.349816
Au	-12.950661	24.092773	-2.349816
Au	12.950661	14.123350	-2.349816
Au	-1.438962	19.108061	-2.349816
Au	14.389623	11.630994	-2.349816
Au	-8.633774	21.600416	-2.349816
Au	15.828585	9.138637	-2.349816
Au	0.000000	16.615706	-2.349816
Au	17.267548	6.646282	-2.349816

Au -5.755849 11.630994 -2.349816
Au 18.706511 4.153926 -2.349816
Au 1.438962 14.123350 -2.349816
Au 20.145472 1.661571 -2.349816
Au -7.194811 19.108061 -2.349816
Au 4.316887 24.092773 -2.349816
Au 2.877925 11.630994 -2.349816
Au 5.755849 21.600416 -2.349816
Au -11.511698 21.600416 -2.349816
Au 7.194811 19.108061 -2.349816
Au 4.316887 9.138637 -2.349816
Au 8.633774 16.615706 -2.349816
Au -5.755849 16.615706 -2.349816
Au 10.072736 14.123350 -2.349816
Au 5.755849 6.646282 -2.349816
Au 11.511698 11.630994 -2.349816
Au 0.000000 1.661571 -2.349816
Au 12.950661 9.138637 -2.349816
Au 7.194811 4.153926 -2.349816
Au 14.389623 6.646282 -2.349816
Au -4.316887 14.123350 -2.349816
Au 15.828585 4.153926 -2.349816
Au 8.633774 1.661571 -2.349816
Au 17.267548 1.661571 -2.349816
Au -10.072736 19.108061 -2.349816
Au 1.438962 24.092773 -2.349816
Au -7.194811 24.092773 -2.349816
Au 2.877925 21.600416 -2.349816
Au -2.877925 11.630994 -2.349816
Au 4.316887 19.108061 -2.349816
Au -5.755849 21.600416 -2.349816
Au 5.755849 16.615706 -2.349816
Au -4.316887 9.138637 -2.349816
Au 7.194811 14.123350 -2.349816

Au	-4.316887	19.108061	-2.349816
Au	8.633774	11.630994	-2.349816
Au	-1.438962	9.138637	-2.349816
Au	10.072736	9.138637	-2.349816
Au	-2.877925	16.615706	-2.349816
Au	11.511698	6.646282	-2.349816
Au	-8.633774	16.615706	-2.349816
Au	12.950661	4.153926	-2.349816
Au	-1.438962	14.123350	-2.349816
Au	14.389623	1.661571	-2.349816
Au	12.950661	22.431202	-4.699631
Au	14.389623	19.938847	-4.699631
Au	15.828585	17.446491	-4.699631
Au	17.267548	14.954135	-4.699631
Au	18.706511	12.461779	-4.699631
Au	20.145472	9.969423	-4.699631
Au	21.584435	7.477067	-4.699631
Au	23.023397	4.984712	-4.699631
Au	24.462359	2.492356	-4.699631
Au	25.901321	0.000000	-4.699631
Au	10.072736	22.431202	-4.699631
Au	11.511698	19.938847	-4.699631
Au	12.950661	17.446491	-4.699631
Au	14.389623	14.954135	-4.699631
Au	15.828585	12.461779	-4.699631
Au	17.267548	9.969423	-4.699631
Au	18.706511	7.477067	-4.699631
Au	20.145472	4.984712	-4.699631
Au	21.584435	2.492356	-4.699631
Au	23.023397	0.000000	-4.699631
Au	7.194811	22.431202	-4.699631
Au	8.633774	19.938847	-4.699631
Au	10.072736	17.446491	-4.699631
Au	11.511698	14.954135	-4.699631

Au	12.950661	12.461779	-4.699631
Au	14.389623	9.969423	-4.699631
Au	15.828585	7.477067	-4.699631
Au	17.267548	4.984712	-4.699631
Au	18.706511	2.492356	-4.699631
Au	20.145472	0.000000	-4.699631
Au	4.316887	22.431202	-4.699631
Au	5.755849	19.938847	-4.699631
Au	7.194811	17.446491	-4.699631
Au	8.633774	14.954135	-4.699631
Au	10.072736	12.461779	-4.699631
Au	11.511698	9.969423	-4.699631
Au	12.950661	7.477067	-4.699631
Au	14.389623	4.984712	-4.699631
Au	15.828585	2.492356	-4.699631
Au	17.267548	0.000000	-4.699631
Au	1.438962	22.431202	-4.699631
Au	2.877925	19.938847	-4.699631
Au	4.316887	17.446491	-4.699631
Au	5.755849	14.954135	-4.699631
Au	7.194811	12.461779	-4.699631
Au	8.633774	9.969423	-4.699631
Au	10.072736	7.477067	-4.699631
Au	11.511698	4.984712	-4.699631
Au	12.950661	2.492356	-4.699631
Au	14.389623	0.000000	-4.699631
Au	-1.438962	22.431202	-4.699631
Au	0.000000	19.938847	-4.699631
Au	1.438962	17.446491	-4.699631
Au	2.877925	14.954135	-4.699631
Au	4.316887	12.461779	-4.699631
Au	5.755849	9.969423	-4.699631
Au	7.194811	7.477067	-4.699631
Au	8.633774	4.984712	-4.699631

Au	10.072736	2.492356	-4.699631
Au	11.511698	0.000000	-4.699631
Au	-4.316887	22.431202	-4.699631
Au	-2.877925	19.938847	-4.699631
Au	-1.438962	17.446491	-4.699631
Au	0.000000	14.954135	-4.699631
Au	1.438962	12.461779	-4.699631
Au	2.877925	9.969423	-4.699631
Au	4.316887	7.477067	-4.699631
Au	5.755849	4.984712	-4.699631
Au	7.194811	2.492356	-4.699631
Au	8.633774	0.000000	-4.699631
Au	-7.194811	22.431202	-4.699631
Au	-5.755849	19.938847	-4.699631
Au	-4.316887	17.446491	-4.699631
Au	-2.877925	14.954135	-4.699631
Au	-1.438962	12.461779	-4.699631
Au	0.000000	9.969423	-4.699631
Au	1.438962	7.477067	-4.699631
Au	2.877925	4.984712	-4.699631
Au	4.316887	2.492356	-4.699631
Au	5.755849	0.000000	-4.699631
Au	-10.072736	22.431202	-4.699631
Au	-8.633774	19.938847	-4.699631
Au	-7.194811	17.446491	-4.699631
Au	-5.755849	14.954135	-4.699631
Au	-4.316887	12.461779	-4.699631
Au	-2.877925	9.969423	-4.699631
Au	-1.438962	7.477067	-4.699631
Au	0.000000	4.984712	-4.699631
Au	1.438962	2.492356	-4.699631
Au	2.877925	0.000000	-4.699631
Au	-12.950661	22.431202	-4.699631
Au	-11.511698	19.938847	-4.699631

Au	-10.072736	17.446491	-4.699631
Au	-8.633774	14.954135	-4.699631
Au	-7.194811	12.461779	-4.699631
Au	-5.755849	9.969423	-4.699631
Au	-4.316887	7.477067	-4.699631
Au	-2.877925	4.984712	-4.699631
Au	-1.438962	2.492356	-4.699631
Au	0.000000	0.000000	-4.699631

5-(4-Nitrophenyl)-10,15,20-tris(3,5-di-t-butylphenyl)porphyrin platinum(II) (2) on Au(111) Surface

C	2.643199	10.699754	2.436800
C	3.887101	11.419146	2.673004
N	3.609713	12.820879	2.814486
C	2.197838	12.956084	2.667417
C	2.301252	17.665590	3.746689
C	1.391471	16.601142	3.716782
C	2.091282	15.457243	3.136891
N	3.443015	15.784267	2.884446
C	3.555506	17.176139	3.176781
C	1.456420	14.190625	2.881274
C	8.312752	17.157821	2.503316
C	7.261012	18.101304	2.509967
C	6.023834	17.374784	2.746477
N	6.307204	15.971583	2.873633
C	7.724379	15.843551	2.732476
C	4.718935	17.994056	2.944724
C	7.588666	11.098660	3.711581
C	8.491056	12.170966	3.764328
C	7.823818	13.331814	3.182304
N	6.479111	13.007438	2.874246
C	6.351286	11.607331	3.132046
C	5.180192	10.794374	2.892713
C	8.480227	14.605149	2.944746
C	4.562586	19.495082	2.974767
C	-0.033006	14.129952	2.874261
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Au	-7.194811	17.446491	-4.699631
Au	-5.755849	14.954135	-4.699631
Au	-4.316887	12.461779	-4.699631
Au	-2.877925	9.969423	-4.699631
Au	-1.438962	7.477067	-4.699631
Au	0.000000	4.984712	-4.699631
Au	1.438962	2.492356	-4.699631
Au	2.877925	0.000000	-4.699631

Au	-12.950661	22.431202	-4.699631
Au	-11.511698	19.938847	-4.699631
Au	-10.072736	17.446491	-4.699631
Au	-8.633774	14.954135	-4.699631
Au	-7.194811	12.461779	-4.699631
Au	-5.755849	9.969423	-4.699631
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Au	-2.877925	4.984712	-4.699631
Au	-1.438962	2.492356	-4.699631
Au	0.000000	0.000000	-4.699631

Azobenzene dimer of 5-(4-nitrophenyl)-10,15,20-triphenylporphyrin platinum (II) on Au(111) Surface
(heterochiral, perpendicular orientation of macrocyclic saddlings, observed experimentally)

C -7.3513399 27.8183945 2.3774980
C -7.7224427 26.4370893 2.3515850
C -6.5259149 25.6706244 2.7079320
N -5.4206418 26.5397693 2.8676570
C -5.9239765 27.8642185 2.6807120
C -1.6547978 29.8576142 3.7591530
C -3.0149440 30.2055265 3.7632250
C -3.7534674 29.0722645 3.2212500
N -2.8674745 27.9838177 2.9825210
C -1.5656395 28.4956994 3.2473010
C -5.1669665 29.0865567 2.9548110
C 0.4274950 24.1958292 2.3628230
C 0.8066972 25.5648158 2.3278600
C -0.3527687 26.3420355 2.7714190
N -1.4519255 25.4683470 2.9815410
C -0.9323577 24.1492251 2.7880840
C -0.3388459 27.7687447 3.0270580
C -5.1713896 22.1842158 3.7496640
C -3.8270886 21.7928041 3.7364300
C -3.0818339 22.9164632 3.2032100
N -3.9448572 24.0111833 2.9015520
C -5.2455761 23.5240366 3.1798160
C -6.4886836 24.2236179 2.8995600
C -1.6558032 22.9172315 3.0192820
C 0.9769354 28.4655345 3.0299820
C -5.8557693 30.4014923 2.8779980
C -7.7298458 23.4003059 2.8147740
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C 3.4684864 28.2601796 2.9964270
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H	10.9336780	14.2811565	3.7459040
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Au 0.0000000 6.6462820 -2.3498160
Au -1.4389620 24.0927730 -2.3498160
Au 0.0000000 11.6309940 -2.3498160
Au 0.0000000 21.6004160 -2.3498160
Au -11.5116980 21.6004160 -2.3498160
Au 2.8779250 34.8929830 -4.6996310
Au 4.3168870 32.4006270 -4.6996310
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Au 7.1948110 27.4159140 -4.6996310
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Au -2.8779250 4.9847120 -4.6996310
Au -1.4389620 2.4923560 -4.6996310
Au 0.0000000 0.0000000 -4.6996310

Azobenzene dimer of 5-(4-nitrophenyl)-10,15,20-triphenylporphyrin platinum (II) on Au(111) Surface
(homochiral, parallel orientation of macrocyclic saddlings, NOT observed experimentally)

Pt	-3.8179545	23.5599047	2.8077760
C	-7.9213164	25.0455921	2.4653280
C	-8.1880230	23.6888695	2.7306750
C	-6.9054765	23.0042998	2.8613560
N	-5.8499930	23.9483907	2.7602650
C	-6.4696502	25.2270765	2.5151830
C	-2.5061311	27.4121840	4.0806110
C	-3.8834546	27.6667322	4.0060110
C	-4.4805591	26.5512936	3.2838460
N	-3.4957634	25.5740195	2.9917930
C	-2.2734694	26.1498721	3.3953610
C	-5.8531088	26.5015054	2.8599710
C	0.2568763	22.2011829	2.4185710
C	0.4958439	23.5954247	2.4946200
C	-0.7716475	24.2185084	2.8256010
N	-1.7888061	23.2139347	2.9578040
C	-1.1442356	21.9527757	2.7407640
C	-0.9666241	25.6364837	3.0605820
C	-5.3253392	19.5315756	2.3354820
C	-3.9201775	19.2002722	2.3983710
C	-3.2028057	20.4499618	2.6895400
N	-4.1605159	21.5249625	2.7935870
C	-5.4556267	20.9277243	2.7216640
C	-6.7392429	21.5709328	2.9464800
C	-1.7533471	20.6118638	2.8095590
C	0.1169954	26.6554756	2.9421640
C	-6.5598928	27.8118872	2.7589330
C	-7.9200190	20.6565809	3.0143680
C	-0.8346039	19.4262619	2.7771420
C	-5.7606970	28.9860675	2.4199570
C	-6.3193125	30.3099839	2.4704070
C	-7.7405776	30.4768432	2.5332660

C -8.5641790 29.3102727 2.6754470
C -7.9824828 28.0152854 2.8745990
C -0.2437091 28.0253981 2.6062260
C 0.7272820 29.0727202 2.5863490
C 2.1233814 28.7630592 2.6637840
C 2.5076418 27.3966446 2.8632930
C 1.5279127 26.3775791 3.0779790
C -1.2188650 18.0442637 2.4834480
C -0.2854359 16.9749551 2.3942840
C 1.5432293 18.5422181 2.9120390
C 0.5680323 19.5399769 3.1688910
C -7.7546780 19.3432458 3.5987620
C -8.7212914 18.3127694 3.4415930
C -10.0125491 18.6044954 2.8884660
C -10.2856589 19.9502194 2.5083200
C -9.2389310 20.9402815 2.4866700
C 1.1503641 17.2076826 2.4778220
N 2.0000000 16.1100000 2.2550000
H -8.7113687 25.8292688 2.2442140
H -9.2196876 23.2844549 2.9776010
H -1.6694096 28.0451859 4.5373890
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H 1.0491042 21.4202139 2.1767870
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H -3.6531694 18.1754086 2.8049970
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H -8.2209832 31.5218463 2.4424610
H -9.7121347 29.4254623 2.6835450
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H -1.3455079 28.2892317 2.4690700
H 0.3739376 30.1501907 2.3765000
H 2.9215097 29.5783103 2.4981470

H 3.6280225 27.1170804 2.8597710
H 1.8740534 25.3595459 3.4593280
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H -0.6688929 15.8998902 2.2477060
H 2.6613968 18.7100512 3.1446010
H 0.9040768 20.4788227 3.7170160
H -6.7768309 19.1246431 4.1424920
H -8.4852665 17.2536844 3.8353700
H -10.8206926 17.7873950 2.7685650
H -11.3476684 20.2643259 2.1925430
H -9.5142260 21.9444524 2.0445330
Pt 8.0904460 8.4861901 2.8156140
C 11.8945087 6.3934263 2.4619530
C 12.3828407 7.7016085 2.7165950
C 11.2322041 8.5680215 2.8774100
N 10.0377756 7.7855003 2.8519440
C 10.4471833 6.4318874 2.6400500
C 6.1041251 4.8856948 3.9796300
C 7.4349652 4.4367381 3.9676720
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N 7.4078928 6.5611108 2.9634340
C 6.0903210 6.1775783 3.3184220
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C 4.2898185 10.5203259 2.3120200
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C 10.1565988 12.3180285 2.8131780
C 8.8496869 12.7685062 3.0331000
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N 8.7591383 10.4236450 2.8620950
C 10.1159342 10.8538136 2.8362880

C 11.2947982 10.0208393 2.9337650
C 6.5259984 11.6811567 2.9288180
C 3.6320738 6.1371712 2.8486970
C 10.0474165 3.8525077 2.7006530
C 12.6053431 10.7478289 3.0865850
C 5.8191313 12.9934386 2.9551560
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C 9.3469083 1.4289816 2.4750020
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C 2.5069589 3.9122094 2.4659860
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C 1.1323570 5.9435678 2.7247190
C 2.3083839 6.7096614 2.9734810
C 6.3833929 14.2711468 2.5567840
C 5.5977824 15.4521800 2.4661260
C 3.6009232 14.1516436 3.1329470
C 4.4442925 13.0518972 3.4059670
C 12.6468119 11.9903148 3.8231410
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H 7.8684158 3.4664377 4.3883860
H 3.5984154 11.4201973 2.2954570
H 2.7530123 8.8433104 2.1851720
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H	7.9457473	3.1322175	2.3636510
H	8.4863691	0.6744072	2.3177350
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H	12.8463260	1.6731463	2.5769870
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H	0.2499543	3.8925861	2.4046210
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H	2.1888697	7.7637401	3.3883640
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Au	-11.5116980	28.2466980	0.0000000
Au	4.3168870	35.7237660	0.0000000
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Au	-10.0727360	35.7237660	0.0000000
Au	5.7558490	33.2314110	0.0000000
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Au	-1.4389620	30.7390560	0.0000000
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Azobenzene dimer of 5-(4-Nitrophenyl)-10,15,20-tris(3,5-di-t-butylphenyl)porphyrin platinum(II) (**2**) on Au(111) Surface
(heterochiral, perpendicular orientation of macrocyclic saddlings, observed experimentally)

C	8.990475	11.524034	3.157556
N	7.949963	10.603513	2.889009
C	8.453895	9.333103	3.262401
C	9.738787	9.488306	3.930793
C	10.083568	10.848975	3.852091
Pt	5.961927	11.076824	2.760976
N	3.964205	11.551493	2.867472
C	3.438633	12.830521	3.196679
C	2.106158	12.680944	3.770214
C	1.760741	11.326859	3.684560
C	2.908391	10.629844	3.118980
C	4.070202	14.105850	2.936475
C	3.187531	15.307319	2.845717
C	3.609826	16.683142	3.025448
C	2.752245	17.797605	2.765589
C	1.337811	17.609244	2.488013
C	0.883869	16.227212	2.363246
C	1.788074	15.136221	2.476550
C	2.950803	9.203517	2.921745
C	4.192439	8.477669	2.746699
C	4.304946	7.040419	2.500295
C	5.678278	6.726154	2.482704
C	6.415589	7.967854	2.695074
N	5.491910	9.056080	2.853545
C	7.844873	8.063685	2.925659
C	8.745594	6.865948	2.907469
C	10.157626	7.063805	2.682940
C	11.110016	6.024305	2.895745
C	10.644140	4.677303	3.030867
C	9.241190	4.423908	3.098649
C	8.318359	5.514295	3.143919

C	12.509557	6.412706	3.395278
C	13.666419	5.492855	2.929171
C	8.706567	3.043688	3.505660
C	7.219955	2.881053	3.086289
N	0.376018	18.624308	2.289201
N	0.988522	19.896428	2.470666
C	-0.000511	20.880119	2.582274
C	-1.447879	20.714375	2.387067
C	-2.338116	21.843893	2.537813
C	-1.863410	23.154304	2.913477
C	-0.440623	23.259872	3.209287
C	0.463012	22.217190	2.939562
C	-2.733373	24.360045	2.944338
C	-2.136855	25.661023	2.687854
N	-2.783391	26.910504	2.902684
C	-1.775746	27.904618	2.732640
C	-0.518213	27.299638	2.334712
C	-0.761936	25.888197	2.254429
Pt	-4.818799	27.265134	2.832320
N	-4.482100	29.277693	3.017158
C	-3.237266	29.864714	3.322837
C	-3.416396	31.155070	3.979620
C	-4.800155	31.382675	4.030770
C	-5.449357	30.253535	3.367608
C	-1.958115	29.310079	2.982426
C	-0.844503	30.256616	2.754091
C	-1.177250	31.550322	2.164521
C	-0.195221	32.673375	2.193778
C	1.197266	32.258417	2.417137
C	1.547200	30.935766	2.812028
C	0.516317	29.964018	3.054052
C	-6.839808	30.189790	2.990350
C	-7.571991	31.500655	2.909482
C	-8.983096	31.672283	3.137558

C	-9.581626	32.971483	3.109714
C	-8.763962	34.139632	3.022464
C	-7.345394	34.005971	2.896492
C	-6.793864	32.705533	2.698341
C	-11.057813	33.105024	3.501573
C	-11.620141	34.485673	3.083445
C	-6.431088	35.128561	3.405825
C	-4.936636	34.807813	3.230200
C	-0.610179	33.833069	3.153630
C	0.240417	35.114663	3.032920
C	2.900982	30.675668	3.482595
C	3.537421	29.324707	3.090163
C	8.987195	12.933121	2.818105
C	10.310991	13.589083	2.702160
C	11.489860	12.792417	2.353562
C	12.815336	13.287778	2.656721
C	12.990468	14.694978	2.828436
C	11.844529	15.553578	2.909178
C	10.534910	14.991583	2.922369
C	13.839541	12.345499	3.316455
C	13.591053	12.676936	4.818774
C	11.997621	16.937328	3.544115
C	12.271541	16.627711	5.038427
C	1.665901	8.436099	2.958412
C	0.373600	8.996783	2.604595
C	-0.825575	8.231159	2.789018
C	-0.729146	6.807973	2.968326
C	0.541225	6.237691	3.280228
C	1.667634	7.083425	3.417219
C	0.735006	4.765736	3.653011
C	-0.482041	3.931965	3.213492
C	-2.071349	8.924027	3.366066
C	-2.092425	10.449975	3.198532
N	6.440212	13.104637	2.831541

C	5.510983	14.194604	2.713256
C	6.240153	15.429774	2.479671
C	7.620382	15.111866	2.430457
C	7.738498	13.671487	2.655718
C	12.826540	7.905465	3.172723
C	12.384605	6.216969	4.933001
C	9.614823	1.882277	3.017745
C	8.766033	3.060788	5.054204
C	13.587468	10.835843	3.129604
C	15.322238	12.668056	3.015804
C	13.172588	17.786128	3.025930
C	10.704028	17.770893	3.446347
C	2.061432	4.263563	3.033259
C	0.906284	4.685190	5.186233
C	-3.434837	8.307577	2.977484
C	-1.862195	8.661782	4.886930
C	-4.153631	24.233763	3.166504
N	-5.131483	25.231955	2.875538
C	-6.383470	24.626614	3.133234
C	-6.186801	23.292239	3.689944
C	-4.803367	23.041971	3.687742
C	-7.683830	25.216264	2.862091
C	-7.868793	26.654032	2.723208
N	-6.852807	27.634075	2.924023
C	-7.474314	28.908729	2.751420
C	-8.873029	28.724085	2.387238
C	-9.126352	27.320517	2.398602
C	-8.828342	24.284080	2.703240
C	-10.178922	24.648391	3.007929
C	-11.264509	23.740180	2.813970
C	-11.007331	22.372352	2.453741
C	-9.646745	21.889887	2.321413
C	-8.600781	22.918359	2.206542
C	-12.579413	24.053292	3.535949

C	-12.436710	23.349922	4.910590
C	-9.282330	20.661363	3.189060
C	-9.481885	21.275128	4.611034
C	-11.902217	31.907383	2.980545
C	-11.083454	33.039278	5.049091
C	-6.759387	36.559316	2.919660
C	-6.709316	35.119392	4.935200
C	-12.776142	25.567113	3.745382
C	-13.853361	23.489153	2.883259
C	-10.238300	19.459806	3.040482
C	-7.834161	20.146183	3.071803
C	-2.093201	34.241101	3.097155
C	-0.290447	33.193476	4.544713
C	3.912778	31.814422	3.280834
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Au	2.877925	34.892983	-4.699631
Au	4.316887	32.400627	-4.699631
Au	5.755849	29.908270	-4.699631
Au	7.194811	27.415914	-4.699631
Au	8.633774	24.923557	-4.699631
Au	10.072736	22.431202	-4.699631
Au	11.511698	19.938847	-4.699631

Au	12.950661	17.446491	-4.699631
Au	14.389623	14.954135	-4.699631
Au	15.828585	12.461779	-4.699631
Au	17.267548	9.969423	-4.699631
Au	18.706511	7.477067	-4.699631
Au	20.145472	4.984712	-4.699631
Au	21.584435	2.492356	-4.699631
Au	23.023397	0.000000	-4.699631
Au	0.000000	34.892983	-4.699631
Au	1.438962	32.400627	-4.699631
Au	2.877925	29.908270	-4.699631
Au	4.316887	27.415914	-4.699631
Au	5.755849	24.923557	-4.699631
Au	7.194811	22.431202	-4.699631
Au	8.633774	19.938847	-4.699631
Au	10.072736	17.446491	-4.699631
Au	11.511698	14.954135	-4.699631
Au	12.950661	12.461779	-4.699631
Au	14.389623	9.969423	-4.699631
Au	15.828585	7.477067	-4.699631
Au	17.267548	4.984712	-4.699631
Au	18.706511	2.492356	-4.699631
Au	20.145472	0.000000	-4.699631
Au	-2.877925	34.892983	-4.699631
Au	-1.438962	32.400627	-4.699631
Au	0.000000	29.908270	-4.699631
Au	1.438962	27.415914	-4.699631
Au	2.877925	24.923557	-4.699631
Au	4.316887	22.431202	-4.699631
Au	5.755849	19.938847	-4.699631
Au	7.194811	17.446491	-4.699631
Au	8.633774	14.954135	-4.699631
Au	10.072736	12.461779	-4.699631
Au	11.511698	9.969423	-4.699631

Au	12.950661	7.477067	-4.699631
Au	14.389623	4.984712	-4.699631
Au	15.828585	2.492356	-4.699631
Au	17.267548	0.000000	-4.699631
Au	-5.755849	34.892983	-4.699631
Au	-4.316887	32.400627	-4.699631
Au	-2.877925	29.908270	-4.699631
Au	-1.438962	27.415914	-4.699631
Au	0.000000	24.923557	-4.699631
Au	1.438962	22.431202	-4.699631
Au	2.877925	19.938847	-4.699631
Au	4.316887	17.446491	-4.699631
Au	5.755849	14.954135	-4.699631
Au	7.194811	12.461779	-4.699631
Au	8.633774	9.969423	-4.699631
Au	10.072736	7.477067	-4.699631
Au	11.511698	4.984712	-4.699631
Au	12.950661	2.492356	-4.699631
Au	14.389623	0.000000	-4.699631
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Au	-5.755849	29.908270	-4.699631
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Au	-2.877925	24.923557	-4.699631
Au	-1.438962	22.431202	-4.699631
Au	0.000000	19.938847	-4.699631
Au	1.438962	17.446491	-4.699631
Au	2.877925	14.954135	-4.699631
Au	4.316887	12.461779	-4.699631
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Au	8.633774	4.984712	-4.699631
Au	10.072736	2.492356	-4.699631
Au	11.511698	0.000000	-4.699631

Au -11.511698 34.892983 -4.699631
Au -10.072736 32.400627 -4.699631
Au -8.633774 29.908270 -4.699631
Au -7.194811 27.415914 -4.699631
Au -5.755849 24.923557 -4.699631
Au -4.316887 22.431202 -4.699631
Au -2.877925 19.938847 -4.699631
Au -1.438962 17.446491 -4.699631
Au 0.000000 14.954135 -4.699631
Au 1.438962 12.461779 -4.699631
Au 2.877925 9.969423 -4.699631
Au 4.316887 7.477067 -4.699631
Au 5.755849 4.984712 -4.699631
Au 7.194811 2.492356 -4.699631
Au 8.633774 0.000000 -4.699631
Au -14.389623 34.892983 -4.699631
Au -12.950661 32.400627 -4.699631
Au -11.511698 29.908270 -4.699631
Au -10.072736 27.415914 -4.699631
Au -8.633774 24.923557 -4.699631
Au -7.194811 22.431202 -4.699631
Au -5.755849 19.938847 -4.699631
Au -4.316887 17.446491 -4.699631
Au -2.877925 14.954135 -4.699631
Au -1.438962 12.461779 -4.699631
Au 0.000000 9.969423 -4.699631
Au 1.438962 7.477067 -4.699631
Au 2.877925 4.984712 -4.699631
Au 4.316887 2.492356 -4.699631
Au 5.755849 0.000000 -4.699631
Au -17.267548 34.892983 -4.699631
Au -15.828585 32.400627 -4.699631
Au -14.389623 29.908270 -4.699631
Au -12.950661 27.415914 -4.699631

Au -11.511698 24.923557 -4.699631
Au -10.072736 22.431202 -4.699631
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Au -7.194811 17.446491 -4.699631
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Au -2.877925 9.969423 -4.699631
Au -1.438962 7.477067 -4.699631
Au 0.000000 4.984712 -4.699631
Au 1.438962 2.492356 -4.699631
Au 2.877925 0.000000 -4.699631
Au -20.145472 34.892983 -4.699631
Au -18.706511 32.400627 -4.699631
Au -17.267548 29.908270 -4.699631
Au -15.828585 27.415914 -4.699631
Au -14.389623 24.923557 -4.699631
Au -12.950661 22.431202 -4.699631
Au -11.511698 19.938847 -4.699631
Au -10.072736 17.446491 -4.699631
Au -8.633774 14.954135 -4.699631
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Au -5.755849 9.969423 -4.699631
Au -4.316887 7.477067 -4.699631
Au -2.877925 4.984712 -4.699631
Au -1.438962 2.492356 -4.699631
Au 0.000000 0.000000 -4.699631

Azobenzene dimer of 5-(4-Nitrophenyl)-10,15,20-tris(3,5-di-t-butylphenyl)porphyrin platinum(II) (**2**) on Au(111) Surface
(homochiral, parallel orientation of macrocyclic saddlings, NOT observed experimentally)

C	10.180149	11.110578	2.349078
C	8.943258	11.832974	2.687931
N	7.896188	10.899753	2.905392
C	8.479462	9.598411	2.772024
C	4.370369	7.471041	4.028418
C	5.736470	7.155639	4.001343
C	6.413903	8.271968	3.346055
N	5.475297	9.281965	3.008795
C	4.217628	8.746375	3.347446
C	7.812958	8.340527	3.022045
C	1.875344	12.780365	2.211432
C	1.562073	11.369139	2.256104
C	2.785050	10.704309	2.703026
N	3.832093	11.656665	2.880177
C	3.248028	12.941765	2.646331
C	2.947461	9.286095	2.923490
C	7.350912	15.216958	3.666571
C	5.972217	15.475756	3.718915
C	5.299095	14.309900	3.173443
N	6.252696	13.304745	2.833514
C	7.518739	13.889641	3.089436
C	8.803844	13.278387	2.804626
C	3.882123	14.218049	2.956417
C	1.849967	8.307895	2.730764
C	8.557339	7.047948	2.946828
C	10.022702	14.147705	2.820520
C	3.058237	15.450743	2.926667
C	9.950328	6.909945	3.253020
C	10.607467	5.649760	3.131990
C	9.829631	4.462921	2.947453
C	8.405950	4.555532	2.805321

C	7.819400	5.848391	2.622952
C	2.164045	6.923024	2.441882
C	1.171535	5.883146	2.531358
C	-0.214168	6.262808	2.690096
C	-0.564663	7.638812	2.847794
C	0.460620	8.635478	2.898215
C	3.592135	16.739923	2.549385
C	2.749629	17.904425	2.423571
C	0.766767	16.453477	2.835160
C	1.628655	15.394685	3.184414
C	11.295970	13.601057	3.193454
C	12.504379	14.345017	3.091465
C	12.438480	15.753438	2.868512
C	11.158173	16.383396	2.753927
C	9.988019	15.577186	2.518131
C	1.610906	4.613169	3.293686
C	-1.928709	8.055080	3.416345
C	3.113301	4.285677	3.216838
C	-3.108515	7.140899	2.991062
C	12.093715	5.589476	3.509236
C	12.843921	6.877053	3.054301
C	7.541984	3.393436	3.323236
C	8.158700	1.999500	3.014207
C	13.806961	13.652497	3.502024
C	13.764719	12.162257	3.079029
C	11.017516	17.787417	3.355984
C	12.112552	18.805811	2.953180
C	1.283120	5.037998	4.759529
C	-1.752409	7.922817	4.951713
C	12.145623	5.551315	5.055970
C	7.682216	3.577838	4.865353
C	15.050968	14.408751	2.966373
C	9.610087	18.376788	3.195949
C	0.799335	3.333139	3.010613

C	-2.221286	9.549821	3.136509
C	12.748756	4.286963	2.998507
C	6.018011	3.506871	3.021771
C	13.864333	13.694921	5.046752
C	11.203770	17.495714	4.871609
C	1.297492	17.771349	2.514534
N	0.347328	18.797416	2.320204
C	9.882006	9.722772	2.446493
H	11.222666	11.540875	2.242954
H	3.494912	6.877920	4.457865
H	6.264336	6.222194	4.394518
Pt	5.866625	11.279985	2.812891
H	1.103417	13.603045	2.090218
H	0.493880	10.985365	2.273333
H	8.220667	15.809297	4.107958
H	5.408948	16.369734	4.161358
H	10.588657	8.861208	2.218860
H	10.546285	7.780807	3.673280
H	10.330703	3.435786	3.030676
H	6.703221	5.965249	2.465152
H	3.256711	6.614726	2.365565
H	-0.992797	5.457829	2.912480
H	0.179452	9.643884	3.335143
H	4.713169	16.845163	2.347796
H	3.190153	18.961909	2.343461
H	-0.378757	16.347024	2.940462
H	1.200160	14.452964	3.661479
H	11.345194	12.570353	3.659143
H	13.375829	16.383456	3.038770
H	8.987565	16.102458	2.386119
H	3.267634	3.318805	3.815381
H	3.457955	4.073713	2.132455
H	3.786104	5.098283	3.656252
H	-3.875361	7.718870	2.352069

H	-2.771993	6.230274	2.374546
H	-3.647023	6.761589	3.937093
H	13.852503	6.626915	2.555778
H	12.233637	7.479222	2.286472
H	13.040091	7.551603	3.966330
H	7.345361	1.245213	2.699746
H	8.950532	2.042541	2.179164
H	8.675326	1.599168	3.960960
H	14.830777	11.736996	2.985170
H	13.185136	11.546132	3.855480
H	13.245764	12.043201	2.056332
H	11.684150	19.587766	2.222678
H	12.477340	19.359101	3.892122
H	13.025468	18.313510	2.464110
H	1.850749	4.356562	5.493909
H	0.151121	4.921273	4.916679
H	1.536247	6.147386	4.931632
H	-2.699414	8.334506	5.458433
H	-0.832138	8.530666	5.276740
H	-1.599312	6.817624	5.231452
H	13.247895	5.488666	5.379926
H	11.574273	4.628048	5.434618
H	11.665243	6.504468	5.481298
H	7.117089	2.718312	5.376824
H	7.241652	4.586314	5.196640
H	8.796588	3.554384	5.143133
H	15.537659	15.007410	3.820768
H	14.768944	15.145098	2.127937
H	15.826959	13.674972	2.534103
H	9.620722	19.443078	3.625281
H	8.834741	17.753188	3.767869
H	9.298848	18.441137	2.077833
H	1.342853	2.661126	2.249824
H	0.715583	2.752421	4.001088

H	-0.265113	3.561464	2.634563
H	-1.821918	9.863616	2.095875
H	-3.356488	9.734194	3.164281
H	-1.725055	10.204537	3.937846
H	13.865349	4.451290	2.771507
H	12.636279	3.455432	3.784269
H	12.243159	3.923819	2.024351
H	5.615236	2.563878	2.498417
H	5.450315	3.619884	4.012413
H	5.719585	4.407442	2.380256
H	12.940689	13.168709	5.485361
H	14.826873	13.164681	5.389859
H	13.883127	14.791267	5.392330
H	12.289062	17.166367	5.054004
H	10.967343	18.458034	5.456102
H	10.504503	16.641401	5.195707
C	-9.000461	27.541333	2.338294
C	-7.749358	26.853644	2.671164
N	-6.732349	27.825962	2.894637
C	-7.347241	29.109878	2.751698
C	-3.289658	31.317025	4.022728
C	-4.660335	31.608907	3.990624
C	-5.322883	30.480074	3.337570
N	-4.366044	29.479553	3.017266
C	-3.117905	30.032712	3.365051
C	-6.720836	30.394707	2.990239
C	-0.660453	26.077945	2.208638
C	-0.398069	27.498942	2.278077
C	-1.646008	28.100847	2.724091
N	-2.662267	27.115347	2.893891
C	-2.027498	25.860310	2.665027
C	-1.833248	29.497512	2.991160
C	-6.087650	23.488196	3.636687
C	-4.700886	23.264776	3.709353

C	-4.049369	24.451856	3.181105
N	-5.025555	25.436750	2.847114
C	-6.280641	24.819600	3.074612
C	-7.577789	25.408813	2.795358
C	-2.630419	24.567681	2.953140
C	-0.753471	30.477047	2.734654
C	-7.501520	31.677268	2.928095
C	-8.771733	24.506040	2.755909
C	-1.775043	23.354312	2.910536
C	-8.915314	31.775272	3.181520
C	-9.589386	33.029139	3.101435
C	-8.837174	34.233936	2.968232
C	-7.413021	34.187019	2.848923
C	-6.786142	32.913420	2.687907
C	-1.154898	31.781358	2.230595
C	-0.228899	32.924111	2.260350
C	1.177660	32.606045	2.442232
C	1.612506	31.282586	2.756073
C	0.641767	30.243786	2.969853
C	-2.281854	22.054424	2.540382
C	-1.419208	20.902461	2.399401
C	0.537049	22.393735	2.831747
C	-0.342751	23.446044	3.156941
C	-10.068572	25.016985	3.096460
C	-11.262674	24.257166	2.959039
C	-11.162886	22.853128	2.684280
C	-9.866059	22.243234	2.614844
C	-8.697978	23.080393	2.420419
C	-0.703479	34.088519	3.172638
C	2.968547	31.127247	3.460774
C	-2.205116	34.421434	3.114034
C	3.913355	32.321804	3.250765
C	-11.059385	33.108102	3.523360
C	-11.888560	31.883224	3.040799

C	-6.608876	35.415177	3.311599
C	-7.288641	36.768676	2.941645
C	-12.540110	24.877542	3.534505
C	-12.554533	26.412063	3.339850
C	-9.725534	20.870041	3.293472
C	-10.806114	19.814980	2.945413
C	-0.354464	33.511487	4.584529
C	2.593150	31.144086	4.966421
C	-11.021930	33.076169	5.071406
C	-6.730532	35.303061	4.859698
C	-13.858677	24.269143	3.004552
C	-8.320239	20.263145	3.182019
C	0.083757	35.402436	3.014761
C	3.705135	29.809584	3.146870
C	-11.684741	34.460125	3.109644
C	-5.084971	35.348816	3.003294
C	-12.464537	24.585962	5.053762
C	-9.931838	21.257689	4.785894
C	0.034215	21.064588	2.516189
N	1.006693	20.059274	2.354322
C	-8.743666	28.938239	2.392669
H	-10.025938	27.083598	2.175166
H	-2.424112	31.944603	4.419605
H	-5.203559	32.529840	4.392967
Pt	-4.702781	27.469431	2.820134
H	0.147654	25.289271	2.113968
H	0.641889	27.957493	2.295999
H	-6.940709	22.867633	4.068309
H	-4.130447	22.377441	4.151320
H	-9.504648	29.760401	2.200962
H	-9.507980	30.888362	3.572063
H	-9.376398	35.232679	3.089242
H	-5.667205	32.837753	2.513594
H	-2.265217	32.028378	2.283536

H	1.928890	33.457377	2.545548
H	0.971733	29.308031	3.528205
H	-3.402499	21.937323	2.342551
H	-1.849114	19.835857	2.354322
H	1.681514	22.519051	2.933596
H	0.073780	24.391855	3.633413
H	-10.137630	26.029283	3.594987
H	-12.068274	22.182733	2.872106
H	-7.680425	22.576103	2.347438
H	-2.358242	35.379305	3.727134
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H	-2.888813	33.606465	3.528452
H	4.922072	32.054194	3.735194
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H	3.495601	33.248543	3.781830
H	-12.822724	32.218624	2.454576
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H	-12.225399	31.262552	3.951264
H	-6.577483	37.459963	2.353995
H	-8.234267	36.634240	2.301316
H	-7.597782	37.308170	3.911748
H	-13.633509	26.786020	3.474885
H	-11.887388	26.933855	4.113464
H	-12.208420	26.699321	2.275766
H	-10.359384	19.002535	2.259727
H	-11.163407	19.309146	3.913706
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H	1.911389	32.048607	5.167630
H	-12.089868	33.226442	5.473054

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H	-0.385626	36.082778	2.208272
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