

Insights into the Intermolecular Interactions Between Stacked Antiaromatic 24- π Hexaphyrin Macrocycles. Variation of the Magnetic Response Properties

Alvaro Muñoz-Castro^{*a}

^a Facultad de Ingeniería, Universidad San Sebastián, Bellavista 7, Santiago, 8420524, Chile

Content

Figure S1. Distance between naphthorosarin rings, obtained from the distance between the respective centroids from each 24- π electron backbone. Page S2

Figure S2. Anisotropic term (NICS_{aniso}) for benzene, under two views. Isosurface values set to 9.0, 18.0, and 26.0 ppm. Page S3

Figure S3. Frontier orbitals from **1** and the resulting **1**₂, denoting the paramagnetic contribution to the overall NICS_{zz} probe at the center of each naphthorosarin (**1**) unit. Page S3

Table S1. Optimized coordinates for the studied species. Page S4

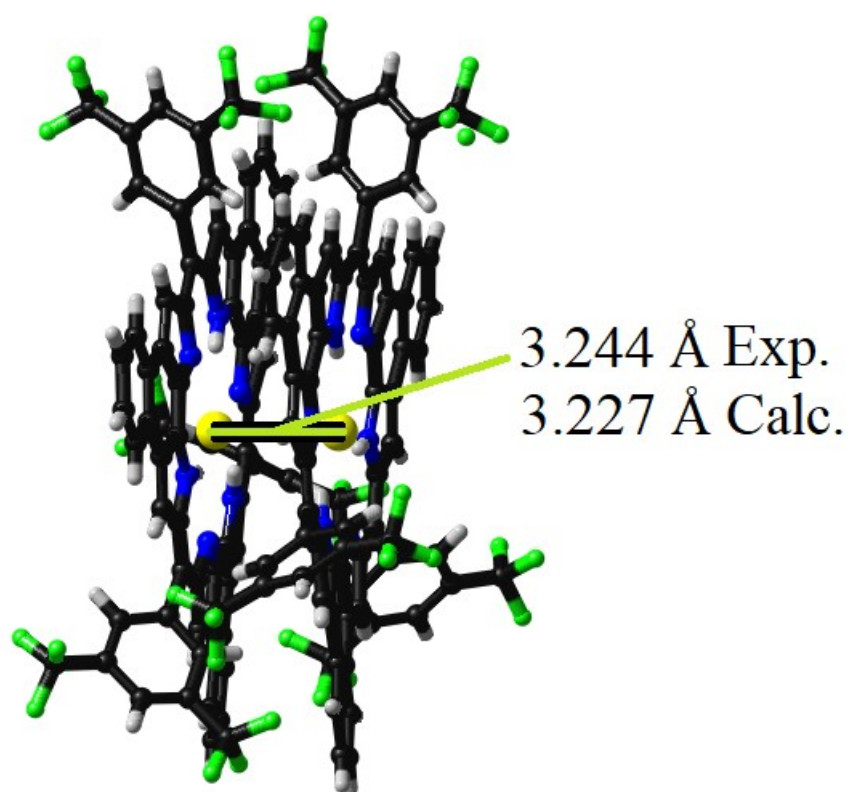


Figure S1. Distance between naphthorosarin rings, obtained from the distance between the respective centroids (yellow spheres) from each 24- π electron backbone in the dimer **1₂**.

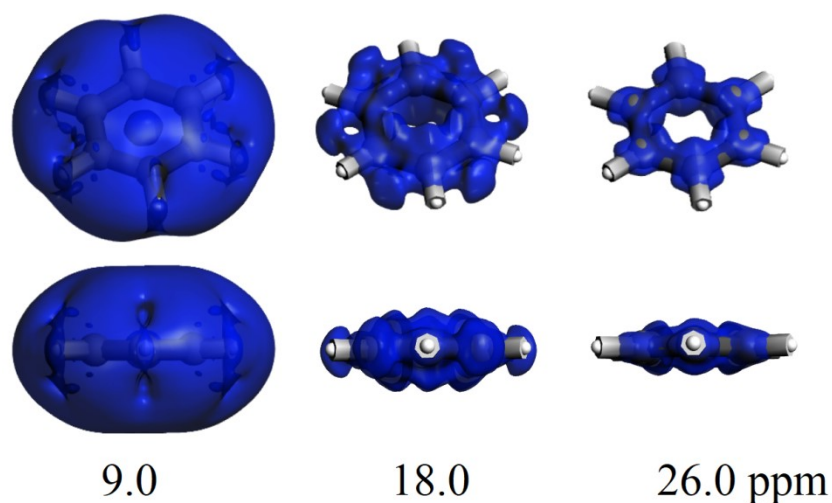


Figure S2. Anisotropic term ($\text{NICS}_{\text{aniso}}$) for benzene, under two views. Isosurface values set to 9.0, 18.0, and 26.0 ppm.

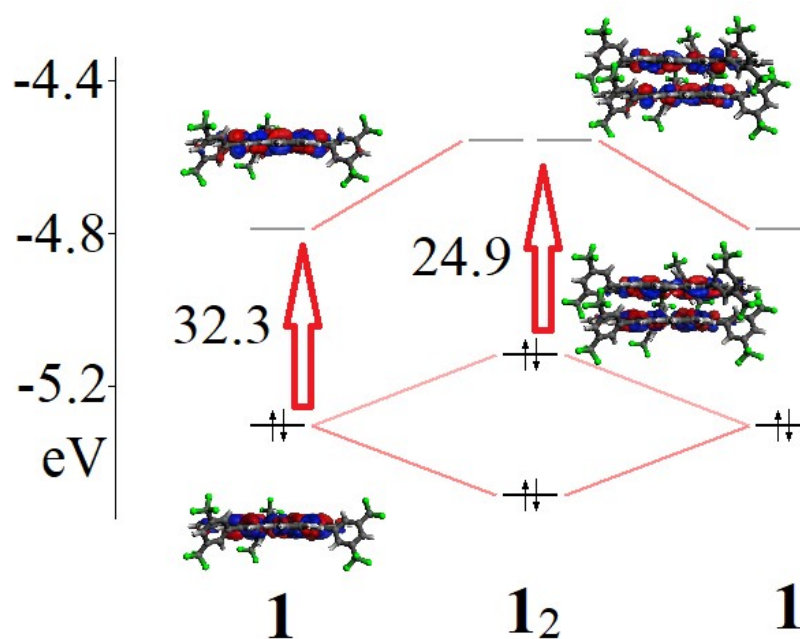


Figure S3. Frontier orbitals from **1** and the resulting **1₂**, denoting the paramagnetic contribution to the overall NICS_{zz} probe at the center of each naphthorosarin (**1**) unit.

Table S1. Optimized coordinates for the studied species in a multipleXYZ format.

Values in Angstrom (Å).

123

1

C	4.113028000	-2.252079000	-0.064028000
C	4.159409000	-0.835738000	-0.038179000
C	5.294982000	0.003102000	-0.125727000
H	6.316194000	-0.348297000	-0.218766000
C	4.852689000	1.331030000	-0.098443000
C	3.426149000	1.285232000	-0.006823000
C	2.666085000	2.488489000	0.001117000
C	3.410123000	3.746914000	-0.088455000
C	2.442256000	4.729907000	-0.101413000
H	2.586621000	5.801567000	-0.189536000
C	1.172089000	4.052758000	0.000383000
C	-0.081966000	4.674157000	0.014552000
C	-1.328130000	3.999135000	0.072291000
C	-2.621079000	4.561816000	0.190837000
H	-2.829596000	5.622943000	0.262638000
C	-3.546262000	3.512293000	0.220606000
C	-2.793399000	2.300596000	0.128423000
C	-3.455329000	1.041007000	0.136497000
C	-4.915626000	1.056006000	0.253474000
C	-5.284101000	-0.272790000	0.248956000
H	-6.283214000	-0.684714000	0.345323000
C	-4.065476000	-1.033561000	0.117616000
C	-3.983870000	-2.430250000	0.090990000
C	-2.781239000	-3.177529000	0.038741000
C	-2.622558000	-4.581889000	-0.019126000
H	-3.439273000	-5.294296000	-0.047939000
C	-1.250596000	-4.859120000	-0.040733000
C	-0.577648000	-3.597544000	-0.013053000
C	0.844358000	-3.537951000	-0.034823000
C	1.563507000	-4.813103000	-0.053035000
C	2.898405000	-4.466765000	-0.052017000
H	3.756248000	-5.130816000	-0.038640000
C	2.945322000	-3.024145000	-0.055245000
C	5.589302000	2.582105000	-0.154866000
C	4.857596000	3.805972000	-0.150516000
C	5.564283000	5.023785000	-0.198747000
H	5.010849000	5.963602000	-0.189087000
C	6.953473000	5.042677000	-0.252090000
H	7.484291000	5.994877000	-0.285960000
C	7.672266000	3.836618000	-0.256867000
H	8.762240000	3.849862000	-0.294786000
C	6.995000000	2.622595000	-0.208325000
H	7.561300000	1.690410000	-0.206652000
C	-0.150385000	6.157699000	-0.049646000
C	-0.825457000	6.780290000	-1.110125000
H	-1.276374000	6.171516000	-1.892968000
C	-0.916816000	8.170815000	-1.165660000
C	-0.335940000	8.966971000	-0.177431000
H	-0.409764000	10.051091000	-0.224877000
C	0.340622000	8.345749000	0.871938000
C	0.432302000	6.953304000	0.945175000
H	0.947441000	6.480755000	1.781244000
C	-1.713974000	8.796309000	-2.283554000
C	1.008369000	9.165418000	1.948140000

C	-4.995509000	3.524392000	0.322999000
C	-5.688756000	2.278814000	0.342957000
C	-7.094297000	2.282001000	0.437424000
H	-7.631737000	1.332914000	0.449019000
C	-7.803105000	3.475797000	0.509678000
H	-8.891436000	3.458815000	0.579842000
C	-7.119040000	4.701840000	0.488061000
H	-7.674416000	5.638892000	0.540646000
C	-5.731342000	4.721780000	0.395120000
H	-5.206945000	5.678038000	0.374544000
C	-5.250411000	-3.207499000	0.136523000
C	-6.190242000	-3.094630000	-0.896145000
H	-5.982336000	-2.445309000	-1.745832000
C	-7.386455000	-3.813205000	-0.835645000
C	-7.664098000	-4.652325000	0.242931000
H	-8.598216000	-5.208151000	0.285462000
C	-6.724979000	-4.761739000	1.269518000
C	-5.525206000	-4.051049000	1.221464000
H	-4.805730000	-4.135951000	2.034940000
C	-8.406085000	-3.620973000	-1.931038000
C	-6.975901000	-5.697916000	2.425253000
C	-0.533529000	-6.122267000	-0.076224000
C	-1.199263000	-7.361817000	-0.105758000
H	-2.289876000	-7.387013000	-0.105968000
C	-0.485786000	-8.555698000	-0.133638000
H	-1.018517000	-9.507109000	-0.156314000
C	0.918044000	-8.533888000	-0.132227000
H	1.479378000	-9.468684000	-0.154587000
C	1.594275000	-7.319355000	-0.103474000
H	2.685131000	-7.308632000	-0.105474000
C	0.892223000	-6.098242000	-0.074776000
C	5.422984000	-2.953852000	-0.123136000
C	5.749108000	-3.750677000	-1.229218000
H	5.041191000	-3.845571000	-2.051404000
C	6.978421000	-4.410005000	-1.279872000
C	7.900107000	-4.287871000	-0.239936000
H	8.856776000	-4.804200000	-0.284000000
C	7.574713000	-3.489111000	0.856486000
C	6.348171000	-2.825164000	0.921489000
H	6.101956000	-2.213541000	1.788613000
C	7.279315000	-5.310507000	-2.452203000
C	8.577455000	-3.285520000	1.965046000
N	3.037660000	-0.020548000	0.036819000
H	2.095565000	-0.431674000	0.059331000
N	1.338878000	2.664311000	0.057107000
N	-1.470644000	2.618294000	0.041956000
H	-0.641967000	2.010571000	0.006956000
N	-2.946237000	-0.195884000	0.055217000
N	-1.514171000	-2.608792000	0.036379000
H	-1.402774000	-1.586256000	0.047859000
N	1.658818000	-2.473201000	-0.037018000
F	2.373098000	9.060402000	1.870738000
F	0.700866000	10.488625000	1.865412000
F	0.652547000	8.738966000	3.196911000
F	-1.451039000	10.123808000	-2.433562000
F	-3.060838000	8.676621000	-2.048469000
F	-1.470292000	8.188839000	-3.481170000
F	-7.823862000	-3.574795000	-3.164690000
F	-9.081221000	-2.438209000	-1.767945000
F	-9.338923000	-4.612749000	-1.953984000
F	-6.477382000	-5.207206000	3.596733000

F	-8.303015000	-5.943381000	2.613799000
F	-6.368790000	-6.911059000	2.214262000
F	6.782673000	-4.809611000	-3.619648000
F	6.710107000	-6.546821000	-2.278308000
F	8.616306000	-5.507823000	-2.624862000
F	9.512619000	-4.274725000	2.006981000
F	7.979274000	-3.230646000	3.189779000
F	9.253111000	-2.102763000	1.801225000
246			
1_2 (dimer)			
C	-4.518368521	-0.969282521	-1.939336667
C	-4.128313922	0.397035409	-1.914427975
C	-4.961959156	1.540354329	-1.987053062
H	-6.039664049	1.514410762	-2.094242216
C	-4.149489867	2.673630600	-1.894837252
C	-2.802011893	2.205684278	-1.780228323
C	-1.729842842	3.129023257	-1.731594386
C	-2.079530325	4.555776070	-1.751964672
C	-0.874028317	5.217936863	-1.747384724
H	-0.708803049	6.289355232	-1.720459835
C	0.152988117	4.198702215	-1.746989654
C	1.529168843	4.447881165	-1.782792191
C	2.527636708	3.445641163	-1.713062989
C	3.932146721	3.599641147	-1.801677075
H	4.437607990	4.547710757	-1.950923358
C	4.509815823	2.328549351	-1.697104861
C	3.430144140	1.394044164	-1.580486790
C	3.687936187	0.001298993	-1.556766146
C	5.095602044	-0.411318954	-1.615966973
C	5.062721410	-1.783552846	-1.693769447
H	5.908611309	-2.454727364	-1.788221396
C	3.667156611	-2.163914276	-1.656383753
C	3.184918554	-3.473671771	-1.771890783
C	1.810391603	-3.832289321	-1.749089009
C	1.244372816	-5.130937753	-1.798247600
H	1.807486741	-6.052662852	-1.884886191
C	-0.145171042	-4.998240322	-1.729012347
C	-0.424552242	-3.597510072	-1.653262266
C	-1.764799987	-3.136347698	-1.664505495
C	-2.819426307	-4.155110805	-1.765492517
C	-3.994119885	-3.443925404	-1.862508327
H	-4.997445438	-3.839438824	-1.978744076
C	-3.633521936	-2.044974736	-1.804325208
C	-4.496892272	4.084082016	-1.880844223
C	-3.445023096	5.039363626	-1.792167129
C	-3.767041051	6.407060920	-1.746032203
H	-2.967636895	7.142141098	-1.650101466
C	-5.092600350	6.829572144	-1.787896241
H	-5.323865529	7.894338333	-1.739353430
C	-6.127485853	5.888357127	-1.882382527
H	-7.167553329	6.214279977	-1.915603097
C	-5.829117118	4.528904826	-1.932434288
H	-6.641442562	3.807653751	-2.017151158
C	1.969100271	5.857720176	-1.951062494
C	2.704075821	6.511581112	-0.954602490
H	3.010191574	5.962612268	-0.068716389
C	2.996927688	7.869954631	-1.073664038
C	2.621146358	8.588159276	-2.210559944
H	2.852084620	9.647566273	-2.300024990
C	1.936332907	7.922349717	-3.225808317
C	1.597903699	6.573075799	-3.097930581

H	1.037519663	6.071717721	-3.886298534
C	3.720360586	8.570541684	0.047109630
C	1.483691504	8.669054513	-4.456032052
C	5.903626787	1.918053262	-1.680113161
C	6.199806244	0.526393225	-1.622015860
C	7.542197560	0.114849221	-1.555882035
H	7.771685480	-0.947592962	-1.470560410
C	8.575553416	1.047376630	-1.558948155
H	9.610750158	0.710619727	-1.493710833
C	8.284081301	2.416780143	-1.628367298
H	9.089193528	3.152112801	-1.624507057
C	6.960011169	2.844269052	-1.691166286
H	6.746240864	3.910868926	-1.743753395
C	4.167483693	-4.566294152	-2.006776998
C	5.198493653	-4.823837017	-1.093941130
H	5.261533299	-4.231212377	-0.183958341
C	6.131255697	-5.831269380	-1.346415235
C	6.070423571	-6.586725603	-2.514547815
H	6.798854665	-7.371279645	-2.707016178
C	5.050495133	-6.322474220	-3.430780759
C	4.100491363	-5.332900947	-3.182244766
H	3.316144147	-5.134303310	-3.911253580
C	7.224844705	-6.066048703	-0.336611576
C	4.947889951	-7.167344450	-4.678153768
C	-1.189792580	-6.007892887	-1.732941496
C	-0.901696906	-7.383202060	-1.690905111
H	0.136753756	-7.715411305	-1.645122808
C	-1.928193148	-8.324883922	-1.698660977
H	-1.689904168	-9.388832970	-1.665207768
C	-3.265615133	-7.904489213	-1.747451704
H	-4.070989597	-8.640063940	-1.745299385
C	-3.568460491	-6.546756181	-1.774903973
H	-4.610305486	-6.225290430	-1.772006983
C	-2.547510371	-5.579371572	-1.767838228
C	-5.966568135	-1.220690434	-2.162739870
C	-6.733240822	-1.936472085	-1.234903192
H	-6.245578601	-2.364017625	-0.362772239
C	-8.111084038	-2.071248353	-1.411438996
C	-8.751813343	-1.525284406	-2.523276952
H	-9.827353245	-1.622750832	-2.650485714
C	-7.981159869	-0.848392128	-3.468398294
C	-6.604712308	-0.696090210	-3.297196605
H	-6.020935041	-0.159108877	-4.044388151
C	-8.894276989	-2.820032034	-0.365476911
C	-8.619956187	-0.231175663	-4.687612448
N	-2.822369960	0.838173934	-1.786728785
H	-2.054144613	0.159229459	-1.699823689
N	-0.402967617	2.917865531	-1.712505490
N	2.257576281	2.094909411	-1.578313102
H	1.284830222	1.761448752	-1.546140099
N	2.839740318	-1.041832351	-1.560016751
N	0.767524852	-2.924976804	-1.651299089
H	0.961097475	-1.916826284	-1.592384680
N	-2.251124486	-1.883716097	-1.670309206
F	0.144975767	8.959949060	-4.390275998
F	2.142786224	9.849949617	-4.619484746
F	1.672105767	7.933571429	-5.590158890
F	3.406336163	9.894479632	0.112092344
F	5.079238438	8.489896088	-0.088647249
F	3.411330892	8.020571971	1.263834574
F	6.724806937	-6.114284161	0.941134964

F	8.145745570	-5.051531388	-0.352690838
F	7.900877591	-7.223870773	-0.550174937
F	4.339204764	-6.503456688	-5.701019977
F	6.173769453	-7.569297998	-5.121183277
F	4.216481734	-8.301695624	-4.448195898
F	-8.581639834	-2.380029437	0.899364660
F	-8.614541652	-4.159865869	-0.387930539
F	-10.238258516	-2.684878455	-0.515833303
F	-9.935894022	-0.526371620	-4.799967432
F	-8.016040156	-0.645885716	-5.828767272
F	-8.514497187	1.121831598	-4.663844987
C	-4.592389660	0.969282521	1.756883039
C	-4.201650544	-0.397035409	1.747610657
C	-5.037535022	-1.540354329	1.786801451
H	-6.118667296	-1.514410762	1.850757357
C	-4.222025171	-2.673630600	1.727187835
C	-2.871039054	-2.205684278	1.666618817
C	-1.797782517	-3.129023257	1.660949547
C	-2.148005180	-4.555776070	1.667303310
C	-0.943286348	-5.217936863	1.710990864
H	-0.777115581	-6.289355232	1.690702570
C	0.082922468	-4.198702215	1.751714041
C	1.456566408	-4.447881165	1.842585044
C	2.457025426	-3.445641163	1.812886701
C	3.856861560	-3.599641147	1.957661110
H	4.355942296	-4.547710757	2.127024527
C	4.438254186	-2.328549351	1.876300468
C	3.364117111	-1.394044164	1.716549848
C	3.622652154	-0.001298993	1.703169261
C	5.026819200	0.411318954	1.818680342
C	4.990850006	1.783552846	1.895104018
H	5.832280187	2.454727364	2.023346533
C	3.597900918	2.163914276	1.801875059
C	3.111425035	3.473671771	1.897982455
C	1.738913041	3.832289321	1.820168002
C	1.171379946	5.130937753	1.846625885
H	1.730573693	6.052662852	1.955740004
C	-0.214277889	4.998240322	1.721813961
C	-0.490402336	3.597510072	1.634939226
C	-1.830025644	3.136347698	1.592514892
C	-2.887849538	4.155110805	1.651197618
C	-4.065485431	3.443925404	1.701105268
H	-5.072660192	3.839438824	1.777078388
C	-3.702847163	2.044974736	1.657405803
C	-4.568588809	-4.084082016	1.699297321
C	-3.514012693	-5.039363626	1.652804267
C	-3.833925391	-6.407060920	1.593813927
H	-3.031321464	-7.142141098	1.529965282
C	-5.160097971	-6.829572144	1.582573920
H	-5.389234254	-7.894338333	1.524811029
C	-6.197936611	-5.888357127	1.635551471
H	-7.238500217	-6.214279977	1.627104961
C	-5.901810987	-4.528904826	1.697508680
H	-6.716876879	-3.807653751	1.749635128
C	1.889408192	-5.857720176	2.028333656
C	2.663689021	-6.511581112	1.062098283
H	3.005026932	-5.962612268	0.189178202
C	2.951539304	-7.869954631	1.192789073
C	2.530542170	-8.588159276	2.313728555
H	2.757713423	-9.647566273	2.412367782
C	1.805631004	-7.922349717	3.300745538

C	1.472592890	-6.573075799	3.159420880
H	0.881094826	-6.071717721	3.924721042
C	3.719263794	-8.570541684	0.101877583
C	1.304098921	-8.669054513	4.511860828
C	5.831627914	-1.918053262	1.915125414
C	6.129895902	-0.526393225	1.868932621
C	7.473858678	-0.114849221	1.856596190
H	7.706578562	0.947592962	1.780530819
C	8.506263260	-1.047376630	1.901031589
H	9.543241869	-0.710619727	1.877292011
C	8.212245554	-2.416780143	1.958725610
H	9.016866813	-3.152112801	1.987102172
C	6.886722789	-2.844269052	1.968463390
H	6.671018487	-3.910868926	2.012449766
C	4.083798406	4.566294152	2.172018609
C	5.150528292	4.823837017	1.301192445
H	5.249949730	4.231212377	0.394463129
C	6.072434344	5.831269380	1.590808456
C	5.964883295	6.586725603	2.755568965
H	6.685024633	7.371279645	2.977046692
C	4.909090041	6.322474220	3.630233145
C	3.969798418	5.332900947	3.343861793
H	3.156893261	5.134303310	4.040883753
C	7.205575335	6.066048703	0.625597679
C	4.756626935	7.167344450	4.872498113
C	-1.258219186	6.007892887	1.683917186
C	-0.968671519	7.383202060	1.653448788
H	0.070779495	7.715411305	1.649278905
C	-1.994655259	8.324883922	1.620101332
H	-1.755217991	9.388832970	1.596215152
C	-3.332958334	7.904489213	1.615307524
H	-4.137600899	8.640063940	1.580912724
C	-3.636659965	6.546756181	1.630612977
H	-4.677553652	6.225290430	1.586006700
C	-2.616245530	5.579371572	1.664427954
C	-6.048372381	1.220690434	1.922126580
C	-6.777283230	1.936472085	0.964339086
H	-6.255095114	2.364017625	0.112431572
C	-8.161089567	2.071248353	1.085569615
C	-8.845819021	1.525284406	2.170863704
H	-9.925589550	1.622750832	2.254909844
C	-8.113622589	0.848392128	3.146081380
C	-6.731424347	0.696090210	3.030124812
H	-6.178029916	0.159108877	3.800089555
C	-8.901778131	2.820032034	0.009090014
C	-8.800719551	0.231175663	4.338742964
N	-2.891641052	-0.838173934	1.672299006
H	-2.120552290	-0.159229459	1.616220482
N	-0.471206896	-2.917865531	1.694999119
N	2.192576413	-2.094909411	1.667432634
H	1.221898364	-1.761448752	1.596340282
N	2.775006203	1.041832351	1.672458642
N	0.700797580	2.924976804	1.680703969
H	0.896573716	1.916826284	1.629586727
N	-2.316192579	1.883716097	1.578843320
F	-0.030910840	-8.959949060	4.392560282
F	1.956121156	-9.849949617	4.701570178
F	1.446955886	-7.933571429	5.652621762
F	3.408092814	-9.894479632	0.024374597
F	5.071616931	-8.489896088	0.291930045
F	3.459195026	-8.020571971	-1.126244227

F	6.757094718	6.114284161	-0.671144055
F	8.125094092	5.051531388	0.678533505
F	7.872515911	7.223870773	0.866055660
F	4.107478006	6.503456688	5.870174717
F	5.963786300	7.569297998	5.364252081
F	4.035011802	8.301695624	4.613441743
F	-8.538752075	2.380029437	-1.242220608
F	-8.623166038	4.159865869	0.042725205
F	-10.250701801	2.684878455	0.105517818
F	-10.120100578	0.526371620	4.398322593
F	-8.242975331	0.645885716	5.503161398
F	-8.694393544	-1.121831598	4.319216747