Electronic Supplementary Information for Dalton Transactions

Frustrated Lewis Pairs Derived from N-Heterocyclic Carbenes and Lewis Acids

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Table S1. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energies for $(F_5C_6)_3BNH_2(Et)$, $(F_5C_6)_2B{=}NH(Et)$, and C_6F_5H

$(F_5C_6)_3BNH_2(Et)$ E = -2343.090421

B	0.661004	-0.102901	-0.101037
N	2.260495	-0.167872	-0.341574
C	0.181712	1.448669	-0.072004
C	0.074056	-0.985736	-1.325265
C	0.350923	-0.683219	1.386805
C	2.725136	0.177765	-1.711562
H	2.732340	0.439070	0.318961
H	2.579967	-1.104363	-0.114757
C	0.955921	2.582806	0.062152
C	-1.183788	1.669056	-0.082848
C	0.426756	3.854473	0.163536
C	-1.750547	2.916355	0.016747
C	-0.934725	4.019351	0.139185
C	0.067941	-2.369731	-1.313839
C	-0.382190	-0.404364	-2.491513
C	-0.411807	-3.131594	-2.356591
C	-0.868333	-1.132502	-3.555741
C	-0.891580	-2.504336	-3.481685
C	1.118571	-0.325621	2.481746
C	-0.755623	-1.463868	1.675724
C	0.843526	-0.719040	3.773107
C	-1.063864	-1.872029	2.955884
C	-0.260453	-1.501423	4.007569
F	2.293239	2.498549	0.105077
F	-2.014784	0.602136	-0.192216
F	1.242663	4.922077	0.288101
F	-3.089701	3.071683	-0.003390
F	-1.473391	5.250501	0.238000
F	0.570427	-3.023950	-0.270677
F	-0.319582	0.944680	-2.656409
F	-0.400744	-4.478786	-2.283050
F	-1.304026	-0.510805	-4.671472
F	-1.360017	-3.230635	-4.515015
F	2.190909	0.458877	2.314005
F	-1.600036	-1.866150	0.699557
F	1.641890	-0.338745	4.792133
F	-2.150979	-2.636790	3.184122
F	-0.555097	-1.900393	5.259966
H	2.656982	-0.719465	-2.318922
H	2.035406	0.910072	-2.120231
C	4.147403	0.715253	-1.677500

$(F_5C_6)_2B{=}NH(Et)$ E = -1614.801763

B	1.150797	-0.148534	-0.102842
N	2.519514	-0.142761	0.056775
C	0.385691	1.227126	-0.255094
C	0.344253	-1.498808	-0.034596
C	3.386454	1.012183	0.174564
H	2.989834	-1.012386	0.242909
C	0.024714	1.838203	-1.437194
C	0.031131	1.860964	0.914681
C	-0.665476	3.032876	-1.453245
C	-0.655962	3.052525	0.935035
C	-1.005455	3.634411	-0.263117
C	0.697946	-2.558686	0.785985
C	-0.813380	-1.658389	-0.777025
C	-0.056212	-3.709064	0.875673
C	-1.580690	-2.799422	-0.714156
C	-1.198773	-3.824799	0.119635
F	0.358176	1.288822	-2.592905
F	0.391470	1.286745	2.097458
F	-1.003998	3.613268	-2.622682
F	-0.984249	3.649850	2.098844
F	-1.677885	4.802028	-0.268804
F	1.793683	-2.492875	1.530741
F	-1.219213	-0.679220	-1.618102
F	0.319791	-4.713615	1.692957
F	-2.697275	-2.921707	-1.459686
F	-1.942295	-4.944083	0.191770
H	4.324263	0.806047	-0.339213
H	2.918288	1.853945	-0.328537
C	3.642999	1.355072	1.642525
H	4.269256	2.242201	1.725822
H	2.694702	1.534651	2.142110
H	4.145779	0.529457	2.145350

C_6F_5H E = -728.283717

C	-0.906852	-1.386529	-0.072212
C	0.467736	-1.454353	-0.041408
C	-1.518809	-0.154703	-0.042174
C	1.233359	-0.308189	0.018683
C	-0.768951	0.999528	0.017770
C	0.605137	0.915788	0.047811
F	1.071394	-2.629293	-0.069563

H	4.485205	0.931562	-2.689002
H	4.175434	1.638619	-1.102973
H	4.835018	-0.007736	-1.238891

F	-2.863749	-0.061668	-0.071468
F	2.579131	-0.380884	0.048464
F	-1.367399	2.207928	0.047041
F	1.339899	2.042958	0.106449
H	-1.503205	-2.280625	-0.119131

Table S2. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energies for the ion pair [*c*-$HCN_2(tBu)_2CHCH$][$(F_5C_6)_3BNH(Et)$] and the carbene *c*-$HCN_2(tBu)_2CHCH$

[*c*-$HCN_2(tBu)_2CHCH$][$(F_5C_6)_3BNH(Et)$] E = -2883.520377

B	-1.644355	0.271639	1.161168	H	-0.895691	1.182170	4.876031
C	-2.754137	-0.470784	0.193756	H	-1.748296	2.702921	5.189488
C	-4.090118	-0.718220	0.468828	H	-2.636110	1.183022	5.143270
C	-4.959692	-1.264539	-0.458569	H	-1.214359	2.475581	2.773898
C	-4.510107	-1.586281	-1.714015	H	-2.937704	2.545838	3.060500
C	-3.191057	-1.363608	-2.033909	H	-2.927282	0.110703	2.863255
C	-2.364975	-0.818170	-1.083989	C	3.544436	-2.056205	-0.383620
F	-1.054363	-0.639319	-1.454319	N	2.970307	-1.338692	-1.397869
F	-2.724555	-1.683946	-3.264076	C	3.265791	-0.061809	-1.215357
F	-5.349608	-2.120489	-2.627771	N	4.011488	0.067095	-0.126402
F	-6.253089	-1.482425	-0.131032	C	4.193410	-1.178300	0.411708
F	-4.617293	-0.443104	1.656360	H	4.694565	-1.346357	1.341781
C	-1.196143	1.578068	0.250200	C	4.525964	1.354157	0.396178
C	-2.078611	2.627416	0.011235	C	5.348828	1.077791	1.647028
C	-1.778822	3.703383	-0.802102	H	4.724707	0.627900	2.413867
C	-0.564192	3.759855	-1.447193	H	6.204749	0.439352	1.429244
C	0.316007	2.724639	-1.268305	H	5.721924	2.028518	2.021903
C	-0.009135	1.679689	-0.437278	C	3.344342	2.257047	0.736608
F	0.948960	0.703468	-0.373154	H	2.681102	1.786639	1.456636
F	1.531919	2.718846	-1.904440	H	3.730691	3.180223	1.165676
F	-0.254164	4.801069	-2.247975	H	2.778799	2.508946	-0.154109
F	-2.674921	4.699259	-0.980135	C	5.399490	1.982292	-0.686108
F	-3.282875	2.615515	0.553165	H	6.216985	1.314554	-0.953676
C	-0.329279	-0.721152	1.431946	H	4.816811	2.212952	-1.577217
C	0.750213	-0.213366	2.148581	H	5.815747	2.914028	-0.308002
C	1.856701	-0.946264	2.490635	H	2.887445	0.756228	-1.795150
C	1.940509	-2.262570	2.109311	C	2.211239	-1.922506	-2.525890
C	0.908215	-2.814866	1.405960	C	3.207823	-2.706002	-3.376491
C	-0.205847	-2.052539	1.098477	H	4.006631	-2.054589	-3.728337
F	-1.149317	-2.698566	0.357959	H	3.642398	-3.527183	-2.807944
F	1.037592	-4.085778	0.935152	H	2.688557	-3.122386	-4.237545
F	3.082972	-2.965814	2.331003	C	1.113098	-2.833560	-1.984012
F	2.914928	-0.363601	3.124185	H	1.475423	-3.552087	-1.254096
F	0.788508	1.078789	2.470016	H	0.318157	-2.252379	-1.531934
N	-2.171255	0.662200	2.504505	H	0.690845	-3.386954	-2.821638
C	-2.047945	1.915202	3.195926	C	1.580383	-0.791765	-3.327729
C	-1.814373	1.736565	4.686112	H	0.979678	-1.231341	-4.121209
H	0.919217	-0.209947	-2.690984	H	3.405510	-3.112432	-0.262977
H	2.333143	-0.153061	-3.790170				

c-$HCN_2(tBu)_2CHCH$ E = -540.411466

C	-2.451605	0.211841	-0.000084	H	3.124228	-1.415328	1.276018	H	-2.619612	0.043354	-2.141403
N	-1.057434	-0.220312	0.000113	H	4.172345	0.007621	1.284706	H	-3.124507	-1.415778	-1.275315
C	-0.000002	0.619216	-0.000142	C	3.137350	-0.328858	-1.255102	H	-4.172559	0.007211	-1.284331
N	1.057435	-0.220305	-0.000206	H	3.126437	-1.418339	-1.270929	C	-2.506946	1.733994	0.001210
C	0.673084	-1.544656	-0.000075	H	2.621653	0.038642	-2.140708	H	-2.002980	2.133512	-0.874603
C	-0.673074	-1.544660	0.000080	H	4.173782	0.005092	-1.282073	H	-3.551490	2.045214	0.000946
H	-1.364469	-2.366509	0.000176	C	2.506936	1.734010	-0.001709	H	-2.003938	2.131970	0.878291
H	1.364485	-2.366500	-0.000098	H	3.551478	2.045236	-0.001345	C	-3.137123	-0.328454	1.255422
C	2.451604	0.211857	0.000098	H	2.004107	2.131679	-0.879034	H	-3.126146	-1.417929	1.271632
C	3.135779	-0.325893	1.257429	H	2.002786	2.133828	0.873859	H	-2.621292	0.039386	2.140809

H	2.619253	0.044133	2.141502	C	-3.136003	-0.326336	-1.257111	H	-4.173568	0.005454	1.282451

Table S3. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energies for $(F_5C_6)_3BNH_2(Ph)$ and $(F_5C_6)_2B{=}NH(Ph)$

$(F_5C_6)_3BNH_2(Ph)$ E = -2495.427672

B	0.359472	0.043376	0.205988
N	2.021677	0.043733	0.196504
C	-0.217062	1.557442	0.209426
C	-0.036106	-0.864205	-1.062276
C	-0.056304	-0.576861	1.651652
C	2.715304	-0.052893	-1.071998
H	2.358002	0.859329	0.697451
H	2.304247	-0.749375	0.762766
C	0.451814	2.748732	0.395481
C	-1.595580	1.663280	0.145758
C	-0.185358	3.971116	0.484341
C	-2.268888	2.856468	0.230548
C	-1.553214	4.021887	0.398566
C	0.268389	-2.212304	-1.086506
C	-0.625294	-0.373126	-2.209126
C	-0.006178	-3.039650	-2.147926
C	-0.926718	-1.174259	-3.291949
C	-0.619930	-2.511554	-3.259657
C	0.505721	-0.087112	2.817971
C	-1.047044	-1.526373	1.824824
C	0.138855	-0.503406	4.078425
C	-1.442020	-1.963397	3.072029
C	-0.846804	-1.452957	4.200765
F	1.787237	2.772121	0.509461
F	-2.325396	0.528561	0.000342
F	0.532213	5.100481	0.659075
F	-3.614076	2.900765	0.154884
F	-2.196552	5.202653	0.483858
F	0.913490	-2.754795	-0.046517
F	-0.920470	0.942922	-2.339640
F	0.329563	-4.346682	-2.109695
F	-1.510589	-0.646131	-4.388084
F	-0.902158	-3.300109	-4.315324
F	1.457350	0.849774	2.741715
F	-1.684164	-2.075332	0.767022
F	0.732883	0.011433	5.174796
F	-2.410518	-2.894282	3.192276
F	-1.227221	-1.880504	5.420011
C	2.896195	1.066816	-1.866716
C	3.172462	-1.295477	-1.482426
C	3.555679	0.932376	-3.080207
C	3.830249	-1.417884	-2.694038
C	4.025093	-0.303219	-3.494630
H	2.537299	2.033206	-1.554371
H	2.980166	-2.163140	-0.872454
H	3.699038	1.801841	-3.699984
H	4.182571	-2.385006	-3.012100
H	4.535678	-0.398356	-4.438386

$(F_5C_6)_2B{=}NH(Ph)$ E = -1767.142226

B	0.619013	-0.408603	-0.054607
N	1.996055	-0.386741	0.097004
C	-0.189248	0.943371	-0.144019
C	-0.136650	-1.787542	-0.075458
C	2.845038	0.736889	0.224611
H	2.491615	-1.262982	0.117439
C	-0.520371	1.600707	-1.309640
C	-0.623641	1.497459	1.036671
C	-1.257687	2.766389	-1.296279
C	-1.355592	2.660150	1.088005
C	-1.674909	3.290436	-0.093986
C	0.258940	-2.883851	0.676102
C	-1.290351	-1.941243	-0.826332
C	-0.453544	-4.063827	0.693522
C	-2.015308	-3.111037	-0.834476
C	-1.593709	-4.172364	-0.067108
F	-0.117378	1.121589	-2.473994
F	-0.276009	0.878751	2.202603
F	-1.568915	3.393459	-2.448855
F	-1.755498	3.183434	2.265107
F	-2.393585	4.429970	-0.071326
F	1.353979	-2.825093	1.420926
F	-1.733461	-0.927718	-1.604773
F	-0.039133	-5.103910	1.444648
F	-3.128704	-3.226899	-1.585379
F	-2.295848	-5.319818	-0.065728
C	2.651479	1.655715	1.250141
C	3.898274	0.907685	-0.666807
C	3.499387	2.747228	1.364736
C	4.748424	1.992466	-0.538096
C	4.548159	2.917958	0.475187
H	1.849708	1.501616	1.953711
H	4.036736	0.196279	-1.465091
H	3.344366	3.457777	2.160288
H	5.561237	2.119527	-1.234367
H	5.207706	3.764556	0.572347

Table S4. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energy for the ion pair [*c*-$HCN_2(tBu)_2CHCH$][$(F_5C_6)_3BNH(Ph)$]

[*c*-$HCN_2(tBu)_2CHCH$][$(F_5C_6)_3BNH(Ph)$] E = -3035.876607

B	-1.785170	-0.075275	0.494409	H	-3.697408	1.070052	-1.101627
C	-0.687197	-0.937950	1.379418	H	-5.778002	2.202697	-1.626118
C	-0.992005	-2.214689	1.852409	H	-7.590071	2.375582	0.049516
C	-0.075891	-3.039193	2.477483	H	-7.251829	1.372712	2.289288
C	1.215218	-2.602249	2.655285	H	-3.108499	-0.478221	2.160574
C	1.557941	-1.353482	2.214386	C	5.487106	-0.505530	0.247864
C	0.620483	-0.563465	1.591788	N	4.301263	-0.948600	-0.273101
F	1.119434	0.629689	1.145205	C	3.488749	0.091654	-0.398986
F	2.843140	-0.917103	2.333935	N	4.119480	1.188169	0.002941
F	2.159653	-3.397950	3.209617	C	5.371116	0.827982	0.424366
F	-0.432623	-4.272904	2.893016	H	6.073850	1.538622	0.810626
F	-2.203757	-2.713503	1.678464	C	3.551714	2.556257	0.103558
C	-1.752645	-0.925993	-0.922212	C	3.143407	2.777328	1.560909
C	-2.748318	-1.755343	-1.419663	H	2.578277	1.921759	1.910323
C	-2.585859	-2.497943	-2.577206	H	4.022683	2.910140	2.190314
C	-1.404544	-2.442712	-3.275760	H	2.504525	3.653505	1.647845
C	-0.391630	-1.637250	-2.811329	C	2.363191	2.666912	-0.841691
C	-0.590284	-0.916524	-1.661981	H	1.552765	2.002445	-0.559442
F	0.476823	-0.145718	-1.242973	H	1.987259	3.686741	-0.797990
F	0.799704	-1.576191	-3.469395	H	2.669067	2.459524	-1.867312
F	-1.232800	-3.171275	-4.399886	C	4.623251	3.553871	-0.325301
F	-3.585111	-3.290810	-3.021769	H	5.476537	3.553941	0.350904
F	-3.903169	-1.881797	-0.798238	H	4.962072	3.347890	-1.339373
C	-1.323855	1.480092	0.238128	H	4.185544	4.549971	-0.299622
C	-0.852622	2.264456	1.283664	H	2.482465	0.044995	-0.769761
C	-0.354241	3.533488	1.102391	C	4.013454	-2.358266	-0.612774
C	-0.381516	4.096976	-0.149126	C	4.894148	-2.738999	-1.799786
C	-0.918843	3.400107	-1.197284	H	4.663203	-2.112716	-2.659755
C	-1.365838	2.111275	-0.985857	H	5.950590	-2.633744	-1.555749
F	-1.847564	1.473796	-2.091310	H	4.705276	-3.777699	-2.064011
F	-0.947725	3.950830	-2.432187	C	4.339482	-3.215227	0.609442
F	0.220311	5.293744	-0.362515	H	5.400588	-3.176465	0.852218
F	0.243179	4.206821	2.120640	H	3.767479	-2.895341	1.474253
F	-0.797725	1.761748	2.508711	H	4.089682	-4.250346	0.384331
N	-3.087853	-0.071678	1.244279	C	2.543936	-2.512928	-0.975421
C	-4.245102	0.569752	0.919720	H	2.355294	-3.571813	-1.143885
C	-5.288086	0.674767	1.859064	H	1.902895	-2.186653	-0.159505
H	-5.155464	0.245925	2.843448	H	2.267883	-1.985851	-1.884696
C	-6.472705	1.313079	1.544809	H	6.308716	-1.163200	0.451148
C	-6.666375	1.876788	0.291927				
C	-5.646407	1.778508	-0.642280				
C	-4.458517	1.136503	-0.346397				

Table S5. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energies for the transition states used to calculate the π bond energy of $(F_5C_6)_2B{=}NH(Et)$, and $(F_5C_6)_2B{=}NH(Ph)$

$(F_5C_6)_2B{=}NH(Et)$ twisted ts E = -1614.749059

B	0.055763	-0.171154	1.172208
N	0.035542	-0.382331	2.594767
C	1.420421	-0.106510	0.405346
C	-1.276008	0.005164	0.313412
C	-0.314118	0.683576	3.522306
H	-0.281285	-1.289939	2.897738
C	2.495421	-0.917928	0.745424
C	1.605674	0.770695	-0.650757
C	3.694099	-0.856933	0.066382
C	2.798940	0.862979	-1.328321
C	3.841335	0.040137	-0.966195
C	-2.006720	1.116264	-0.034393
C	-1.732968	-1.210883	-0.136752
C	-3.154571	1.015740	-0.793937
C	-2.864221	-1.354977	-0.901811
C	-3.575431	-0.220705	-1.229749
F	2.387066	-1.807062	1.710998
F	0.607091	1.605298	-1.022575
F	4.716998	-1.667566	0.405278
F	2.958141	1.744634	-2.336001
F	5.010068	0.114111	-1.626814
F	-1.642138	2.316008	0.401674
F	-0.996624	-2.306299	0.224977
F	-3.862763	2.118121	-1.111346
F	-3.280642	-2.564922	-1.324816
F	-4.693233	-0.325638	-1.974757
H	-0.100520	0.318006	4.524842
H	0.362594	1.521939	3.354415
C	-1.762457	1.178108	3.449817
H	-1.965125	1.861863	4.274394
H	-1.940172	1.711522	2.520927
H	-2.455160	0.340172	3.519083

$(F_5C_6)_2B{=}NH(Ph)$ twisted ts E = -1767.103663

B	0.274578	-0.436231	0.612530
N	0.273187	-0.478504	2.068571
C	1.613240	-0.375090	-0.201568
C	-1.124687	-0.454429	-0.112360
C	-0.246844	0.657458	2.701318
H	-0.053250	-1.338781	2.474314
C	2.811283	0.113121	0.309055
C	1.669403	-0.895858	-1.490478
C	3.981016	0.109916	-0.422485
C	2.825695	-0.926112	-2.231149
C	3.984404	-0.414878	-1.692157
C	-1.414957	0.260476	-1.264704
C	-2.176064	-1.155671	0.457109
C	-2.673451	0.280611	-1.823254
C	-3.438349	-1.167821	-0.088342
C	-3.683644	-0.441345	-1.231049
F	2.877455	0.641500	1.516248
F	0.569280	-1.443120	-2.055401
F	5.115284	0.613704	0.103000
F	2.838588	-1.453123	-3.471630
F	5.119885	-0.431264	-2.409650
F	-0.474415	0.979262	-1.852076
F	-1.986560	-1.894042	1.583250
F	-2.920115	0.998722	-2.936666
F	-4.431773	-1.876823	0.484196
F	-4.915747	-0.436829	-1.768498
C	-1.376185	0.567451	3.521216
C	0.320046	1.911860	2.475121
C	-1.902327	1.700152	4.117084
C	-0.233439	3.043335	3.051792
C	-1.341138	2.946816	3.877884
H	-1.848774	-0.393493	3.660328
H	1.231270	1.977824	1.910235
H	-2.766752	1.610944	4.755626
H	0.221280	4.003985	2.869524
H	-1.759916	3.828377	4.334164

Table S6. Optimized Cartesian Coordinates [ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G)] and M06/6-311++G(d,p) Energies for the components used to calculate the dative bond dissociation energies of $(F_5C_6)_3B–NH_2(Et)$, and $(F_5C_6)_3B–NH_2(Ph)$

$B(C_6F_5)_3$ E = -2207.930071

B	0.000223	-0.001085	0.026771
C	-1.227797	-0.959520	-0.002730
C	1.444542	-0.583992	-0.002752
C	-0.216210	1.541837	-0.002700
C	-1.228064	-2.184923	-0.655733
C	-2.399673	-0.610608	0.652300
C	-2.330683	-3.009638	-0.671464
C	-3.507717	-1.422820	0.666564
C	-3.469823	-2.624691	-0.003419
C	2.503244	0.027180	-0.660553
C	1.730240	-1.771292	0.654983
C	3.769456	-0.513758	-0.676733
C	2.988647	-2.322607	0.669586
C	4.008588	-1.689704	-0.004425
C	-1.276161	2.154018	-0.657788
C	0.671237	2.382482	0.653225
C	-1.440169	3.521401	-0.672694
C	0.520237	3.747865	0.668748
C	-0.539305	4.315601	-0.002351
F	-0.158406	-2.590868	-1.316314
F	-2.471633	0.555990	1.332647
F	-2.297847	-4.184141	-1.330969
F	-4.624676	-1.055710	1.324760
F	-4.549800	-3.423314	-0.004671
F	2.316229	1.153734	-1.324961
F	0.757851	-2.414533	1.340365
F	4.768164	0.101183	-1.339972
F	3.232383	-3.470255	1.332266
F	5.241510	-2.222646	-0.004127
F	-2.159507	1.429792	-1.321686
F	1.716771	1.861552	1.335006
F	-2.472987	4.079771	-1.333752
F	1.394219	4.532182	1.329445
F	-0.692787	5.649978	-0.000952

NH_2Et E = -135.106807

N	-0.765080	-0.212109	1.016136
C	-0.253311	-0.414430	-0.324079
H	-1.095147	0.734839	1.131943
H	-0.037248	-0.356557	1.700569
H	0.062296	-1.453707	-0.411186
H	-1.077373	-0.277846	-1.023734
C	0.905299	0.512874	-0.699804
H	1.256740	0.324806	-1.714743
H	0.591092	1.555673	-0.635873
H	1.743269	0.366895	-0.016634

NH_2Ph E = -287.456432

N	-1.096581	-0.439210	1.992077
C	-0.433276	-0.168481	0.814003
H	-1.520094	0.348605	2.447478
H	-0.610594	-1.034619	2.637502
C	-0.831041	0.897347	0.001487
C	0.620561	-0.975788	0.375782
C	-0.189732	1.143959	-1.199969
C	1.251502	-0.723183	-0.828240
C	0.855935	0.339058	-1.626820
H	-1.650631	1.529345	0.312887
H	0.935570	-1.809728	0.983961
H	-0.514148	1.973178	-1.808763
H	2.061346	-1.362294	-1.142971
H	1.350672	0.534741	-2.563373