Unveiling the promising anticancer activity of lipophilic platinum(II) complexes containg (1S, 4R, 5R)-4-(4-phenyl-1H-1,2,3-triazol-1-yl)-2-((S)-1-phenylethyl)-2-azabicyclo[3.2.1]octane: spectroscopical characterization and DFT calulation

Adriana Kaszuba[1], Jerzy Sitkowski[2,3], Tadeusz Muzioł[1], Elżbieta Wojaczyńska[4], Franz Steppeler[4], Karolina Pokrzywka[5], Łukasz Kaźmierski[5], Małgorzata Maj[5], Marcin Hoffmann[6], Iwona Łakomska[1*]

[1]*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland; iwona.lakomska@umk.pl (I.Ł.); akaszuba@doktorant.umk.pl (A.K.);*

[2]*National Institutes of Medicines, Chełmska 30/34, 00-725 Warszawa, Poland j.sitkowski@nil.gov.pl*

[3]*Institutes of Organic Chemistry, Polish Academic of Science, Kasprzaka 44/52, 01-224 Warszawa, Poland elzbieta.wojaczynska@pwr.edu.pl (E.W.), franz.steppeler@pwr.edu.pl (F.S)*

[4]F*aculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50 370 Wrocław, Poland*

[5]*Faculty of Medicine, Tissue Engineering Department, Collegium Medicum, Nicolaus Copernicus University, Karłowicza 24, 85-092 Bydgoszcz, Poland, m.maj@cm.umk.pl (M.M.); lukasz.kazmierski@cm.umk.pl (Ł.K.); karolinakowalska@doktorant.umk.pl (K.P.)*

[6]*Faculty of Chemistry, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 8, 61-614 Poznań Poland mmh@amu.edu.pl*

** Correspondence: iwona.lakomska@umk.pl; tel.: +48-56-611-4510*

Video S1. Real-time cell growth of 5637 cell line during 72h incubation with tested compounds

Video S2. Real-time cell growth of T24 cell line during 72h incubation with tested compounds

Video S3. Real-time cell growth of HT1376 cell line during 72h incubation with tested compounds

Video S4. Real-time cell growth of SV-HUC cell line during 72h incubation with tested compounds

Figure S1. NMR spectra of ligand (L) in $CDCl_3$

Table 1. Relative energies [kcal/mol] Cartesian coordinates [Å], and Mulliken point charges [*e*] in vaccuo and aquaeous solution for the studied systems:

(2) cis N3' 0.0 0.5

Atom	X	Y	Z	in vaccuo	aqua
Pt	1.459560	-0.706384	-0.630014	-0.081692	-0.009143
N	0.403358	0.899834	-0.068206	-0.457956	-0.464661
N	-0.888084	0.762867	0.209782	0.089847	0.065283
N	-1.277392	1.957181	0.699588	-0.126511	-0.128056
C	-0.237080	2.846451	0.735010	-0.323963	-0.299882
H	-0.335048	3.855895	1.090833	0.296950	0.330356
C	0.860419	2.161710	0.241557	0.253847	0.234612
C	2.274703	2.545145	0.108996	0.301631	0.310834
C	2.957976	2.337556	-1.104272	-0.318193	-0.328840
H	2.430363	1.935134	-1.963668	0.285723	0.269912
C	2.960885	3.054091	1.225811	-0.359208	-0.368806
H	2.440550	3.156436	2.171749	0.259390	0.268746
C	4.322061	2.642655	-1.195255	-0.240841	-0.256884
H	4.846152	2.473392	-2.129019	0.238572	0.253882
C	4.322898	3.369053	1.125739	-0.248232	-0.258185
H	4.851164	3.758634	1.989326	0.231109	0.254635
C	5.005698	3.161238	-0.083589	-0.237466	-0.249309
H	6.061874	3.398053	-0.158194	0.233554	0.256669
C	-2.680734	2.165792	1.119465	-0.099850	-0.104661
H	-2.633593	2.605919	2.121540	0.254400	0.288014
C	-3.428650	0.823232	1.218514	-0.407986	-0.407809
H	-4.263680	0.977605	1.930795	0.193737	0.219261
H	-2.772209	0.068066	1.658266	0.267273	0.249345

C	-3.394831	3.139997	0.150982	-0.149204	-0.155710
H	-2.851474	4.089478	0.112114	0.247856	0.272251
C	-4.874129	3.334338	0.591203	-0.443292	-0.449472
H	-4.984130	3.319958	1.681752	0.196286	0.208336
H	-5.231130	4.308514	0.244060	0.225813	0.232804
C	-3.537877	2.455240	-1.221000	-0.472203	-0.474816
H	-3.935451	3.161872	-1.957693	0.206979	0.219101
H	-2.613766	2.021306	-1.609589	0.260840	0.234869
C	-5.662499	2.174781	-0.100405	-0.445875	-0.449737
H	-6.187400	1.537711	0.619512	0.208095	0.213504
H	-6.412145	2.572778	-0.791399	0.224518	0.229670
C	-4.579062	1.369946	-0.885237	-0.117545	-0.125060
H	-4.978779	0.910677	-1.786768	0.257062	0.259830
N	-3.908943	0.337269	-0.076212	-0.180471	-0.193850
C	-4.482902	-1.018334	0.034009	-0.148556	-0.146922
H	-5.214643	-1.056078	0.868152	0.177292	0.198919
C	-3.371486	-2.024130	0.346684	0.433477	0.419360
C	-5.220892	-1.463893	-1.241286	-0.723035	-0.731164
H	-4.566127	-1.382348	-2.115237	0.227475	0.216662
H	-5.508511	-2.513698	-1.134291	0.232994	0.229987
H	-6.131069	-0.880943	-1.417638	0.200685	0.220256
C	-3.508817	-2.940280	1.401375	-0.448822	-0.457110
H	-4.391790	-2.901921	2.035608	0.226331	0.252507
C	-2.221145	-2.076644	-0.461313	-0.337674	-0.348843
H	-2.087284	-1.346098	-1.251669	0.284918	0.269904
C	-2.518457	-3.907561	1.642578	-0.237932	-0.260875
H	-2.638128	-4.613159	2.459070	0.217767	0.243736
C	-1.237856	-3.047785	-0.234349	-0.210244	-0.215744
H	-0.367196	-3.091191	-0.881293	0.278384	0.255218
C	-1.384118	-3.966802	0.819336	-0.299258	-0.307531
H	-0.627090	-4.728098	0.983356	0.233593	0.252921
S	2.245461	-0.903667	1.614197	0.688192	0.696468
C	4.104028	-0.829854	1.636626	-0.717727	-0.704226
H	4.429318	-1.004722	2.662195	0.269051	0.301277
H	4.470751	-1.576732	0.932954	0.292075	0.290544
H	4.356029	0.178434	1.307172	0.300478	0.299175
C	1.859903	-2.592580	2.292020	-0.722906	-0.709908
H	2.293908	-3.325031	1.611868	0.285497	0.287956
H	2.267895	-2.639549	3.301673	0.272761	0.304311
H	0.772327	-2.664368	2.293795	0.310937	0.304806
O	1.700423	0.208789	2.735304	-0.648165	-0.693937
Cl	0.646330	-0.431964	-2.840878	-0.208799	-0.299136
Cl	2.757382	-2.668029	-1.146280	-0.251782	-0.315643

(2) cis N3' 0.3 0.0

Atom	X	Y	Z	in vaccuo	aqua
Pt	2.781193	-0.405980	-0.494725	-0.059072	0.005014
N	0.810564	-0.276409	-0.863663	-0.443795	-0.446584
N	0.093043	-1.344535	-1.212677	0.023687	-0.008522
N	-1.197706	-0.946404	-1.126501	-0.133622	-0.125984
C	-1.298572	0.354858	-0.729364	-0.246552	-0.233526
H	-2.234251	0.857216	-0.568577	0.334334	0.344504
C	-0.000142	0.795571	-0.560143	0.229117	0.222193
C	0.498562	2.082467	-0.053566	0.316066	0.321916
C	1.556158	2.754973	-0.693764	-0.320561	-0.331744
H	1.998179	2.340564	-1.594702	0.288961	0.271247
C	-0.073092	2.621479	1.113706	-0.367419	-0.375803
H	-0.853158	2.069893	1.627705	0.258158	0.270410
C	2.039320	3.957619	-0.161391	-0.245548	-0.260108
H	2.860278	4.466916	-0.653136	0.240006	0.255285
C	0.404176	3.831707	1.634202	-0.257166	-0.262641
H	-0.035201	4.242012	2.537295	0.231948	0.257050
C	1.464218	4.499758	0.999394	-0.238663	-0.248966
H	1.839856	5.432638	1.406454	0.233863	0.257916
C	-2.261207	-1.951426	-1.339618	-0.102129	-0.111006
H	-2.165754	-2.301325	-2.371714	0.272987	0.295547
C	-3.645771	-1.314112	-1.153511	-0.459082	-0.467161
H	-4.377588	-1.984669	-1.640702	0.218504	0.242948
H	-3.707896	-0.364384	-1.695233	0.258485	0.262368
C	-2.056079	-3.129905	-0.354055	-0.157850	-0.150187
H	-1.087742	-3.593307	-0.547628	0.293717	0.282021
C	-3.234297	-4.137032	-0.462976	-0.457773	-0.463098
H	-3.602895	-4.236605	-1.490401	0.196691	0.209594
H	-2.891643	-5.127254	-0.149307	0.230508	0.234472
C	-2.208515	-2.588733	1.079479	-0.499654	-0.509070
H	-1.967845	-3.373477	1.805010	0.206344	0.219449
H	-1.588200	-1.718959	1.308298	0.292981	0.263791
C	-4.329677	-3.594361	0.513771	-0.450882	-0.454291
H	-5.284671	-3.403539	0.011030	0.204926	0.216312
H	-4.524976	-4.312270	1.316397	0.227314	0.233383
C	-3.717823	-2.287348	1.105180	-0.120027	-0.124416
H	-4.065915	-2.084402	2.115929	0.253220	0.263777
N	-3.975382	-1.091462	0.264661	-0.193967	-0.205442
C	-5.281658	-0.400056	0.393482	-0.152239	-0.153331
H	-6.029583	-0.876856	-0.271353	0.187526	0.208982
C	-5.113491	1.051432	-0.056373	0.466654	0.457031
C	-5.854915	-0.436930	1.820891	-0.721220	-0.729332
H	-5.131348	-0.051296	2.546773	0.216182	0.216246
H	-6.744359	0.198549	1.861682	0.232793	0.232289
H	-6.148745	-1.448432	2.117396	0.214149	0.225068
C	-5.909429	1.598794	-1.072970	-0.451380	-0.458915
H	-6.656795	0.979420	-1.562415	0.234992	0.256883
C	-4.148163	1.865263	0.566131	-0.416917	-0.429581
H	-3.527453	1.437390	1.348496	0.272176	0.281795
C	-5.743019	2.936799	-1.469191	-0.219996	-0.244334

H	-6.361702	3.347321	-2.260410	0.225707	0.246227
C	-3.974457	3.197379	0.171849	-0.212782	-0.237075
H	-3.216802	3.809781	0.650571	0.230930	0.246837
C	-4.773296	3.737895	-0.850595	-0.250003	-0.273987
H	-4.637320	4.768289	-1.161213	0.232063	0.250891
S	2.262033	-0.536790	1.843411	0.685045	0.692455
C	3.015235	0.931820	2.702541	-0.718875	-0.705949
H	2.822684	0.824783	3.770118	0.266954	0.300739
H	4.076176	0.944639	2.453282	0.291644	0.289681
H	2.505641	1.804468	2.293495	0.302426	0.298216
C	3.107569	-1.978566	2.661446	-0.709725	-0.699777
H	4.166707	-1.919908	2.412417	0.293061	0.288184
H	2.906712	-1.910446	3.730578	0.268098	0.300008
H	2.653654	-2.868589	2.229008	0.288355	0.299704
O	0.653366	-0.597725	2.300305	-0.656257	-0.690050
Cl	3.241793	-0.151165	-2.798716	-0.199571	-0.298363
Cl	5.097974	-0.536815	0.143204	-0.257846	-0.321195

(2) trans N3' 1.9 1.9

Atom	X	Y	Z	in vaccuo	aqua
Pt	-1.590722	-0.404685	-0.091054	-0.039781	0.020345
N	-0.228022	1.027188	-0.338670	-0.451109	-0.451152
N	1.002683	0.643782	-0.664592	0.092055	0.054783
N	1.706942	1.782184	-0.820793	-0.133548	-0.132723
C	0.923439	2.883067	-0.603505	-0.307165	-0.274348
H	1.287481	3.892363	-0.654765	0.298959	0.329100
C	-0.336601	2.399832	-0.285562	0.204582	0.192605
C	-1.570609	3.133791	0.039885	0.352585	0.335614
C	-2.325857	2.798455	1.178921	-0.320001	-0.329593
H	-1.994698	1.995843	1.830940	0.278894	0.269603
C	-1.989301	4.186494	-0.792507	-0.360361	-0.372936
H	-1.421620	4.424505	-1.686878	0.233725	0.261082
C	-3.494025	3.512447	1.473504	-0.252246	-0.265967
H	-4.070679	3.253653	2.355029	0.229427	0.252445
C	-3.156112	4.900644	-0.491092	-0.229850	-0.250369
H	-3.479713	5.705871	-1.141706	0.226649	0.253201
C	-3.911864	4.563440	0.642109	-0.227068	-0.245827
H	-4.817644	5.113835	0.873986	0.229415	0.255578
C	3.144949	1.717889	-1.185095	-0.087862	-0.090993
H	3.216143	2.019674	-2.236005	0.266176	0.297442
C	3.668192	0.276706	-1.055762	-0.413139	-0.409037
H	4.579734	0.211242	-1.681252	0.194094	0.221189
H	2.944988	-0.423161	-1.476501	0.296250	0.266466
C	3.962874	2.688230	-0.298967	-0.161264	-0.171048
H	3.617189	3.717312	-0.438031	0.239507	0.270891

C	5.478789	2.554949	-0.624319	-0.451405	-0.457799
H	5.655481	2.359878	-1.688087	0.199607	0.209374
H	5.984748	3.493791	-0.380122	0.225689	0.235092
C	3.889378	2.199238	1.160205	-0.466542	-0.473503
H	4.364069	2.925055	1.829600	0.205220	0.220599
H	2.877762	1.995289	1.518897	0.252874	0.236444
C	5.992537	1.393093	0.286743	-0.448036	-0.451648
H	6.441602	0.576956	-0.289112	0.211346	0.214376
H	6.752302	1.754599	0.986627	0.224258	0.231629
C	4.728884	0.911248	1.065445	-0.116585	-0.123994
H	4.974171	0.523581	2.051919	0.255318	0.259243
N	3.933627	-0.097525	0.337864	-0.181521	-0.198025
C	4.320559	-1.524447	0.442225	-0.144997	-0.142533
H	5.167315	-1.737829	-0.243289	0.177744	0.200517
C	3.146065	-2.405083	0.015370	0.439535	0.426292
C	4.766778	-1.914424	1.862962	-0.726157	-0.731273
H	4.007712	-1.623928	2.596955	0.224755	0.216110
H	4.882488	-3.000846	1.910347	0.235588	0.229307
H	5.725456	-1.462188	2.139029	0.195096	0.219000
C	3.308164	-3.383311	-0.977800	-0.454003	-0.460340
H	4.270596	-3.492677	-1.473544	0.220958	0.251763
C	1.895540	-2.268380	0.644657	-0.356421	-0.367975
H	1.747664	-1.490519	1.387011	0.269220	0.266095
C	2.236522	-4.216897	-1.341318	-0.230988	-0.260306
H	2.371285	-4.963970	-2.117623	0.212725	0.240959
C	0.830643	-3.107859	0.297335	-0.205999	-0.228906
H	-0.127081	-3.018434	0.799657	0.268115	0.265359
C	0.996107	-4.081236	-0.701794	-0.269444	-0.301274
H	0.158187	-4.716044	-0.969274	0.244151	0.249699
S	-3.158586	-2.180069	0.214609	0.706094	0.706389
C	-4.398455	-2.301237	-1.166587	-0.729428	-0.719864
H	-5.103408	-3.081864	-0.879909	0.268180	0.295922
H	-4.865530	-1.328664	-1.310634	0.273352	0.293931
H	-3.828946	-2.575842	-2.051679	0.316785	0.302973
C	-4.239075	-1.816811	1.685212	-0.723536	-0.711721
H	-4.725629	-0.853936	1.531504	0.256991	0.288780
H	-4.947973	-2.640259	1.771430	0.274328	0.298617
H	-3.560357	-1.776189	2.535794	0.316697	0.298317
O	-2.579005	-3.727751	0.438584	-0.620466	-0.700555
Cl	-1.070979	-0.502546	2.270482	-0.266590	-0.314561
Cl	-2.161319	-0.179630	-2.415113	-0.241434	-0.298862

(2) cis N2' 3.0 3.4

Atom	X	Y	Z	in vaccuo	aqua
Pt	-2.580225	-0.179368	0.726461	-0.051407	0.031585

N	-0.507390	1.886869	0.233170	-0.090596	-0.098645
N	-0.749225	0.584645	0.360531	-0.325972	-0.331714
N	0.399218	-0.111589	0.158196	-0.074267	-0.072224
C	1.399816	0.760842	-0.105289	-0.227009	-0.213469
H	2.396506	0.411516	-0.311027	0.346287	0.354903
C	0.826744	2.032511	-0.055473	0.034756	0.024546
C	1.452337	3.346438	-0.254661	0.356225	0.342457
C	0.755914	4.519777	0.087788	-0.350995	-0.362846
H	-0.240678	4.440027	0.508165	0.260506	0.268669
C	2.751477	3.444460	-0.786126	-0.328954	-0.340971
H	3.294022	2.546402	-1.066615	0.213749	0.240312
C	1.352431	5.772495	-0.099418	-0.234358	-0.257668
H	0.810496	6.672504	0.170593	0.228207	0.252136
C	3.347263	4.697749	-0.970182	-0.241819	-0.261507
H	4.348093	4.764338	-1.383588	0.225875	0.253681
C	2.649583	5.866573	-0.627985	-0.235308	-0.253104
H	3.110905	6.837807	-0.771075	0.230043	0.254812
C	0.435036	-1.592859	0.178208	-0.109942	-0.102692
H	-0.184213	-1.896113	1.027520	0.315308	0.300491
C	1.872969	-2.072395	0.418936	-0.464178	-0.464049
H	1.808125	-3.102756	0.810999	0.223818	0.241712
H	2.338841	-1.475114	1.208961	0.269178	0.266884
C	-0.137822	-2.166128	-1.140303	-0.124085	-0.131096
H	-1.166488	-1.828184	-1.276699	0.294956	0.292051
C	-0.014372	-3.714617	-1.129158	-0.454786	-0.457490
H	-0.169748	-4.133678	-0.129272	0.209942	0.211902
H	-0.784050	-4.141399	-1.778131	0.231411	0.235953
C	0.784755	-1.766494	-2.301140	-0.481865	-0.491951
H	0.342297	-2.075671	-3.253291	0.223262	0.226893
H	0.990404	-0.696483	-2.361817	0.249546	0.241038
C	1.414556	-4.014286	-1.692441	-0.450917	-0.454649
H	2.029094	-4.592879	-0.993480	0.204722	0.215691
H	1.354017	-4.590410	-2.621006	0.226394	0.234673
C	2.030428	-2.610520	-1.979040	-0.116616	-0.120209
H	2.731744	-2.625113	-2.811411	0.249927	0.264421
N	2.709838	-2.013594	-0.798090	-0.213077	-0.219853
C	4.089678	-2.469564	-0.487969	-0.144808	-0.147013
H	4.052416	-3.417193	0.085210	0.190667	0.209341
C	4.763691	-1.418988	0.394109	0.463393	0.448731
C	4.941383	-2.729231	-1.742493	-0.725784	-0.732861
H	4.935309	-1.862443	-2.411954	0.210836	0.215485
H	5.975694	-2.913710	-1.437953	0.233133	0.232172
H	4.593048	-3.604905	-2.298192	0.215371	0.225004
C	5.232873	-1.737735	1.676598	-0.436637	-0.447923
H	5.112333	-2.749169	2.055797	0.235534	0.256559
C	4.921535	-0.102713	-0.079287	-0.399697	-0.413353
H	4.568108	0.144773	-1.077441	0.245786	0.266580
C	5.844304	-0.760078	2.479271	-0.221969	-0.247792
H	6.196237	-1.018977	3.472346	0.226959	0.246917
C	5.527716	0.876085	0.716717	-0.216523	-0.245847

H	5.639094	1.889220	0.343042	0.222135	0.246472
C	5.990160	0.549789	2.002972	-0.248947	-0.273467
H	6.454602	1.308161	2.624073	0.231069	0.251082
S	-3.192310	0.580796	-1.462403	0.681337	0.692242
C	-3.514638	2.412486	-1.398331	-0.723490	-0.711238
H	-3.717101	2.743116	-2.417020	0.275165	0.299669
H	-4.349747	2.590628	-0.721554	0.268314	0.289078
H	-2.594486	2.846976	-1.007511	0.317841	0.308712
C	-4.785201	-0.109224	-2.130054	-0.720001	-0.709824
H	-5.590942	0.145237	-1.444694	0.286355	0.293912
H	-4.906146	0.313952	-3.127381	0.270738	0.299277
H	-4.653198	-1.188721	-2.162537	0.300784	0.302174
O	-2.038196	0.346518	-2.648716	-0.639734	-0.692882
Cl	-1.832642	-0.910407	2.852834	-0.201035	-0.291589
Cl	-4.793668	-0.991150	1.085580	-0.214750	-0.290292

(2) trans N3' 3.0 2.7

Atom	X	Y	Z	in vaccuo	aqua
Pt	-2.599816	-0.333137	0.175957	-0.025576	0.034239
N	-0.618551	-0.273386	0.378471	-0.438097	-0.437321
N	0.050966	-1.357670	0.774341	0.023998	-0.006097
N	1.356308	-1.012461	0.698088	-0.135961	-0.127173
C	1.513872	0.270230	0.261874	-0.252434	-0.228006
H	2.475000	0.730938	0.125849	0.343942	0.351232
C	0.234949	0.761477	0.057665	0.193626	0.187843
C	-0.166181	2.089952	-0.430671	0.365814	0.344696
C	-1.253852	2.782777	0.130675	-0.307278	-0.321897
H	-1.816811	2.348547	0.950640	0.279090	0.270149
C	0.574086	2.679910	-1.472031	-0.355988	-0.368026
H	1.395385	2.132244	-1.925638	0.225782	0.260094
C	-1.603916	4.046316	-0.361241	-0.246836	-0.271559
H	-2.453388	4.566212	0.066801	0.237013	0.253843
C	0.228443	3.948226	-1.952465	-0.241607	-0.257125
H	0.794578	4.391821	-2.764771	0.224157	0.254710
C	-0.865657	4.632705	-1.399950	-0.228799	-0.247824
H	-1.144075	5.609751	-1.780526	0.228574	0.255736
C	2.376858	-2.031344	1.019079	-0.101790	-0.111109
H	2.128907	-2.411012	2.014338	0.273882	0.295622
C	3.775248	-1.397866	1.063307	-0.459553	-0.466500
H	4.420248	-2.075906	1.651950	0.217294	0.242283
H	3.747108	-0.454332	1.617924	0.265339	0.265522
C	2.314889	-3.182363	-0.015131	-0.156528	-0.151232
H	1.320217	-3.630675	0.007321	0.295694	0.282115
C	3.445593	-4.211946	0.261225	-0.452154	-0.456782
H	3.636618	-4.339349	1.332833	0.197678	0.210391

H	3.147646	-5.189100	-0.129324	0.232013	0.235513
C	2.708859	-2.619626	-1.392410	-0.479682	-0.486749
H	2.572071	-3.382008	-2.166478	0.218514	0.227386
H	2.154304	-1.726720	-1.689058	0.250159	0.237117
C	4.695019	-3.665608	-0.506086	-0.451725	-0.455009
H	5.552849	-3.495195	0.154043	0.206372	0.216885
H	5.016970	-4.371715	-1.277628	0.228865	0.234609
C	4.205716	-2.340932	-1.167750	-0.119185	-0.122651
H	4.718148	-2.129959	-2.104267	0.254981	0.265552
N	4.331403	-1.157786	-0.280617	-0.199651	-0.210609
C	5.650766	-0.483526	-0.183477	-0.150974	-0.151309
H	6.280819	-0.994875	0.571558	0.188601	0.209637
C	5.430351	0.953754	0.288374	0.465753	0.454547
C	6.435124	-0.485397	-1.506940	-0.721763	-0.730462
H	5.833454	-0.072801	-2.323661	0.214467	0.216106
H	7.323421	0.142548	-1.392966	0.234535	0.232467
H	6.766588	-1.490491	-1.785039	0.213142	0.224872
C	6.039788	1.440354	1.453903	-0.446323	-0.453835
H	6.679576	0.784901	2.039379	0.234260	0.256905
C	4.602579	1.814383	-0.457085	-0.418105	-0.432451
H	4.129854	1.439080	-1.360752	0.264751	0.281029
C	5.822625	2.763053	1.875778	-0.220629	-0.245497
H	6.295819	3.125974	2.782228	0.226076	0.246614
C	4.377583	3.131160	-0.038406	-0.211297	-0.239056
H	3.724486	3.779158	-0.614114	0.232434	0.247150
C	4.987861	3.609749	1.133658	-0.247229	-0.271975
H	4.810188	4.627681	1.463406	0.233095	0.251024
S	-4.980248	-0.327762	-0.076903	0.700466	0.700200
C	-5.776668	-1.216179	1.352235	-0.724044	-0.713175
H	-6.851098	-1.211553	1.168520	0.270198	0.297258
H	-5.361560	-2.221418	1.417309	0.257511	0.289402
H	-5.512702	-0.635583	2.234552	0.317742	0.298835
C	-5.541961	-1.347296	-1.529161	-0.730122	-0.719088
H	-5.107549	-2.342778	-1.454780	0.266302	0.291457
H	-6.631836	-1.349836	-1.502461	0.267191	0.295736
H	-5.159902	-0.837877	-2.411105	0.315660	0.301390
O	-5.772937	1.130697	-0.215511	-0.619040	-0.710137
Cl	-2.867177	0.247526	2.501564	-0.262208	-0.316653
Cl	-2.270762	-0.963703	-2.124387	-0.260388	-0.310861

(2) trans N2' 3.1 5.4

Atom	X	Y	Z	in vaccuo	aqua
Pt	-2.436629	0.291488	0.212237	-0.030743	0.046055
N	-0.141624	2.139414	-0.151490	-0.046389	-0.088686
N	-0.548221	0.883374	-0.039766	-0.332543	-0.327240

N	0.521194	0.041561	-0.102032	-0.083802	-0.077532
C	1.643184	0.781702	-0.266861	-0.239377	-0.220542
H	2.604910	0.310905	-0.377776	0.345578	0.355765
C	1.225308	2.113856	-0.293369	0.035493	0.028862
C	2.022035	3.338463	-0.445656	0.350332	0.341823
C	1.391710	4.555882	-0.760365	-0.344873	-0.364609
H	0.314742	4.576547	-0.885269	0.269167	0.269386
C	3.418304	3.303116	-0.276325	-0.332667	-0.335345
H	3.908754	2.372794	-0.004429	0.221409	0.239205
C	2.153003	5.721237	-0.910886	-0.235485	-0.257898
H	1.661218	6.656820	-1.154657	0.227624	0.251717
C	4.177485	4.469111	-0.431698	-0.240914	-0.261597
H	5.253654	4.435331	-0.297137	0.221061	0.252564
C	3.547349	5.682171	-0.750569	-0.236327	-0.253610
H	4.135042	6.586288	-0.869100	0.228036	0.254399
C	0.370860	-1.430154	-0.016588	-0.096824	-0.090772
H	-0.364701	-1.609628	0.773088	0.315082	0.305096
C	1.701859	-2.065621	0.408314	-0.463966	-0.464363
H	1.462379	-3.051077	0.845972	0.222718	0.241891
H	2.157218	-1.477986	1.211540	0.268236	0.266837
C	-0.133153	-2.011182	-1.359515	-0.146075	-0.144975
H	-1.093269	-1.562839	-1.621159	0.320420	0.296543
C	-0.216350	-3.558857	-1.257504	-0.448813	-0.453139
H	-0.532694	-3.888698	-0.262341	0.208785	0.212461
H	-0.964286	-3.925008	-1.965506	0.239798	0.237353
C	0.954861	-1.805994	-2.425655	-0.488541	-0.496188
H	0.583552	-2.117714	-3.407386	0.223299	0.231160
H	1.318013	-0.779153	-2.509130	0.242504	0.241741
C	1.211656	-4.072007	-1.638014	-0.452165	-0.454975
H	1.666889	-4.675929	-0.844880	0.204484	0.216696
H	1.174662	-4.696138	-2.536268	0.227152	0.235202
C	2.035562	-2.779545	-1.924332	-0.118211	-0.122188
H	2.811437	-2.935754	-2.671534	0.252576	0.267560
N	2.662238	-2.196529	-0.707613	-0.208305	-0.215394
C	3.920391	-2.818118	-0.219214	-0.143686	-0.146752
H	3.683411	-3.711333	0.392504	0.189270	0.208574
C	4.649173	-1.820747	0.680514	0.469197	0.454209
C	4.852621	-3.278915	-1.353288	-0.725872	-0.732655
H	5.045616	-2.466977	-2.062459	0.212005	0.215694
H	5.810255	-3.586465	-0.923277	0.232951	0.232253
H	4.439709	-4.132230	-1.899426	0.215767	0.225166
C	4.927737	-2.123178	2.021442	-0.435434	-0.446890
H	4.604000	-3.075040	2.434416	0.235377	0.256474
C	5.069054	-0.581150	0.161892	-0.407330	-0.417978
H	4.859132	-0.342787	-0.877722	0.255741	0.271458
C	5.612271	-1.206376	2.836543	-0.222573	-0.248202
H	5.814781	-1.451352	3.873851	0.226884	0.247146
C	5.757731	0.332988	0.968312	-0.224305	-0.250619
H	6.091528	1.279247	0.553090	0.220281	0.245887
C	6.029576	0.024177	2.311916	-0.250572	-0.276356

H	6.558744	0.734026	2.938627	0.231177	0.251829
S	-4.682126	-0.471627	0.511966	0.699001	0.701528
C	-5.869033	0.403790	-0.623820	-0.723563	-0.714446
H	-6.867071	0.050590	-0.364291	0.269453	0.297133
H	-5.750446	1.478993	-0.497688	0.266833	0.293045
H	-5.581977	0.108535	-1.630773	0.317668	0.302138
C	-5.334401	-0.004789	2.191968	-0.722105	-0.712962
H	-5.227390	1.071040	2.324748	0.264648	0.292646
H	-6.371848	-0.337127	2.229012	0.271090	0.297939
H	-4.710639	-0.538718	2.906056	0.317596	0.301362
O	-4.980224	-2.100239	0.331189	-0.617991	-0.705912
Cl	-1.949824	-0.162146	2.530522	-0.256099	-0.305374
Cl	-2.864902	0.704431	-2.117186	-0.243146	-0.299599

(2) cis N3' 3.5 3.0

Atom	X	Y	Z	in vaccuo	aqua
Pt	-1.699108	-0.333617	-1.100990	-0.055068	0.011100
N	-0.482436	-0.829706	0.417509	-0.457094	-0.458150
N	0.813651	-1.042575	0.201150	0.046594	0.015119
N	1.327111	-1.389289	1.402718	-0.099798	-0.103035
C	0.361532	-1.379219	2.375139	-0.321713	-0.290759
H	0.556574	-1.634712	3.400766	0.295151	0.327164
C	-0.814900	-1.019112	1.741051	0.267781	0.248831
C	-2.184404	-0.844974	2.254795	0.285422	0.294512
C	-3.246057	-1.578537	1.690566	-0.320886	-0.326306
H	-3.050441	-2.290318	0.894262	0.286563	0.270949
C	-2.436944	0.083630	3.278926	-0.342515	-0.355668
H	-1.623894	0.686032	3.667427	0.259540	0.267465
C	-4.553234	-1.382722	2.155523	-0.247872	-0.259951
H	-5.367624	-1.946470	1.714889	0.240636	0.255985
C	-3.744585	0.267637	3.748770	-0.243131	-0.255774
H	-3.937105	0.988380	4.535857	0.232677	0.255476
C	-4.804031	-0.463730	3.187782	-0.242244	-0.251790
H	-5.816232	-0.317347	3.549829	0.235372	0.258128
C	2.761652	-1.724804	1.560040	-0.103180	-0.107833
H	2.872634	-1.957708	2.624622	0.221430	0.264464
C	3.659456	-0.513145	1.243624	-0.394762	-0.402362
H	4.609296	-0.656640	1.794714	0.200642	0.225093
H	3.200018	0.389895	1.650165	0.264829	0.259044
C	3.173213	-2.964398	0.727460	-0.160760	-0.166417
H	2.538918	-3.813862	0.995234	0.254381	0.266974
C	4.686015	-3.251874	0.967756	-0.438881	-0.444923
H	4.992993	-3.043276	1.999515	0.191195	0.207836
H	4.881807	-4.311783	0.781001	0.230372	0.234773
C	3.151673	-2.627348	-0.776432	-0.485706	-0.487347

H	3.394632	-3.524495	-1.357240	0.204342	0.212331
H	2.211951	-2.215260	-1.136885	0.305345	0.266008
C	5.440881	-2.356645	-0.070936	-0.457583	-0.462593
H	6.136672	-1.656511	0.404123	0.204458	0.213577
H	6.023443	-2.972776	-0.762554	0.226835	0.231573
C	4.306790	-1.614800	-0.848011	-0.087041	-0.093848
H	4.584607	-1.400856	-1.877435	0.242821	0.247840
N	3.874094	-0.355335	-0.196625	-0.194645	-0.208738
C	4.591763	0.886929	-0.550613	-0.123744	-0.125602
H	5.612215	0.887758	-0.113432	0.182332	0.203396
C	3.856251	2.105954	0.007909	0.414671	0.406103
C	4.730904	1.053984	-2.078491	-0.711029	-0.717180
H	3.757546	0.904984	-2.557182	0.231468	0.215729
H	5.073904	2.068604	-2.300735	0.229150	0.230322
H	5.454120	0.357099	-2.512980	0.200091	0.217288
C	4.589497	3.205969	0.480116	-0.441224	-0.450612
H	5.676525	3.170956	0.470691	0.227652	0.252347
C	2.450304	2.159924	0.031647	-0.414265	-0.420576
H	1.887501	1.299886	-0.321920	0.296428	0.292029
C	3.933610	4.345909	0.970581	-0.226934	-0.251826
H	4.512730	5.190547	1.330742	0.217906	0.242650
C	1.790620	3.281826	0.552823	-0.226287	-0.251450
H	0.707598	3.270527	0.640869	0.274809	0.278164
C	2.532232	4.381767	1.015459	-0.272969	-0.293696
H	2.021561	5.249137	1.421739	0.223982	0.245761
S	-2.063050	1.857082	-0.207502	0.683022	0.692811
C	-3.873697	2.065302	0.163767	-0.716386	-0.705248
H	-4.022651	3.092752	0.495970	0.269026	0.301068
H	-4.425334	1.818735	-0.742951	0.291939	0.290380
H	-4.091100	1.356226	0.962958	0.300417	0.297307
C	-1.732728	3.168435	-1.487847	-0.722613	-0.709581
H	-2.314162	2.916510	-2.374011	0.297611	0.293264
H	-2.005283	4.126891	-1.045919	0.269965	0.300830
H	-0.664075	3.118292	-1.692715	0.297092	0.299959
O	-1.241527	2.327043	1.169978	-0.650176	-0.686260
Cl	-1.420982	-2.536632	-1.920311	-0.200360	-0.294600
Cl	-3.190765	0.309800	-2.875198	-0.245084	-0.311521

(2) trans N3' 3.7 2.8

Atom	X	Y	Z	in vaccuo	aqua
Pt	-1.564881	-0.479730	0.022927	-0.058907	0.005181
N	-0.334209	1.025328	-0.415973	-0.454769	-0.458657
N	0.943057	0.750967	-0.663427	0.081997	0.057710
N	1.537948	1.944560	-0.859212	-0.134554	-0.133054
C	0.638375	2.970249	-0.749872	-0.309595	-0.276690

H	0.904400	4.006532	-0.848249	0.299890	0.330978
C	-0.582624	2.381173	-0.457877	0.209637	0.196252
C	-1.895841	3.004162	-0.230226	0.359665	0.338400
C	-2.709190	2.602020	0.845275	-0.302107	-0.315147
H	-2.366129	1.838197	1.535953	0.278382	0.271444
C	-2.338547	4.015575	-1.101372	-0.360375	-0.369601
H	-1.724812	4.304785	-1.949360	0.228611	0.260978
C	-3.961484	3.198663	1.032939	-0.244348	-0.270631
H	-4.588875	2.872007	1.854346	0.237056	0.253745
C	-3.586987	4.617588	-0.903090	-0.232698	-0.253631
H	-3.929100	5.388888	-1.584689	0.224652	0.253484
C	-4.402815	4.206407	0.162348	-0.225693	-0.246391
H	-5.376250	4.662409	0.308181	0.229822	0.255803
C	3.005261	2.025195	-1.062572	-0.096110	-0.098715
H	3.164559	2.423456	-2.070476	0.262136	0.295344
C	3.650007	0.628834	-0.985332	-0.409561	-0.408732
H	4.624715	0.701831	-1.505868	0.196978	0.223028
H	3.045620	-0.087614	-1.544020	0.281827	0.260525
C	3.618212	2.980163	-0.008136	-0.153285	-0.162628
H	3.185919	3.980538	-0.106217	0.243248	0.271611
C	5.166390	3.013566	-0.149023	-0.452190	-0.458396
H	5.486474	2.929640	-1.193847	0.198514	0.209732
H	5.543903	3.968772	0.227642	0.227238	0.234901
C	3.417088	2.353018	1.384441	-0.476058	-0.480634
H	3.730412	3.053022	2.166367	0.207745	0.221671
H	2.395708	2.025995	1.593454	0.262566	0.237041
C	5.682597	1.827124	0.728194	-0.447699	-0.451628
H	6.280875	1.111692	0.153772	0.208434	0.213781
H	6.310686	2.193178	1.546182	0.225672	0.231501
C	4.390214	1.163497	1.297532	-0.106873	-0.115374
H	4.551749	0.713202	2.274423	0.252123	0.256160
N	3.803665	0.150735	0.395491	-0.183127	-0.198675
C	4.356244	-1.221446	0.447186	-0.137697	-0.139006
H	5.342460	-1.259562	-0.061598	0.179200	0.201580
C	3.422783	-2.183246	-0.286061	0.403198	0.393652
C	4.552340	-1.717308	1.893121	-0.722058	-0.727072
H	3.632202	-1.570983	2.468541	0.233650	0.216964
H	4.778666	-2.787340	1.875998	0.230218	0.229348
H	5.378884	-1.210488	2.401342	0.198602	0.218291
C	3.932503	-3.105369	-1.213436	-0.446225	-0.455569
H	4.998050	-3.116407	-1.430691	0.227582	0.253063
C	2.043019	-2.170873	-0.016164	-0.328398	-0.340902
H	1.640965	-1.442950	0.680231	0.299942	0.286644
C	3.078697	-4.005669	-1.870952	-0.230133	-0.253879
H	3.484105	-4.711798	-2.588626	0.218735	0.243676
C	1.189904	-3.055595	-0.685119	-0.160987	-0.200113
H	0.120229	-2.998059	-0.503025	0.188519	0.218169
C	1.700732	-3.978190	-1.611770	-0.274504	-0.303411
H	1.034400	-4.656393	-2.135538	0.219895	0.248291
S	-3.054594	-2.256535	0.607534	0.704607	0.703188

C	-2.224511	-3.458856	1.762979	-0.730087	-0.717952
H	-2.933584	-4.268597	1.935216	0.272789	0.300857
H	-1.291822	-3.800004	1.314813	0.260129	0.282966
H	-2.024435	-2.895225	2.672107	0.317955	0.302027
C	-3.450184	-3.336604	-0.855946	-0.727719	-0.717735
H	-2.519351	-3.674658	-1.309388	0.260671	0.288495
H	-4.065723	-4.154842	-0.481903	0.269773	0.297889
H	-3.995826	-2.701165	-1.550285	0.319648	0.303247
O	-4.517361	-1.882482	1.311141	-0.615321	-0.705678
Cl	-0.680590	-0.453730	2.272431	-0.262770	-0.309307
Cl	-2.351898	-0.480406	-2.245569	-0.237459	-0.298410

(2) trans N3' 4.6 2.6 (optimized crystal structure)

Atom	X	Y	Z	in vaccuo	aqua
Pt	2.601960	-0.361769	-0.297564	-0.059601	0.019348
Cl	2.872743	-1.496918	1.843929	-0.310279	-0.336486
Cl	2.275444	0.795516	-2.352316	-0.202489	-0.298213
H	-5.130249	-1.976672	2.031093	0.255446	0.265962
C	-3.086303	-2.608551	1.575583	-0.485361	-0.491706
H	-2.514801	-1.751991	1.939383	0.248232	0.240910
H	-3.100260	-3.371277	2.361391	0.220004	0.229760
N	-1.373094	-1.121760	-0.381651	-0.130031	-0.120186
N	-0.076035	-1.456766	-0.566767	0.025720	-0.008577
N	0.619017	-0.416161	-0.103134	-0.431033	-0.432507
C	-0.210582	0.573041	0.380801	0.184289	0.178664
C	-1.501344	0.107885	0.196502	-0.258641	-0.233423
H	-2.459660	0.525330	0.448679	0.351892	0.361611
C	0.235007	1.857276	0.944478	0.351351	0.335741
C	-0.369240	3.044390	0.494888	-0.347955	-0.364498
H	-1.121319	3.001388	-0.287197	0.247496	0.264472
C	0.027066	4.278623	1.024859	-0.235145	-0.252057
H	-0.430272	5.193537	0.663470	0.225680	0.254371
C	1.030122	4.332480	2.004820	-0.229320	-0.249135
H	1.343059	5.289144	2.409796	0.228536	0.255639
C	1.631153	3.146859	2.455740	-0.250933	-0.266982
H	2.402177	3.184064	3.217889	0.227380	0.252952
C	1.235320	1.909664	1.932112	-0.326010	-0.330646
H	1.688955	0.991448	2.292989	0.274504	0.267880
H	-6.114498	0.165954	2.104622	0.213709	0.215865
C	-4.241675	3.252099	-0.027602	-0.236653	-0.254870
H	-3.665823	3.891338	0.634250	0.236382	0.250212
C	-4.590568	1.959913	0.382382	-0.406878	-0.419093
H	-4.284633	1.599529	1.360978	0.256116	0.270880
S	4.996459	-0.282150	-0.470663	0.730689	0.726331
O	5.850991	0.358177	-1.745445	-0.611310	-0.709058

C	5.658766	-2.008531	-0.234229	-0.725535	-0.711716
H	5.368060	-2.556968	-1.128831	0.291701	0.298098
H	5.201896	-2.434110	0.658101	0.282908	0.286646
H	6.743353	-1.922892	-0.166367	0.269996	0.296160
C	5.622554	0.592128	1.051850	-0.729962	-0.713385
H	6.710835	0.535358	1.025005	0.273687	0.298311
H	5.186757	0.111409	1.926811	0.277669	0.286030
H	5.284145	1.622840	0.954928	0.292163	0.297552
C	-4.521057	-2.230810	1.165927	-0.116054	-0.119676
N	-4.452389	-1.048257	0.270601	-0.208161	-0.217502
C	-3.755354	-1.340534	-0.996936	-0.450756	-0.454226
H	-3.581237	-0.404011	-1.536051	0.269452	0.265222
H	-4.376814	-1.968504	-1.660988	0.217618	0.241581
C	-2.423211	-2.076069	-0.784904	-0.113123	-0.123039
H	-2.092758	-2.492165	-1.740205	0.279104	0.294067
C	-2.562849	-3.209871	0.259109	-0.153587	-0.147686
H	-1.605127	-3.724627	0.359499	0.290091	0.278670
C	-3.718188	-4.166304	-0.150271	-0.445864	-0.450450
H	-3.781165	-4.295801	-1.236472	0.200417	0.210956
H	-3.539209	-5.155376	0.280688	0.232615	0.235907
C	-5.013316	-3.525702	0.450033	-0.452945	-0.456116
H	-5.765837	-3.304125	-0.314813	0.207838	0.217250
H	-5.479980	-4.198807	1.175712	0.228784	0.234552
C	-5.704895	-0.293760	0.005526	-0.145564	-0.145727
H	-6.270645	-0.782642	-0.812450	0.189251	0.209054
C	-6.640231	-0.218992	1.224466	-0.723734	-0.732354
H	-7.071457	-1.194288	1.469761	0.212923	0.224665
H	-7.463288	0.464852	0.998173	0.235213	0.232263
C	-5.337487	1.115269	-0.460109	0.471705	0.457274
C	-5.733282	1.591703	-1.718574	-0.440484	-0.450287
H	-6.308011	0.948182	-2.379792	0.234168	0.256299
C	-5.386044	2.887634	-2.135598	-0.222394	-0.248562
H	-5.693429	3.241352	-3.114087	0.227482	0.246711
C	-4.637562	3.720197	-1.292242	-0.245807	-0.271980
H	-4.365374	4.719727	-1.614195	0.233397	0.252279

(3) N3' 0.0 0.0

Atom	X	Y	Z	in vaccuo	aqua
Pt	1.578210	-0.407053	0.231883	0.462691	0.530307
N	0.132128	1.004892	0.279495	-0.463506	-0.470372
N	-1.071414	0.537983	0.614615	0.045137	0.036690
N	-1.868038	1.612071	0.747951	-0.116683	-0.118203
C	-1.177500	2.765203	0.501103	-0.308531	-0.283444
H	-1.620173	3.743405	0.526288	0.303190	0.330571
C	0.120904	2.380731	0.192432	0.179863	0.164796

C	1.282245	3.224359	-0.137158	0.329361	0.320454
C	2.054042	2.971362	-1.285636	-0.332411	-0.332819
H	1.803303	2.139317	-1.934092	0.326536	0.303733
C	1.605514	4.307267	0.701437	-0.369878	-0.374188
H	1.021263	4.488911	1.598875	0.234290	0.260208
C	3.151297	3.790718	-1.581342	-0.252329	-0.265194
H	3.743185	3.582627	-2.465670	0.251916	0.253229
C	2.698983	5.128300	0.397376	-0.232356	-0.252231
H	2.949767	5.957612	1.050116	0.225965	0.252419
C	3.475624	4.868972	-0.743233	-0.227678	-0.249781
H	4.326087	5.501325	-0.975571	0.230960	0.254236
C	-3.275801	1.418710	1.176825	-0.081285	-0.088679
H	-3.290322	1.547313	2.264344	0.284124	0.300788
C	-3.732110	-0.012715	0.843852	-0.414284	-0.413732
H	-4.608831	-0.231535	1.481747	0.203167	0.224460
H	-2.953034	-0.723024	1.122144	0.274385	0.263664
C	-4.200915	2.459682	0.503312	-0.179094	-0.186762
H	-3.913553	3.474093	0.795687	0.249555	0.275055
C	-5.683857	2.169212	0.878298	-0.453926	-0.459932
H	-5.783719	1.796358	1.903606	0.202096	0.209762
H	-6.259870	3.096980	0.815329	0.229422	0.235557
C	-4.196043	2.223218	-1.020202	-0.459353	-0.465038
H	-4.763815	3.010526	-1.528187	0.209371	0.220014
H	-3.201488	2.160628	-1.467390	0.248254	0.237604
C	-6.180334	1.134302	-0.184008	-0.449369	-0.452951
H	-6.543238	0.206772	0.271065	0.211207	0.215592
H	-7.001587	1.549705	-0.776000	0.227637	0.231812
C	-4.941141	0.875981	-1.096078	-0.123107	-0.127330
H	-5.223856	0.633848	-2.118202	0.258284	0.261779
N	-4.034164	-0.168701	-0.581129	-0.199810	-0.209134
C	-4.234650	-1.587479	-0.943452	-0.153573	-0.150404
H	-4.906824	-2.076674	-0.209979	0.185605	0.205115
C	-2.892107	-2.324395	-0.913761	0.441571	0.433219
C	-4.868364	-1.772562	-2.334809	-0.713831	-0.724968
H	-4.278183	-1.258382	-3.100899	0.221409	0.216051
H	-4.876866	-2.838352	-2.579724	0.236095	0.231594
H	-5.900994	-1.409857	-2.370294	0.204102	0.221557
C	-1.761400	-1.753018	-1.522890	-0.361352	-0.371113
H	-1.832146	-0.748106	-1.924845	0.263969	0.267971
C	-2.790131	-3.612478	-0.363365	-0.465417	-0.469083
H	-3.658057	-4.066149	0.110155	0.231733	0.254798
C	-0.553758	-2.458520	-1.596091	-0.204773	-0.211620
H	0.306093	-2.002208	-2.075350	0.276063	0.258502
C	-1.580338	-4.325127	-0.433046	-0.244534	-0.258672
H	-1.516212	-5.323424	-0.011095	0.225027	0.244509
C	-0.459468	-3.750268	-1.051313	-0.273129	-0.295869
H	0.478193	-4.293219	-1.107777	0.252985	0.252910
S	0.982975	-1.055086	2.448405	0.726127	0.733463
C	2.490118	-1.673016	3.345805	-0.717676	-0.709399
H	2.149338	-2.197128	4.238481	0.264798	0.293517

H	3.034351	-2.308756	2.647107	0.321064	0.307300
H	3.064793	-0.785704	3.605410	0.285393	0.296883
C	-0.043508	-2.592016	2.257627	-0.733274	-0.723876
H	0.552615	-3.324088	1.714335	0.296563	0.296978
H	-0.326106	-2.925198	3.256424	0.272585	0.300026
H	-0.910125	-2.300306	1.664753	0.309410	0.306396
O	0.155693	-0.029122	3.470092	-0.638555	-0.699352
O	2.879915	-1.937270	0.298834	-0.487913	-0.491481
O	1.995960	-0.029442	-1.689349	-0.481207	-0.493869
C	3.930142	-2.071042	-0.534974	0.286210	0.291817
C	3.213159	-0.212736	-2.237786	0.285572	0.289934
C	4.310810	-0.848648	-1.376973	-0.544448	-0.543300
H	5.134247	-1.125295	-2.033048	0.275345	0.264541
H	4.665196	-0.070965	-0.686191	0.252455	0.286126
O	4.596746	-3.115537	-0.567197	-0.305649	-0.369414
O	3.450998	0.174219	-3.392516	-0.312564	-0.373728

(3) N2' 8.5 8.5

Atom	X	Y	Z	in vaccuo	aqua
Pt	1.970764	-0.575353	-0.337552	0.468596	0.550689
N	0.805150	2.121854	-0.589734	-0.067211	-0.086379
N	0.697808	0.951464	0.031969	-0.350076	-0.351997
N	-0.292372	1.013914	0.966704	-0.069023	-0.073022
C	-0.820632	2.259867	0.940741	-0.264350	-0.254785
H	-1.614703	2.563617	1.593719	0.298849	0.325018
C	-0.132018	2.964140	-0.049684	0.060412	0.054499
C	-0.299038	4.348710	-0.514252	0.356072	0.343586
C	0.325239	4.766300	-1.704409	-0.346525	-0.361325
H	0.918761	4.054850	-2.267838	0.266383	0.269704
C	-1.077228	5.265430	0.216154	-0.340666	-0.352493
H	-1.554506	4.963806	1.143936	0.213311	0.246712
C	0.170195	6.082118	-2.156062	-0.234149	-0.257808
H	0.651609	6.395185	-3.076203	0.229421	0.251655
C	-1.233825	6.580244	-0.239446	-0.237607	-0.259625
H	-1.835467	7.280137	0.330352	0.227369	0.252207
C	-0.610237	6.993254	-1.426812	-0.231781	-0.251119
H	-0.731676	8.011747	-1.779503	0.231400	0.254553
C	-0.567343	-0.144000	1.862061	-0.039951	-0.042406
H	0.408071	-0.388056	2.298343	0.289920	0.296324
C	-1.098160	-1.362078	1.071866	-0.409456	-0.424482
H	-0.816261	-2.254928	1.662522	0.186017	0.203170
H	-0.596915	-1.453088	0.107661	0.331425	0.317140
C	-1.535289	0.236762	3.007695	-0.221035	-0.219390
H	-1.133530	1.090226	3.562803	0.268893	0.282854
C	-1.709666	-1.006736	3.932789	-0.453868	-0.459405

H	-0.783087	-1.583368	4.023306	0.204474	0.210072
H	-1.979576	-0.668338	4.937646	0.229179	0.239214
C	-2.987303	0.433918	2.503272	-0.475932	-0.481477
H	-3.622887	0.752739	3.338041	0.207213	0.221732
H	-3.123095	1.124433	1.670156	0.233422	0.236115
C	-2.869988	-1.836500	3.293756	-0.453724	-0.456144
H	-2.555395	-2.844101	3.009417	0.218389	0.217436
H	-3.706483	-1.939762	3.991950	0.225976	0.234474
C	-3.318853	-1.000564	2.054591	-0.112520	-0.113538
H	-4.376119	-1.136042	1.819594	0.271680	0.264988
N	-2.527966	-1.247705	0.837594	-0.193561	-0.191540
C	-3.082181	-2.141090	-0.200003	-0.147710	-0.138067
H	-2.343937	-2.140642	-1.013541	0.286809	0.249739
C	-4.366524	-1.519125	-0.755069	0.389458	0.374732
C	-3.236657	-3.602737	0.266685	-0.716829	-0.725710
H	-3.983191	-3.698646	1.064474	0.190072	0.208908
H	-3.528222	-4.249551	-0.566629	0.226518	0.218509
H	-2.277307	-3.972292	0.643386	0.219026	0.224724
C	-5.576598	-2.220407	-0.871373	-0.407973	-0.419358
H	-5.640784	-3.256532	-0.557093	0.241222	0.260947
C	-4.323835	-0.177012	-1.183149	-0.342334	-0.360041
H	-3.387758	0.365038	-1.087576	0.245291	0.258753
C	-6.720739	-1.596753	-1.399105	-0.244591	-0.270526
H	-7.647902	-2.155231	-1.481963	0.217388	0.242818
C	-5.457977	0.447339	-1.712111	-0.242284	-0.266654
H	-5.403027	1.479477	-2.044098	0.218758	0.243957
C	-6.666963	-0.262454	-1.820609	-0.242798	-0.266171
H	-7.549139	0.218020	-2.231498	0.221885	0.247606
S	3.458067	0.304199	1.287625	0.706989	0.719242
C	4.577432	1.583867	0.536212	-0.722455	-0.709893
H	5.194997	1.988728	1.337843	0.282961	0.303014
H	5.166119	1.105434	-0.245822	0.275148	0.294041
H	3.917807	2.344461	0.120361	0.304827	0.299920
C	4.629075	-1.012355	1.888799	-0.702286	-0.698549
H	4.929520	-1.597115	1.019386	0.330242	0.312881
H	5.451684	-0.516311	2.403275	0.259176	0.291351
H	4.043268	-1.623350	2.573336	0.291103	0.298485
O	2.726171	1.008865	2.613260	-0.636632	-0.697144
O	3.332899	-2.012105	-0.637576	-0.508968	-0.509128
O	0.619322	-1.358093	-1.584882	-0.478656	-0.500526
C	3.290563	-2.987101	-1.569933	0.287386	0.290210
C	0.793470	-2.541678	-2.214036	0.289815	0.293217
C	2.214475	-2.891088	-2.658620	-0.534459	-0.531313
H	2.190924	-3.840791	-3.189789	0.272493	0.261242
H	2.537403	-2.107039	-3.356030	0.251828	0.282814
O	4.135888	-3.891288	-1.578801	-0.300844	-0.364979
O	-0.177101	-3.264965	-2.481035	-0.296544	-0.354257

(1) trans N3', N3' 0.0 0.0 (optimized crystal structure)

Atom	X	Y	Z	in vaccuo	aqua
Pt	0.000096	-0.000432	-0.001159	0.223676	0.233555
Cl	-0.066385	0.886601	2.247798	-0.277249	-0.329677
Cl	0.066522	-0.887276	-2.250197	-0.277250	-0.329688
C	6.940702	2.300677	1.301269	-0.116941	-0.121323
H	7.564403	2.063912	2.161103	0.252714	0.265246
N	7.003242	1.167604	0.343953	-0.202436	-0.213892
C	6.282439	1.448724	-0.912684	-0.451155	-0.455889
H	6.208049	0.527206	-1.498891	0.266551	0.264288
H	6.839356	2.169272	-1.539867	0.212647	0.239732
C	4.881606	2.034295	-0.678423	-0.108277	-0.120384
H	4.518117	2.462811	-1.616536	0.272074	0.292372
C	4.901814	3.124916	0.419664	-0.155570	-0.149120
H	3.896148	3.533410	0.535080	0.297423	0.279720
C	5.958138	4.211142	0.073795	-0.447694	-0.452041
H	6.018206	4.399658	-1.004165	0.196378	0.209719
H	5.676584	5.154983	0.549424	0.230579	0.235150
C	7.305963	3.674865	0.660392	-0.452359	-0.455500
H	8.084977	3.570903	-0.103320	0.205032	0.216535
H	7.694065	4.352766	1.426991	0.226386	0.234076
C	5.471641	2.509131	1.709482	-0.483442	-0.489750
H	4.984950	1.581189	2.016744	0.252695	0.239038
H	5.400908	3.224638	2.535628	0.217619	0.228481
N	3.929008	0.967892	-0.324813	-0.134082	-0.124250
N	2.601465	1.225719	-0.407397	0.011921	-0.023317
N	1.998604	0.109490	0.005776	-0.421833	-0.426352
C	2.920912	-0.856029	0.353846	0.180250	0.168636
C	4.167908	-0.291660	0.139034	-0.264870	-0.237466
H	5.161014	-0.663746	0.313583	0.342446	0.354768
C	2.620406	-2.214867	0.833594	0.354271	0.335908
C	3.398379	-3.284986	0.352541	-0.354745	-0.362942
H	4.162521	-3.099306	-0.396987	0.241860	0.262248
C	3.165604	-4.588315	0.807756	-0.245088	-0.258001
H	3.760730	-5.409959	0.422364	0.218974	0.253346
C	2.149193	-4.832489	1.744659	-0.235371	-0.252383
H	1.961478	-5.843151	2.092744	0.222014	0.254448
C	1.373067	-3.766408	2.224136	-0.255725	-0.273215
H	0.585615	-3.947551	2.947639	0.226057	0.251966
C	1.606770	-2.459602	1.777461	-0.301607	-0.322141
H	1.013145	-1.636798	2.163326	0.287660	0.274589
C	8.330451	0.570143	0.052110	-0.143637	-0.146111
H	8.845187	1.161389	-0.731975	0.185827	0.207849
C	9.262224	0.528331	1.275892	-0.724210	-0.731109
H	9.583212	1.529229	1.580140	0.212374	0.224465
H	10.155877	-0.049082	1.021829	0.232699	0.231993

H	8.775148	0.039816	2.126394	0.215492	0.215961
C	8.125015	-0.843670	-0.491943	0.468281	0.454402
C	8.607806	-1.214181	-1.755654	-0.441901	-0.450432
H	9.128362	-0.481478	-2.367150	0.233008	0.256227
C	8.416506	-2.518596	-2.241299	-0.223069	-0.248183
H	8.789841	-2.790253	-3.223226	0.224938	0.246683
C	7.737980	-3.465925	-1.462179	-0.246628	-0.272258
H	7.585285	-4.472396	-1.837244	0.231298	0.252202
C	7.254709	-3.103425	-0.193263	-0.237027	-0.255327
H	6.729957	-3.830423	0.418596	0.237982	0.250876
C	7.448485	-1.802270	0.285472	-0.407395	-0.420676
H	7.072858	-1.521470	1.265675	0.263022	0.274045
C	-6.943084	-2.297419	-1.303480	-0.116899	-0.121276
H	-7.567654	-2.058932	-2.162208	0.252713	0.265244
N	-7.004025	-1.165881	-0.344211	-0.202463	-0.213915
C	-6.281917	-1.449473	0.911158	-0.451068	-0.455784
H	-6.206299	-0.528943	1.498742	0.266603	0.264297
H	-6.838541	-2.170724	1.537782	0.212636	0.239729
C	-4.881643	-2.035379	0.674349	-0.108360	-0.120471
H	-4.517340	-2.465726	1.611301	0.272088	0.292362
C	-4.903563	-3.124082	-0.425612	-0.155516	-0.149070
H	-3.898209	-3.532835	-0.542854	0.297385	0.279696
C	-5.959984	-4.210426	-0.080391	-0.447660	-0.452006
H	-6.018867	-4.400784	0.997309	0.196391	0.209727
H	-5.679427	-5.153567	-0.557992	0.230584	0.235154
C	-7.308246	-3.672501	-0.664471	-0.452364	-0.455508
H	-8.086290	-3.569455	0.100352	0.205034	0.216535
H	-7.697605	-4.348921	-1.431739	0.226387	0.234080
C	-5.474602	-2.505881	-1.713739	-0.483540	-0.489846
H	-4.987832	-1.577672	-2.020060	0.252717	0.239085
H	-5.405182	-3.220050	-2.541153	0.217633	0.228504
N	-3.928889	-0.968827	0.321687	-0.134020	-0.124181
N	-2.601372	-1.226815	0.404199	0.011912	-0.023340
N	-1.998409	-0.110337	-0.008152	-0.421852	-0.426372
C	-2.920616	0.855502	-0.355588	0.180279	0.168667
C	-4.167674	0.291078	-0.141289	-0.264961	-0.237576
H	-5.160815	0.663229	-0.315544	0.342480	0.354825
C	-2.619829	2.214642	-0.834291	0.354279	0.335914
C	-3.397270	3.284626	-0.352098	-0.354799	-0.362964
H	-4.161220	3.098559	0.397530	0.241854	0.262226
C	-3.164134	4.588258	-0.806263	-0.245035	-0.257999
H	-3.758831	5.409804	-0.419999	0.218957	0.253343
C	-2.147899	4.832849	-1.743248	-0.235367	-0.252375
H	-1.959908	5.843738	-2.090522	0.222014	0.254451
C	-1.372297	3.766895	-2.223856	-0.255700	-0.273197
H	-0.584971	3.948370	-2.947413	0.226052	0.251968
C	-1.606358	2.459798	-1.778225	-0.301657	-0.322166
H	-1.013122	1.637098	-2.164916	0.287656	0.274577
C	-8.330839	-0.568772	-0.049756	-0.143558	-0.146025
H	-8.845096	-1.161869	0.733246	0.185819	0.207837

C	-9.263538	-0.523612	-1.272713	-0.724233	-0.731133
H	-9.585337	-1.523616	-1.579034	0.212360	0.224454
H	-10.156675	0.053712	-1.016646	0.232701	0.231986
H	-8.776812	-0.033427	-2.122456	0.215483	0.215959
C	-8.124594	0.843578	0.497747	0.468203	0.454294
C	-8.605964	1.210789	1.762961	-0.441845	-0.450380
H	-9.125953	0.476524	2.373063	0.233000	0.256221
C	-8.413964	2.513871	2.251886	-0.223081	-0.248199
H	-8.786194	2.782949	3.234941	0.224940	0.246684
C	-7.736163	3.463187	1.474562	-0.246586	-0.272258
H	-7.582921	4.468631	1.852144	0.231294	0.252197
C	-7.254333	3.104008	0.204158	-0.237086	-0.255419
H	-6.730244	3.832608	-0.406364	0.237891	0.250857
C	-7.448781	1.804160	-0.277842	-0.407117	-0.420403
H	-7.074364	1.526008	-1.259263	0.262838	0.273896

(1) trans N3', N3' 4.6 3.6

Atom	X	Y	Z	in vaccuo	aqua
Pt	-0.018373	-0.056073	-0.128034	0.231599	0.239797
N	-2.010837	-0.220584	-0.029107	-0.427564	-0.431522
N	-2.583271	-1.425522	-0.007763	0.012469	-0.025901
N	-3.917896	-1.189078	-0.044903	-0.120859	-0.111165
C	-4.189209	0.148599	-0.082744	-0.293304	-0.255877
H	-5.198231	0.520006	-0.081926	0.355613	0.363095
C	-2.957402	0.782449	-0.070645	0.186176	0.174571
C	-2.679221	2.227654	-0.099274	0.363276	0.340184
C	-3.423513	3.047726	-0.966924	-0.353610	-0.368269
H	-4.144704	2.598158	-1.643623	0.218700	0.253944
C	-1.711898	2.803761	0.744036	-0.307398	-0.325684
H	-1.141465	2.178695	1.424020	0.285285	0.272213
C	-3.206630	4.430675	-0.993826	-0.241558	-0.257284
H	-3.775550	5.054389	-1.675528	0.220696	0.253268
C	-1.493032	4.186555	0.708966	-0.252623	-0.271320
H	-0.741257	4.622312	1.357998	0.225955	0.252090
C	-2.237957	5.003499	-0.155138	-0.233667	-0.251337
H	-2.061964	6.074070	-0.179785	0.222865	0.254825
C	-4.844004	-2.332493	-0.015441	-0.115400	-0.125856
H	-4.273474	-3.173594	-0.417342	0.275666	0.285941
C	-6.058995	-2.059711	-0.924816	-0.440600	-0.443397
H	-6.500757	-3.036215	-1.191452	0.207668	0.230143
H	-5.718701	-1.598676	-1.858264	0.242990	0.250954
C	-5.283707	-2.655323	1.436944	-0.146676	-0.141409
H	-4.396224	-2.880495	2.032728	0.280217	0.272449
C	-6.311344	-3.821609	1.427583	-0.451030	-0.454655
H	-6.086998	-4.564660	0.654150	0.199523	0.210956

H	-6.280038	-4.339718	2.390413	0.231550	0.237094
C	-6.129695	-1.496832	2.002179	-0.493714	-0.500426
H	-6.384414	-1.697604	3.048897	0.217178	0.229342
H	-5.655976	-0.516118	1.950921	0.262512	0.251242
C	-7.699368	-3.134502	1.208482	-0.444793	-0.447868
H	-8.212489	-3.508456	0.318529	0.213172	0.221859
H	-8.360408	-3.311182	2.063005	0.226343	0.233935
C	-7.378324	-1.607946	1.106181	-0.110172	-0.113691
H	-8.202544	-0.983157	1.455221	0.263906	0.267008
N	-7.005107	-1.162767	-0.256063	-0.207566	-0.217391
C	-8.070614	-0.590703	-1.111185	-0.143095	-0.139740
H	-7.586956	-0.391443	-2.077097	0.213861	0.228120
C	-8.492363	0.766265	-0.543604	0.441597	0.416162
C	-9.249117	-1.548934	-1.384711	-0.715706	-0.720990
H	-8.887868	-2.466202	-1.862220	0.211101	0.222201
H	-9.766373	-1.834687	-0.463023	0.203173	0.210310
H	-9.978053	-1.080530	-2.054037	0.226206	0.224253
C	-7.611280	1.854971	-0.690676	-0.364681	-0.378803
H	-6.688326	1.718470	-1.248827	0.213840	0.233563
C	-9.695229	0.969510	0.151008	-0.378504	-0.386171
H	-10.403323	0.155409	0.268229	0.230980	0.253488
C	-7.909773	3.108250	-0.146002	-0.236864	-0.263280
H	-7.212691	3.930920	-0.267268	0.230827	0.247639
C	-10.002921	2.225647	0.699808	-0.250522	-0.276509
H	-10.936117	2.364698	1.236068	0.221994	0.245149
C	-9.110913	3.296748	0.558344	-0.240498	-0.266017
H	-9.347488	4.265685	0.985126	0.228896	0.250183
Cl	-0.172593	0.004995	-2.530269	-0.261516	-0.323166
Cl	0.139119	-0.112836	2.295589	-0.295104	-0.338514
N	1.971346	0.114621	-0.267541	-0.427575	-0.432024
N	2.537108	1.321888	-0.237955	0.015919	-0.021562
N	3.859380	1.105408	-0.437018	-0.119479	-0.110545
C	4.131826	-0.223861	-0.585157	-0.297409	-0.259108
H	5.132472	-0.593688	-0.712735	0.327715	0.344087
C	2.912190	-0.873551	-0.473154	0.201361	0.187917
C	2.636499	-2.317743	-0.546773	0.360671	0.338867
C	3.292136	-3.089910	-1.522962	-0.358846	-0.371995
H	3.948955	-2.606431	-2.240035	0.226606	0.259046
C	1.757974	-2.939957	0.359312	-0.305956	-0.322969
H	1.259039	-2.353146	1.124198	0.286336	0.273290
C	3.072353	-4.470768	-1.597014	-0.237052	-0.256001
H	3.574514	-5.057570	-2.358911	0.220750	0.252444
C	1.535265	-4.319919	0.276516	-0.252995	-0.271127
H	0.851248	-4.790523	0.974290	0.226336	0.252015
C	2.190073	-5.088930	-0.697578	-0.232085	-0.249524
H	2.012152	-6.157718	-0.758666	0.222843	0.254636
C	4.769059	2.263608	-0.393786	-0.098057	-0.110426
H	4.249427	3.065918	-0.924478	0.271826	0.287583
C	6.089863	1.952599	-1.121864	-0.458165	-0.465370
H	6.532413	2.922634	-1.409874	0.209435	0.231351

H	5.883213	1.415578	-2.054789	0.242311	0.255544
C	5.016264	2.695449	1.075210	-0.157875	-0.151878
H	4.055232	2.926678	1.539264	0.290995	0.277022
C	6.006542	3.890873	1.115764	-0.448514	-0.451996
H	5.864010	4.574533	0.271130	0.196487	0.209424
H	5.839995	4.469528	2.028881	0.231517	0.236276
C	5.807834	1.594473	1.808802	-0.483788	-0.491129
H	5.910565	1.849307	2.869179	0.218697	0.227879
H	5.365534	0.598687	1.736450	0.248022	0.240100
C	7.426665	3.237522	1.119845	-0.456493	-0.459678
H	8.041951	3.572034	0.280689	0.211679	0.221096
H	7.967697	3.488491	2.037659	0.228386	0.234167
C	7.162117	1.698677	1.081337	-0.104815	-0.101327
H	7.953936	1.131917	1.573687	0.271019	0.267501
N	6.979315	1.146126	-0.281889	-0.217246	-0.225708
C	8.164051	0.594609	-0.967742	-0.092463	-0.091333
H	7.785850	0.212876	-1.928701	0.220536	0.236261
C	8.713002	-0.620009	-0.204768	0.365923	0.349691
C	9.248217	1.648068	-1.298605	-0.708193	-0.713554
H	8.792429	2.522740	-1.774337	0.211793	0.223283
H	9.772871	1.976504	-0.395277	0.214874	0.213706
H	9.986423	1.249067	-2.001077	0.212873	0.219691
C	7.832405	-1.462985	0.501024	-0.341081	-0.348558
H	6.783062	-1.197727	0.557216	0.243570	0.250551
C	10.076919	-0.961148	-0.233335	-0.389197	-0.403341
H	10.789356	-0.334719	-0.758387	0.227304	0.250154
C	8.295069	-2.613120	1.150694	-0.249786	-0.276080
H	7.595148	-3.244950	1.687636	0.229589	0.245736
C	10.546174	-2.113252	0.417383	-0.244563	-0.270383
H	11.603339	-2.356294	0.382094	0.221484	0.244575
C	9.657928	-2.946649	1.109909	-0.242047	-0.267303
H	10.019997	-3.837499	1.612256	0.228016	0.249288

(1) cis N3', N3' 11.6 2.5

Atom	X	Y	Z	in vaccuo	aqua
Pt	0.172381	-3.232420	-0.023200	0.160555	0.192116
N	1.397172	-1.695406	-0.496176	-0.435381	-0.446753
N	1.009275	-0.847419	-1.455861	-0.008043	-0.015484
N	1.974800	0.102796	-1.511643	-0.122708	-0.111360
C	2.958499	-0.132264	-0.597858	-0.281348	-0.239894
H	3.770443	0.558138	-0.455677	0.342881	0.351038
C	2.594222	-1.297140	0.063944	0.172469	0.165450
C	3.313504	-1.950920	1.167882	0.385859	0.358755
C	4.720733	-1.933801	1.159599	-0.352960	-0.367324
H	5.249836	-1.506714	0.311985	0.213972	0.253491

C	2.635298	-2.552746	2.241688	-0.279893	-0.310652
H	1.551278	-2.580121	2.252252	0.275551	0.276758
C	5.442820	-2.510163	2.210598	-0.244259	-0.261104
H	6.527587	-2.508543	2.186751	0.220885	0.253236
C	3.359375	-3.137384	3.286585	-0.255115	-0.279778
H	2.826898	-3.618909	4.099157	0.229683	0.252057
C	4.761952	-3.115636	3.278047	-0.230627	-0.250989
H	5.318537	-3.578340	4.086305	0.225538	0.254730
C	1.783614	1.251538	-2.410677	-0.125551	-0.137300
H	1.241407	0.861925	-3.276183	0.273844	0.287805
C	3.140100	1.818127	-2.872367	-0.447516	-0.452194
H	2.961161	2.382678	-3.804553	0.211045	0.232797
H	3.814357	0.993090	-3.126737	0.243653	0.252503
C	0.922266	2.333490	-1.707614	-0.143923	-0.140189
H	-0.037303	1.888793	-1.433371	0.288511	0.286773
C	0.766085	3.573154	-2.629254	-0.465376	-0.467795
H	0.681413	3.294617	-3.685339	0.206635	0.215144
H	-0.150199	4.110561	-2.365254	0.228066	0.236516
C	1.699220	2.923637	-0.513414	-0.478283	-0.484481
H	1.067445	3.638099	0.028887	0.204817	0.224465
H	2.076363	2.187965	0.198873	0.259938	0.249609
C	2.029878	4.448416	-2.343126	-0.445163	-0.447603
H	2.622687	4.627312	-3.243798	0.216964	0.222452
H	1.744664	5.426648	-1.942992	0.226723	0.234981
C	2.830899	3.655102	-1.260136	-0.125187	-0.127942
H	3.410167	4.309720	-0.606673	0.266221	0.267112
N	3.744178	2.630493	-1.813332	-0.203699	-0.214106
C	5.163441	3.007501	-2.013244	-0.145182	-0.139812
H	5.635666	2.120721	-2.457646	0.216063	0.229300
C	5.820683	3.218767	-0.647595	0.440538	0.415353
C	5.376316	4.175869	-2.998591	-0.715559	-0.722090
H	4.947448	3.930751	-3.976281	0.211525	0.222808
H	4.901867	5.098239	-2.648051	0.202416	0.210722
H	6.444379	4.372920	-3.135707	0.229452	0.224786
C	6.091211	2.088533	0.147498	-0.352689	-0.368815
H	5.884195	1.097512	-0.248445	0.206206	0.227354
C	6.131196	4.487392	-0.132609	-0.379953	-0.386284
H	5.951989	5.377857	-0.726551	0.231702	0.253850
C	6.638615	2.216704	1.428278	-0.240259	-0.266298
H	6.834642	1.331292	2.023925	0.233276	0.247533
C	6.682992	4.624540	1.152079	-0.251163	-0.276533
H	6.916873	5.612760	1.534697	0.223272	0.245236
C	6.933319	3.492308	1.938423	-0.239793	-0.264956
H	7.358178	3.598534	2.930915	0.230708	0.250237
Cl	1.894911	-4.760276	-0.649684	-0.226574	-0.317633
Cl	-1.332558	-4.966669	0.632219	-0.226705	-0.317473
N	-1.235301	-1.856859	0.451872	-0.436316	-0.448751
N	-0.917092	-0.939737	1.373296	-0.007171	-0.011704
N	-2.003047	-0.136651	1.479486	-0.120555	-0.109061
C	-2.997590	-0.533253	0.636695	-0.286502	-0.246309

H	-3.922542	0.006802	0.553137	0.324550	0.340523
C	-2.508612	-1.645746	-0.037675	0.179461	0.171034
C	-3.181636	-2.409971	-1.099141	0.384708	0.359727
C	-4.580413	-2.555860	-1.047220	-0.357408	-0.369062
H	-5.135251	-2.163866	-0.199495	0.220607	0.256941
C	-2.468066	-2.958705	-2.178816	-0.277794	-0.307167
H	-1.388826	-2.861147	-2.222707	0.275285	0.275109
C	-5.258363	-3.243210	-2.060271	-0.241430	-0.261042
H	-6.335097	-3.363225	-2.004383	0.221305	0.252436
C	-3.147014	-3.654077	-3.185046	-0.253983	-0.278860
H	-2.584383	-4.093177	-4.001285	0.229815	0.251963
C	-4.541557	-3.796600	-3.132379	-0.229421	-0.249612
H	-5.062822	-4.343969	-3.910717	0.225454	0.254489
C	-1.912777	1.042558	2.356294	-0.115126	-0.128086
H	-1.357133	0.711751	3.237847	0.271645	0.287391
C	-3.310641	1.519073	2.793264	-0.454953	-0.461565
H	-3.175600	2.089740	3.729006	0.210438	0.231711
H	-3.936666	0.654780	3.042128	0.245680	0.255518
C	-1.118714	2.171463	1.647573	-0.144073	-0.140300
H	-0.133575	1.785994	1.373654	0.289021	0.284531
C	-1.037797	3.419151	2.567398	-0.462574	-0.465226
H	-0.937339	3.147014	3.623807	0.205793	0.214551
H	-0.154653	4.009580	2.304145	0.228195	0.236125
C	-1.931889	2.707706	0.452144	-0.479507	-0.485881
H	-1.343355	3.450216	-0.100173	0.208206	0.225481
H	-2.269172	1.940116	-0.248218	0.249170	0.244027
C	-2.350742	4.216829	2.279427	-0.457765	-0.460164
H	-2.955177	4.361618	3.178300	0.216124	0.221691
H	-2.124207	5.210231	1.879462	0.228543	0.235901
C	-3.101379	3.380229	1.194613	-0.116371	-0.113020
H	-3.714484	4.004785	0.543036	0.272749	0.267836
N	-3.958045	2.301183	1.736623	-0.214018	-0.222172
C	-5.386706	2.604252	1.960028	-0.099493	-0.095976
H	-5.829532	1.656404	2.302105	0.224603	0.237038
C	-6.073022	2.951841	0.631179	0.368098	0.352041
C	-5.642162	3.647944	3.072278	-0.712129	-0.718387
H	-5.077328	3.387811	3.973536	0.213334	0.224789
H	-5.344578	4.652581	2.753516	0.212534	0.213641
H	-6.699676	3.674028	3.352532	0.218175	0.221128
C	-5.694068	2.279652	-0.547498	-0.336371	-0.341823
H	-4.872251	1.574003	-0.510063	0.233743	0.242595
C	-7.117419	3.889448	0.552607	-0.392918	-0.407324
H	-7.435739	4.433151	1.434899	0.233074	0.254595
C	-6.340655	2.527316	-1.763486	-0.249022	-0.274351
H	-6.031551	1.992696	-2.655704	0.230518	0.246208
C	-7.768377	4.143524	-0.665449	-0.244060	-0.270421
H	-8.572610	4.871219	-0.702170	0.223653	0.244752
C	-7.386065	3.462308	-1.828238	-0.241538	-0.267112
H	-7.891184	3.656013	-2.768572	0.229959	0.249481