

Electronic supplementary information

Twisted Hexaazatrianthrylene: Synthesis, Optoelectronic Properties and Near-infrared Electroluminescent Heterojunctions Thereof

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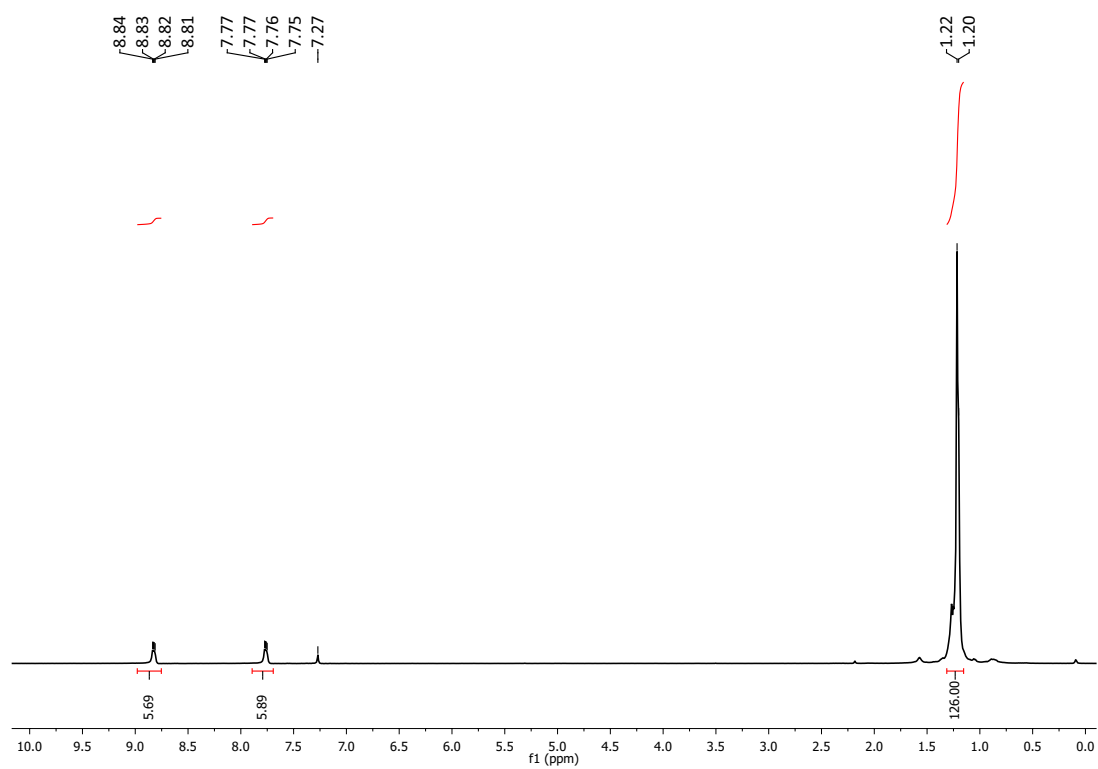


Figure S1. ^1H -NMR of *twisted*-HATANT (400 MHz, CDCl_3)

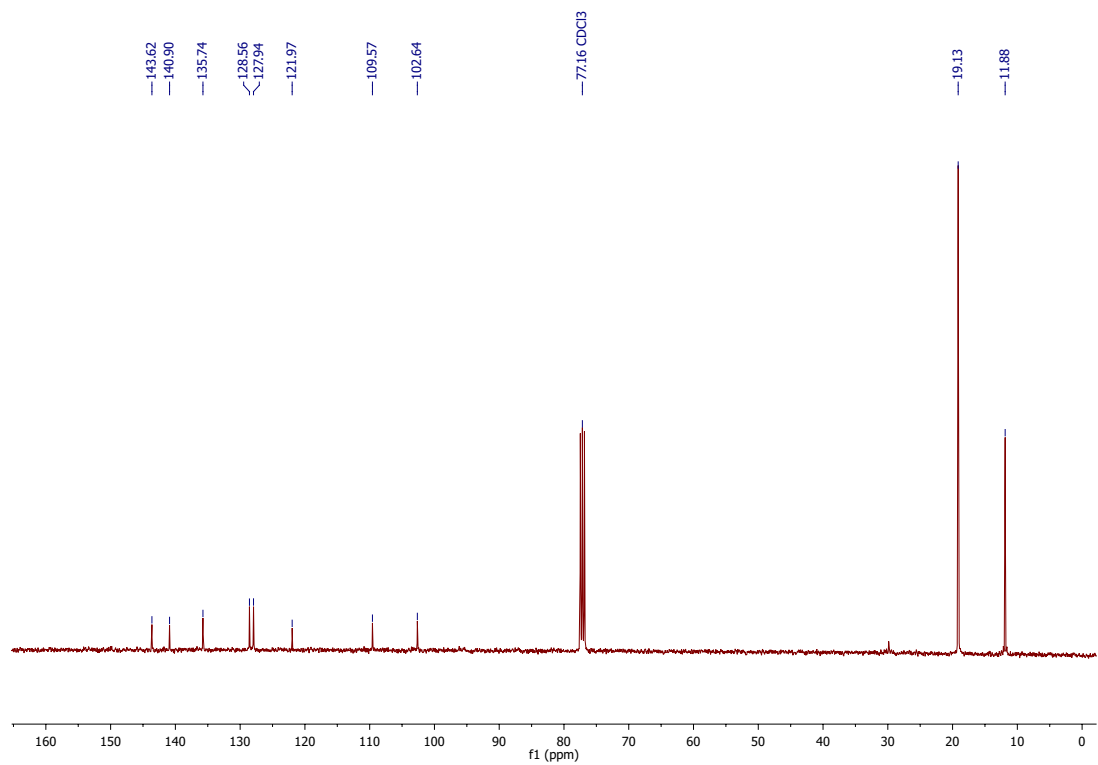


Figure S2. ^{13}C -NMR of *twisted*-HATANT (400 MHz, CDCl_3)

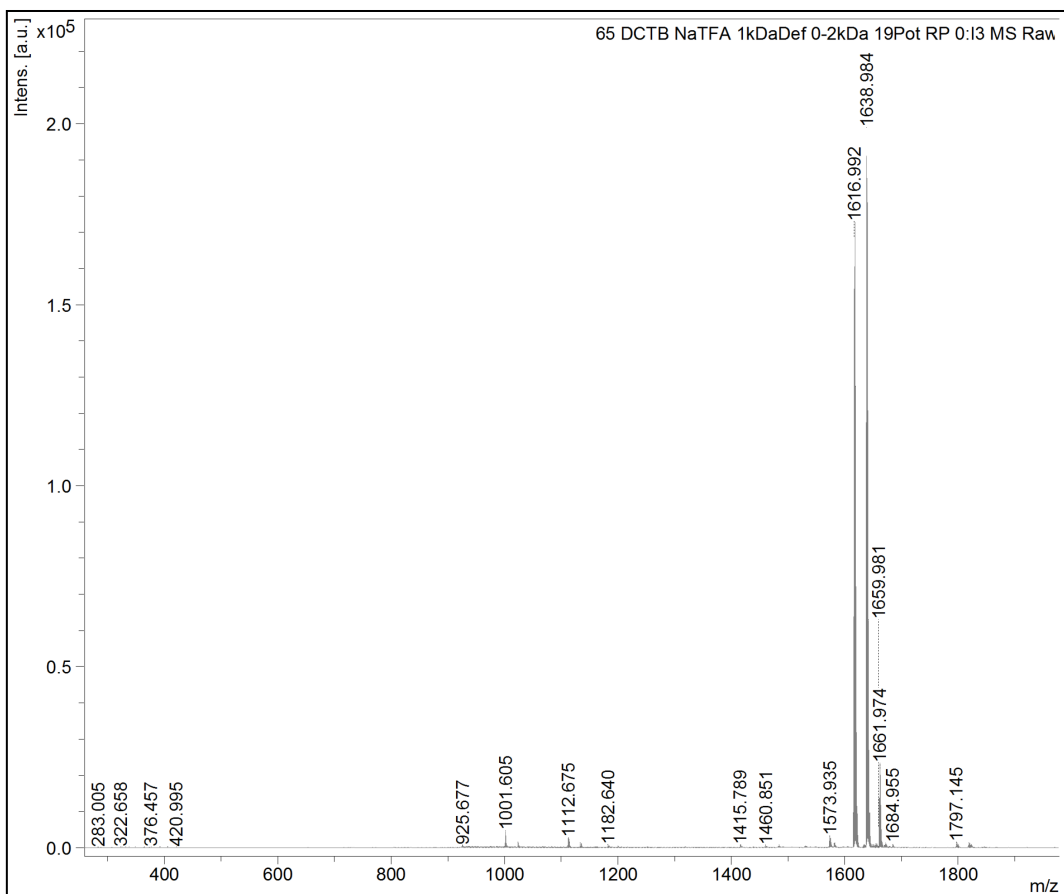


Figure S3. MALDI-TOF *twisted*-HATANT (400 MHz, CDCl_3)

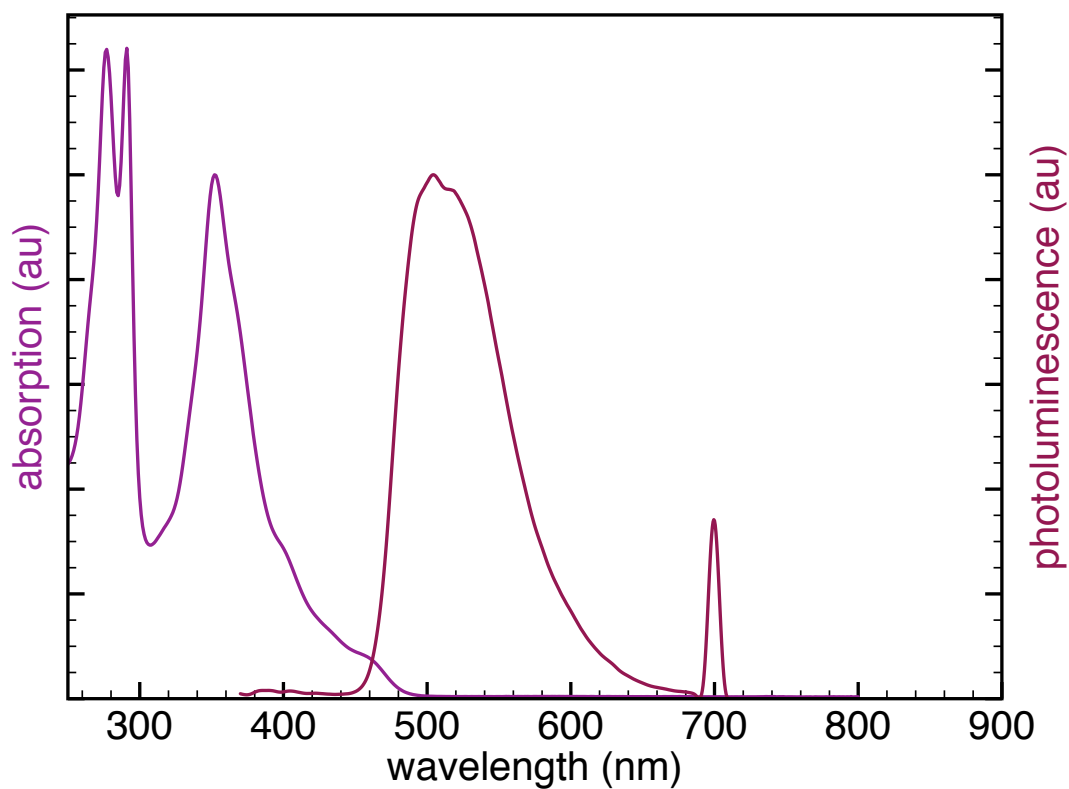


Figure S4. Absorption and photoluminescence of *twisted*-HATNA

DFT Calculations

DFT geometry optimizations were performed with a B3LYP-6-31g(d,p) Hamiltonian for the *twisted*-HATNA and *twisted*-HATANT molecules. The spectrum and frontier orbitals were computed at the B3LYP-CHCl₃-6-31g(d,p). All calculation were performed with the program Gaussian 09.

	LUMO+2	LUMO+1	LUMO	HOMO	HOMO-1	HOMO-2	HOMO-LUMO gap
<i>twisted</i> -HATNA	-2.71	-2.72	-3.08	-5.92	-5.96	-5.97	2.8
<i>twisted</i> -HATANT	-2.89	-2.9	-3.37	-5.48	-5.57	-5.58	2.1

Table 1. Frontier orbitals for *twisted*-HATNA and *twisted*-HATNA in CHCl₃. All energies in eV.

Twisted-HATNA geometry (cartesian coordinates in xyz format):

```
Si  -5.98472  -3.78897  2.58261
N   1.00233  -2.59668  -0.23280
N  -1.73158  -2.15110  0.23370
C  -0.30433  -6.01124  -0.27707
H   0.01894  -7.02159  -0.50330
C   0.57267  -4.95792  -0.51600
C   0.13013  -3.62670  -0.19512
C   0.52348  -1.37779  -0.04149
C   1.83784  -5.17824  -1.12426
C   2.87784  -5.38713  -1.73156
C  -1.58896  -5.80216  0.25716
H  -2.22005  -6.65703  0.47473
C  -2.08377  -4.52434  0.49579
C  -1.23363  -3.40464  0.18808
C  -0.88999  -1.14691  0.04980
C  -3.36501  -4.31959  1.07412
C  -4.43624  -4.15583  1.63898
Si   4.39440  -5.58590  -2.76848
C   4.89492  -3.83695  -3.36190
H   5.77092  -3.98006  -4.01319
C   3.98282  -6.77911  -4.22061
H   4.14616  -7.78468  -3.80435
C   5.75012  -6.33473  -1.63999
H   5.86197  -5.60024  -0.82935
Si   6.33747  -3.14688  2.89174
C   6.21506  -2.53601  4.70801
H   6.81532  -1.61370  4.70221
```

C	4.79081	-2.14291	5.14169
H	4.31916	-1.45918	4.42928
H	4.80685	-1.64708	6.12065
H	4.14417	-3.02177	5.23725
C	6.85585	-3.49263	5.73280
H	6.30421	-4.43607	5.80636
H	6.85568	-3.04198	6.73344
H	7.89431	-3.73668	5.48577
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H	5.50232	-4.81821	1.36343
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H	6.56108	-6.17588	3.20943
H	4.94383	-6.75192	2.79336
H	5.18705	-5.79989	4.25619
C	3.70850	-4.29534	2.39433
H	3.32517	-4.12099	3.40567
H	3.14277	-5.13547	1.97321
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H	8.84977	-1.48059	2.21779
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N	2.74008	-0.45937	0.27656
C	5.37159	2.70350	-0.24757
H	6.08768	3.48430	-0.47998
C	4.02506	2.92672	-0.51636
C	3.09066	1.88330	-0.18632
C	0.94536	1.10081	-0.04563
C	3.58974	4.11754	-1.15769
C	3.25654	5.10823	-1.79129
C	5.82361	1.50299	0.32997
H	6.87422	1.39395	0.57633
C	4.96255	0.43938	0.57997
C	3.57528	0.60043	0.23288
C	1.45260	-0.23756	0.06602
C	5.42108	-0.74508	1.21653
C	5.82166	-1.71650	1.84075
Si	2.68163	6.49833	-2.86454
C	0.92404	6.04436	-3.46957
H	0.61433	6.86438	-4.13566
C	0.89508	4.73773	-4.28604
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H	-0.12558	4.51487	-4.62210

H	1.23330	3.88920	-3.68144
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H	3.89303	4.70310	-5.19773
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H	-0.70721	8.82585	5.30820
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N	-0.95688	2.56654	0.25540
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H	-8.80995	0.33279	-3.71206
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C	-9.13573	-2.95303	-2.23867
H	-9.79351	-3.44728	-1.51243
H	-9.77728	-2.57907	-3.04489
H	-8.48259	-3.72224	-2.66437
C	-5.19132	-3.14798	-2.17447
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H	5.62614	-1.94191	-2.56243
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H	6.15462	-3.33864	-1.62260
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H	-4.11974	-4.69673	5.86758
H	-3.53906	-4.77248	4.19481
H	-3.92287	-3.21514	4.92811

***Twisted-HATANT* geometry (cartesian coordinates in xyz format):**

Si	5.71683	-3.93822	-2.63888
N	-1.14515	-2.52811	0.24798
N	1.60858	-2.23561	-0.24931
C	-0.04363	-6.04656	0.27332
C	-0.84532	-4.89831	0.52542
C	-0.33054	-3.61598	0.20153
C	-0.60298	-1.34500	0.05127
C	-2.11719	-5.01193	1.14408
C	-3.16840	-5.12553	1.75966
C	1.27270	-5.90463	-0.30023
C	1.81892	-4.61197	-0.53092
C	1.04104	-3.46978	-0.20746
C	0.83084	-1.19289	-0.05155
C	3.10100	-4.44375	-1.11461
C	4.17467	-4.30295	-1.68361
Si	-4.69107	-5.16914	2.80614
C	-5.03941	-3.37310	3.36528
C	-4.37291	-6.36353	4.28102
C	-6.11048	-5.82323	1.69636
Si	-6.32702	-2.79092	-2.94539
C	-6.12457	-2.16159	-4.74850
C	-4.68556	-1.75555	-5.11704
C	-6.71502	-3.11017	-5.81044
C	-5.25422	-4.29098	-2.43165
C	-5.55635	-5.56997	-3.23715
C	-3.74080	-4.00569	-2.39163
C	-8.17932	-3.16732	-2.62146
C	-8.45138	-3.60770	-1.17099
C	-9.09679	-1.99158	-3.00698
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N	-2.75745	-0.29751	-0.26977
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C	-3.83187	3.13869	0.59207
C	-2.98046	2.06046	0.23692
C	-0.87916	1.16255	0.06635
C	-3.29115	4.27583	1.24598
C	-2.85454	5.22180	1.88734
C	-5.75835	1.84370	-0.29528
C	-4.91252	0.73146	-0.56359

C	-3.53932	0.81361	-0.21388
C	-1.46675	-0.15290	-0.05671
C	-5.40483	-0.42648	-1.21966
C	-5.82486	-1.38036	-1.86052
Si	-2.10149	6.52547	2.95911
C	-0.37060	5.89463	3.47489
C	-0.43011	4.56295	4.24813
C	0.58256	5.76791	2.27050
C	-3.26567	6.82147	4.46235
C	-4.04903	5.57526	4.91681
C	-2.53331	7.46446	5.65831
C	-1.95638	8.11022	1.89074
C	-1.25257	9.27759	2.60849
C	-3.30794	8.56052	1.30674
Si	0.65794	6.90211	-2.85385
C	1.06687	6.46159	-4.67799
C	0.69311	5.02222	-5.07777
C	0.51945	7.47439	-5.70295
C	-1.16701	6.70465	-2.31014
C	-2.14052	7.62282	-3.07510
C	-1.67119	5.24893	-2.29873
C	1.26148	8.68644	-2.49360
C	1.04756	9.10146	-1.02600
C	2.72901	8.90788	-2.90601
N	2.72702	0.27267	0.24140
N	1.09836	2.50996	-0.26972
C	5.23298	2.97395	0.21644
C	4.63566	1.71192	0.48788
C	3.26413	1.51971	0.17728
C	1.43054	0.15161	0.05153
C	5.36907	0.66905	1.11107
C	5.99060	-0.18396	1.73022
C	4.45327	4.03690	-0.37015
C	3.05877	3.86540	-0.59540
C	2.45260	2.63142	-0.24244
C	0.58360	1.31782	-0.05469
C	2.28401	4.88129	-1.21307
C	1.65243	5.73538	-1.82016
Si	6.76555	-1.48331	2.79283
C	5.34454	-2.58059	3.45348
C	7.75410	-0.60720	4.19117
C	7.93492	-2.49781	1.66202
C	8.02823	-1.53610	5.39202
C	7.14203	0.72401	4.66725
C	8.53671	-3.74247	2.34164
C	4.61826	-3.32577	2.31643
C	9.03788	-1.63554	1.02128
C	-5.80142	-7.20248	1.08584
C	-7.48705	-5.82527	2.38796
C	-2.90963	-6.40808	4.76059

C	-5.32224	-6.10260	5.46879
C	4.33104	-1.79450	4.30737
C	-3.87750	-2.76739	4.17636
C	-5.39405	-2.45629	2.17833
C	6.01740	-2.06552	-2.36129
C	7.12891	-4.99341	-1.86936
C	5.38945	-4.48164	-4.45741
C	7.38622	-1.53472	-2.82853
C	4.86832	-1.19449	-2.90538
C	6.64596	-6.38728	-1.42386
C	8.37144	-5.13284	-2.77131
C	6.33643	-3.82348	-5.48183
C	3.92509	-4.31657	-4.90785
C	-6.12015	4.09689	0.64169
C	-7.15105	1.80239	-0.60128
C	-7.97597	2.85277	-0.29306
C	-7.45454	4.01350	0.33955
C	5.10565	5.26615	-0.68380
C	6.61487	3.20852	0.48250
C	7.20188	4.40809	0.17385
C	6.43810	5.44917	-0.41955
C	2.01985	-7.08380	-0.59437
C	-0.52784	-7.35983	0.54951
C	1.51422	-8.32845	-0.32225
C	0.22563	-8.46792	0.26051
H	-5.91788	-3.43013	4.02649
H	-4.61260	-7.36151	3.88362
H	-6.15723	-5.10127	0.86828
H	-6.72948	-1.24227	-4.75911
H	-4.24792	-1.07926	-4.37655
H	-4.03008	-2.62925	-5.19796
H	-4.66441	-1.24635	-6.08902
H	-7.76008	-3.36780	-5.60879
H	-6.15121	-4.04709	-5.87404
H	-6.67921	-2.64623	-6.80434
H	-5.56693	-4.47788	-1.39332
H	-5.02674	-6.42950	-2.80775
H	-6.62347	-5.81823	-3.25180
H	-5.22434	-5.47753	-4.27724
H	-3.20513	-4.86061	-1.96135
H	-3.50219	-3.12943	-1.78239
H	-3.33506	-3.84204	-3.39598
H	-8.43004	-4.01376	-3.27911
H	-7.89125	-4.50793	-0.89905
H	-8.17793	-2.81959	-0.45979
H	-9.51633	-3.82746	-1.02232
H	-10.15046	-2.24562	-2.83508
H	-8.87536	-1.10257	-2.40476
H	-8.99562	-1.70987	-4.05986
H	0.03678	6.66008	4.15335

H	-0.86223	3.76921	3.62923
H	-1.02687	4.63531	5.16312
H	0.57759	4.24041	4.53934
H	1.57595	5.43774	2.60000
H	0.71640	6.71709	1.74155
H	0.21820	5.03129	1.54648
H	-4.00432	7.55229	4.09960
H	-4.74934	5.83226	5.72200
H	-3.38246	4.79707	5.30440
H	-4.62387	5.13205	4.09898
H	-3.24290	7.71279	6.45769
H	-1.79123	6.78220	6.08770
H	-2.01128	8.38766	5.38745
H	-1.31926	7.80772	1.04716
H	-0.27423	8.99280	3.01008
H	-1.85527	9.65902	3.44081
H	-1.09145	10.11721	1.92054
H	-3.79556	7.75807	0.74414
H	-4.00002	8.88391	2.09357
H	-3.17669	9.41216	0.62710
H	2.16504	6.52785	-4.70793
H	1.07432	4.28603	-4.36367
H	-0.39256	4.89252	-5.14143
H	1.10505	4.77562	-6.06468
H	0.82250	8.50282	-5.48011
H	-0.57485	7.45531	-5.74549
H	0.88376	7.23797	-6.71080
H	-1.15503	7.04193	-1.26280
H	-3.14148	7.58042	-2.62799
H	-1.82478	8.67206	-3.06961
H	-2.24492	7.31470	-4.12141
H	-2.67271	5.19801	-1.85451
H	-1.02011	4.59186	-1.71539
H	-1.74573	4.84060	-3.31255
H	0.63788	9.34302	-3.11962
H	-0.00567	9.05568	-0.73151
H	1.61074	8.45301	-0.34481
H	1.39034	10.13022	-0.85667
H	3.03674	9.94363	-2.71412
H	3.40296	8.25861	-2.33479
H	2.89981	8.70709	-3.96838
H	5.82193	-3.33044	4.10317
H	8.72590	-0.36878	3.73313
H	7.28010	-2.84750	0.85055
H	8.67521	-1.03875	6.12565
H	7.10143	-1.80509	5.91090
H	8.52274	-2.46825	5.10076
H	7.79895	1.20985	5.40018
H	6.17190	0.57353	5.15303
H	6.98590	1.42206	3.84012

H	7.77086	-4.39110	2.77973
H	9.23507	-3.46680	3.14014
H	9.10183	-4.34513	1.61921
H	3.82881	-3.97063	2.72312
H	5.29170	-3.96605	1.73766
H	4.14327	-2.62814	1.61836
H	8.62389	-0.77356	0.48849
H	9.74140	-1.25704	1.77244
H	9.62410	-2.22103	0.30152
H	-4.85216	-7.20251	0.54073
H	-5.74338	-7.98094	1.85611
H	-6.58888	-7.50551	0.38406
H	-7.74575	-4.84721	2.80740
H	-7.52607	-6.55728	3.20287
H	-8.27891	-6.09606	1.67813
H	-2.78404	-7.16451	5.54599
H	-2.59255	-5.44823	5.18266
H	-2.21928	-6.64871	3.94747
H	-5.18369	-6.86258	6.24817
H	-5.12716	-5.12873	5.93140
H	-6.37758	-6.12188	5.17886
H	3.53649	-2.45822	4.67124
H	4.79337	-1.32809	5.18320
H	3.85290	-1.00285	3.72039
H	-2.96270	-2.72001	3.57578
H	-3.65365	-3.34136	5.08134
H	-4.11808	-1.74349	4.48943
H	-5.62081	-1.44200	2.53070
H	-6.26992	-2.80953	1.62457
H	-4.56208	-2.37659	1.47048
H	5.98996	-1.97047	-1.26528
H	7.43357	-4.44501	-0.96494
H	5.60827	-5.56123	-4.45481
H	7.49190	-0.47503	-2.56398
H	8.22031	-2.06808	-2.36137
H	7.50948	-1.60840	-3.91423
H	5.02107	-0.14441	-2.62686
H	3.90146	-1.50415	-2.49837
H	4.81078	-1.23372	-3.99963
H	7.46278	-6.95043	-0.95452
H	5.82398	-6.32443	-0.70542
H	6.29620	-6.98193	-2.27717
H	9.16964	-5.67330	-2.24680
H	8.78162	-4.16766	-3.08325
H	8.14254	-5.70398	-3.67827
H	7.39298	-3.94811	-5.22704
H	6.18630	-4.25918	-6.47790
H	6.14131	-2.74922	-5.57004
H	3.23025	-4.83460	-4.24187
H	3.78720	-4.71758	-5.92026

H	3.62881	-3.26217	-4.93371
H	-5.71240	4.98275	1.11559
H	-7.54229	0.91009	-1.07683
H	-9.03423	2.79890	-0.53002
H	-8.11795	4.83852	0.58081
H	4.51428	6.05778	-1.12984
H	7.19266	2.40545	0.92609
H	8.25636	4.56493	0.37988
H	6.91419	6.39448	-0.66181
H	3.00398	-6.96792	-1.03453
H	-1.51588	-7.45861	0.98481
H	2.10011	-9.21376	-0.55011
H	-0.16370	-9.45889	0.47361