

Supplementary Information

Endohedral pnictogen and triel bonds in doped C₆₀ fullerenes

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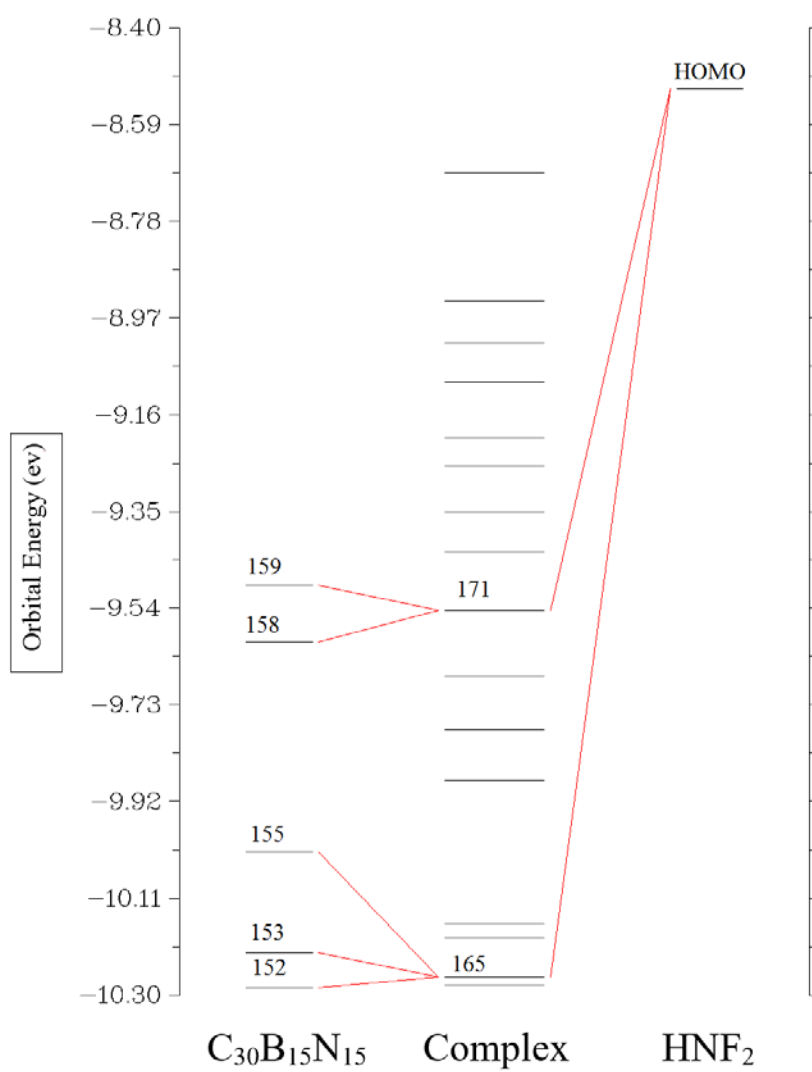


Figure S1. Molecular Orbital diagram for $HNF_2@C_{30}B_{15}N_{15}$ system.

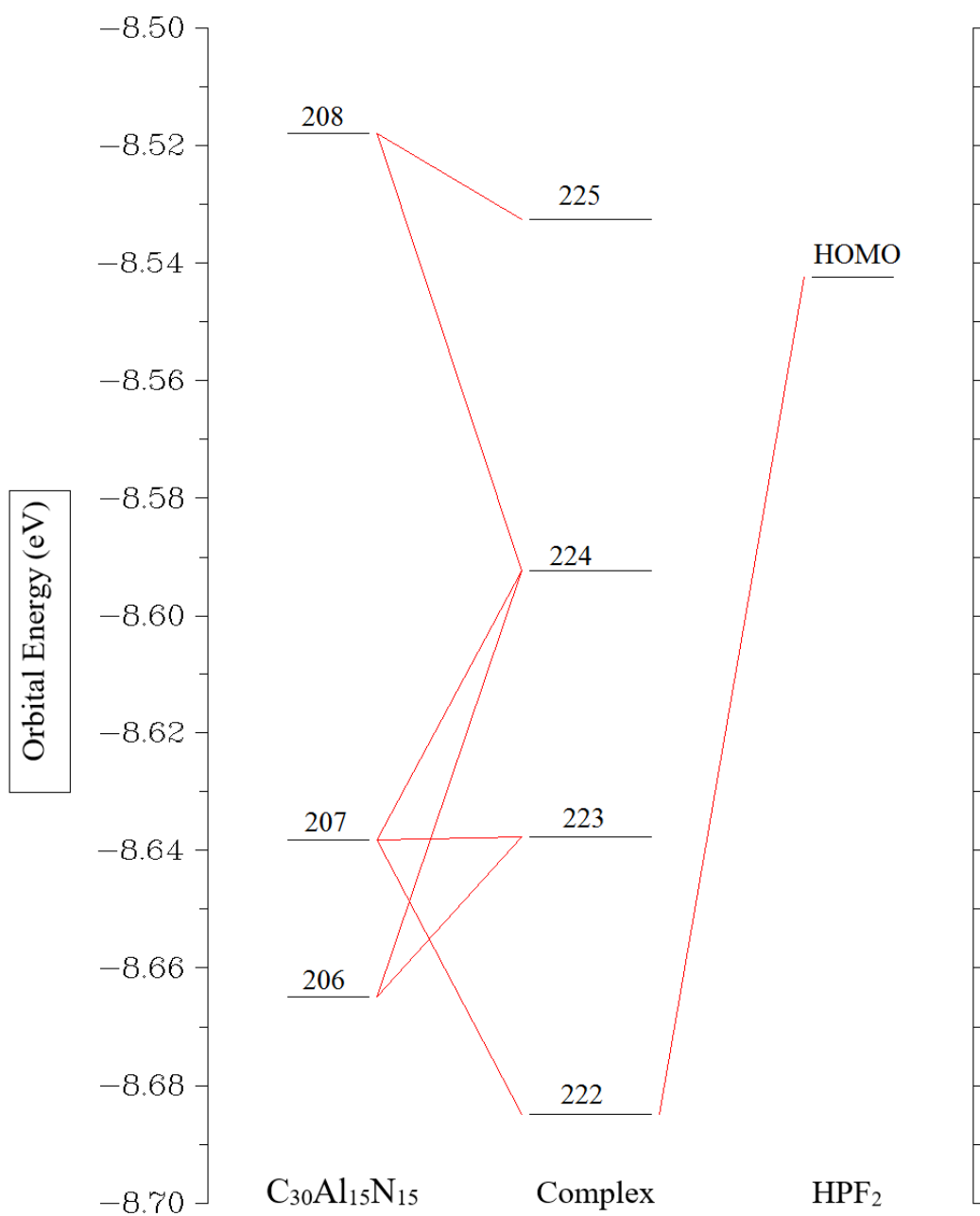


Figure S2. Molecular Orbital diagram for HPF₂@C₃₀Al₁₅N₁₅ system.

Cartesian coordinates of isolated heterofullerenes and endohedral complexes.

C₃₀B₁₅N₁₅

6	2.187612	-1.994271	-1.957002
6	2.982283	0.340534	-1.890215
6	3.061848	-1.051253	-1.443460
6	1.582308	-2.990241	-1.071196
6	-1.276576	-1.746272	-2.835778
6	-0.196745	0.356765	-3.541837
6	2.557668	2.389756	-0.583420
6	3.252033	1.201733	-0.737587
6	1.883997	-2.989278	0.280211
6	0.825003	-3.208986	1.266720
6	1.094752	-2.347786	2.419358
6	2.302862	1.973216	1.835024
6	2.069882	2.786244	0.738657
6	-0.079229	1.749204	-3.105555
6	-1.615063	2.997455	1.056951
6	-1.916758	2.996506	-0.294446
6	-3.094613	1.058497	1.429218
6	-0.857719	3.216199	-1.280982
6	-3.284761	-1.194500	0.723338
6	-3.015014	-0.333307	1.875957
6	1.243859	1.753497	2.821536
6	1.323439	0.361708	3.268265
6	0.164056	-0.349554	3.527587
6	0.046532	-1.741985	3.091326
6	-2.590397	-2.382542	0.569190
6	-2.102617	-2.778992	-0.752844
6	-2.335580	-1.965974	-1.849225
6	-1.127448	2.355016	-2.433574
6	-1.356124	-0.354486	-3.282510
6	-2.220367	2.001527	1.942750
5	2.431639	-0.278756	2.557848
5	2.808263	-1.992286	0.823139
5	3.498334	0.342193	0.421522
5	-0.237110	3.218226	1.499182
5	-1.216537	1.606730	2.932441
5	-2.065496	-0.706720	2.812060
5	-1.586574	-2.777323	1.558871
5	-0.797283	-3.418833	-0.580260
5	-0.041920	-2.351471	-2.672551
5	1.108564	-0.283049	-3.369288

5	1.298679	1.969938	-2.663354
5	0.445650	3.424990	-0.862701
5	-2.353183	1.603032	-2.159418
5	-3.413538	1.057455	0.000508
5	-3.069628	-0.710006	-1.686271
7	3.036954	0.717199	1.672046
7	2.320477	-1.595830	2.145195
7	3.380800	-1.050222	-0.014734
7	-0.478361	-3.417802	0.848443
7	-1.331417	-1.962723	2.649110
7	-1.141257	0.290272	3.355001
7	0.009184	2.358695	2.658284
7	0.764578	3.426046	0.566054
7	1.553829	2.784538	-1.573086
7	2.032792	0.713955	-2.826340
7	1.183803	-1.599522	-2.946705
7	0.204395	-3.211002	-1.513397
7	-3.531034	-0.334982	-0.435752
7	-2.840987	1.999509	-0.837378
7	-2.464331	0.285984	-2.572082

C₃₀B₁₅P₁₅

6	-2.620335	-0.059286	-2.288050
6	-2.817966	1.323495	-1.864613
6	-1.764448	2.220900	-2.362852
6	-1.065852	3.163091	-1.607513
6	1.252757	2.303488	-2.286891
6	2.799531	0.422804	-2.367875
6	3.268163	-0.654825	-1.615883
6	2.588493	-1.998880	-1.610780
6	1.361940	-2.231165	-2.292738
6	0.263132	-3.094972	-1.873160
6	-1.039728	-2.629643	-2.370613
6	-2.205730	-2.498597	-1.615975
6	-3.030403	-1.238525	-1.606706
6	2.550034	1.782611	-1.867051
6	2.854553	0.052846	2.530746
6	3.109229	1.229028	1.787939
6	2.193116	2.458593	1.804903
6	0.968882	2.516542	2.511003
6	1.701693	-2.102754	2.503154
6	2.891489	-1.335567	2.056972
6	-0.290415	3.163944	2.065921
6	-1.474605	2.436326	2.537942

6	1.037140	-3.131902	1.795856
6	-0.485621	-3.309525	1.782276
6	-1.374393	-2.502986	2.529464
6	-2.597141	-1.840289	2.060210
6	-2.666364	-0.427577	2.509710
6	-3.227481	0.663754	1.806144
6	-2.620206	2.071272	1.793929
6	0.437844	3.246791	-1.601680
5	0.936400	-1.336723	-3.465202
5	-1.634671	-0.135284	-3.462670
5	0.691930	1.490067	-3.461865
5	3.694533	-1.685892	0.865553
5	1.644585	-3.678588	0.510710
5	-0.985722	-3.935874	0.516088
5	-3.305439	-2.358386	0.869441
5	-4.007367	0.413968	0.522360
5	-2.915459	2.819760	0.529805
5	-0.388075	4.039341	0.877932
5	2.362709	3.261856	0.522626
5	3.902337	1.113347	0.522301
5	0.978406	-1.381827	3.670216
5	-1.676865	-0.163413	3.674557
5	0.706353	1.525798	3.674945
15	-0.853116	-1.767560	-4.010951
15	1.960610	0.157021	-4.009166
15	-1.113838	1.631097	-4.005500
15	3.267787	-3.150537	-0.282894
15	0.403406	-4.472023	-0.700624
15	-2.697869	-3.761657	-0.267567
15	-4.363029	-1.253741	-0.274044
15	-4.077201	1.887370	-0.686271
15	-1.910713	4.216916	-0.253997
15	1.094914	4.405617	-0.268046
15	3.671081	2.588127	-0.690096
15	4.607476	-0.454268	-0.265943
15	-0.799191	-1.791444	4.149425
15	1.950163	0.189889	4.150688
15	-1.140621	1.579544	4.155206

C₃₀Al₁₅N₁₅

6	-2.453881	-1.133072	-2.354822
6	-1.931712	-2.394981	-1.827712
6	-2.454658	-2.569687	-0.471574
6	-1.655604	-3.127666	0.512019

6	-2.455847	-1.472088	2.157009
6	-2.456051	0.877133	2.459517
6	-1.656649	2.007731	2.451483
6	-1.656195	2.895603	1.287581
6	-2.455175	2.604822	0.194701
6	-1.932254	2.779493	-1.161416
6	-2.454186	1.692175	-1.991043
6	-1.654311	1.119705	-2.965616
6	-1.654154	-0.332219	-3.152561
6	-1.933880	-0.384757	2.986647
6	2.371982	1.133036	2.354796
6	1.572269	0.332192	3.152543
6	1.572398	-1.119712	2.965583
6	2.372294	-1.692180	1.991016
6	2.372732	2.569660	0.471561
6	1.849811	2.394993	1.827664
6	1.850330	-2.779487	1.161361
6	2.373259	-2.604831	-0.194718
6	1.573684	3.127664	-0.512051
6	1.574281	2.563604	-1.862907
6	2.373899	1.472093	-2.157057
6	1.851956	0.384771	-2.986697
6	2.374142	-0.877156	-2.459549
6	1.574766	-2.007746	-2.451526
6	1.574290	-2.895615	-1.287623
6	-1.656225	-2.563588	1.862864
7	-3.299670	0.845494	-1.147671
7	-3.300753	0.569738	1.304110
7	-3.300028	-1.415723	-0.160606
7	-0.638054	-2.787751	-2.126844
7	-0.286486	-0.747463	-3.468787
7	-0.286732	1.601779	-3.166303
7	-0.638679	3.235493	-1.351249
7	-0.288594	3.377705	1.086908
7	-0.289375	1.941072	2.970139
7	-0.640557	-0.447787	3.477234
7	-0.288898	-2.630236	2.381521
7	-0.287896	-3.542894	0.195779
7	3.218375	-1.409568	-0.203209
7	3.218668	0.882169	-1.117171
7	3.217625	0.527821	1.324500
13	-3.299521	-0.527835	-1.324490
13	-3.300297	1.409550	0.203192
13	-3.300636	-0.882176	1.117153
13	3.217786	-0.845518	1.147670
13	3.218799	-0.569742	-1.304119

13	3.218100	1.415690	0.160578
13	0.206011	3.542920	-0.195819
13	0.206969	2.630256	-2.381564
13	0.558644	0.447813	-3.477282
13	0.207432	-1.941099	-2.970193
13	0.206732	-3.377680	-1.086940
13	0.556738	-3.235478	1.351169
13	0.204815	-1.601778	3.166240
13	0.204549	0.747445	3.468755
13	0.556151	2.787765	2.126779

$C_{30}Al_{15}P_{15}$

6	-2.424271	-1.203958	-2.318921
6	-1.902029	-2.449301	-1.753851
6	-2.424743	-2.582763	-0.392946
6	-1.625526	-3.110653	0.606989
6	-2.425458	-1.405903	2.201119
6	-2.425574	0.951416	2.432200
6	-1.626156	2.081233	2.389721
6	-1.625891	2.933377	1.199413
6	-2.425065	2.609582	0.115998
6	-1.902377	2.743009	-1.244885
6	-2.424470	1.631027	-2.041044
6	-1.624773	1.029230	-2.997935
6	-1.624670	-0.427699	-3.140734
6	-1.903331	-0.293907	2.997289
6	2.402444	1.203925	2.318925
6	1.602857	0.427674	3.140746
6	1.602932	-1.029234	2.997931
6	2.402650	-1.631030	2.041047
6	2.402889	2.582739	0.392963
6	1.880201	2.449314	1.753832
6	1.880526	-2.743002	1.244860
6	2.403221	-2.609588	-0.115986
6	1.603680	3.110653	-0.606991
6	1.604034	2.505861	-1.940108
6	2.403584	1.405910	-2.201139
6	1.881479	0.293923	-2.997310
6	2.403738	-0.951437	-2.432201
6	1.604346	-2.081246	-2.389736
6	1.604059	-2.933387	-1.199425
6	-1.625904	-2.505843	1.940094
15	-3.269722	-0.567716	-1.307284
15	-3.270204	1.415136	0.160903

15	-3.270420	-0.847800	1.143988
15	3.248600	-0.609119	-1.286779
15	3.248186	1.419845	0.116994
15	3.248008	-0.810366	1.172250
15	0.235199	0.852360	3.444447
15	0.586599	2.851010	2.041114
15	0.236067	3.535342	-0.303269
15	0.236632	2.556771	-2.460313
15	0.588083	0.342075	-3.489359
15	0.236923	-2.030342	-2.909950
15	0.236528	-3.409112	-0.983969
15	0.586959	-3.192996	1.448641
15	0.235376	-1.504962	3.213361
13	-0.608828	3.193012	-1.448692
13	-0.257221	1.504964	-3.213395
13	-3.269820	0.810346	-1.172221
13	-3.270041	-1.419876	-0.116992
13	-3.270482	0.609119	1.286799
13	-0.258317	3.409139	0.983965
13	-0.258793	2.030316	2.909925
13	-0.609924	-0.342047	3.489339
13	-0.258488	-2.556749	2.460298
13	-0.257880	-3.535314	0.303259
13	-0.608430	-2.850994	-2.041150
13	3.248354	-1.415151	-0.160890
13	3.248524	0.847796	-1.143976
13	3.247899	0.567705	1.307324
1**3	-0.257064	-0.852375	-3.444450

H₂NF@ C₃₀B₁₅N₁₅

6	1.631235	0.115070	-3.063230
6	0.899928	2.366005	-2.434961
6	1.933773	1.389843	-2.567570
6	2.202204	-1.069015	-2.537836
6	-1.397189	-1.991075	-2.695729
6	-2.200575	0.377782	-2.869973
6	0.085073	3.492427	-0.434415
6	1.136339	3.158642	-1.282962
6	3.154809	-1.045776	-1.511068
6	3.034334	-1.898231	-0.395722
6	3.285059	-1.162350	0.820983
6	1.378424	2.796197	1.565157
6	0.221498	3.324057	0.984265
6	-2.664228	1.515131	-2.046205

6	-2.346614	1.050636	2.621292
6	-3.167879	0.970791	1.469736
6	-2.054345	-1.426238	2.720038
6	-3.122620	1.952460	0.398221
6	-1.291434	-3.060278	1.237097
6	-1.018238	-2.450057	2.456494
6	1.264836	1.870679	2.655437
6	2.317116	0.923014	2.605252
6	2.041057	-0.424258	2.826684
6	2.556847	-1.452693	1.986044
6	-0.213751	-3.523715	0.362607
6	-0.277094	-3.462819	-1.019711
6	-1.467263	-2.915223	-1.668120
6	-3.351657	1.265972	-0.859282
6	-2.441200	-0.938817	-2.524010
6	-1.747956	-0.162473	3.191711
5	3.114452	1.239270	1.345065
5	3.476755	0.343141	-0.950476
5	2.408124	2.592108	-0.641003
5	-1.224204	2.122481	2.613129
5	-0.250686	0.172553	3.536706
5	0.447994	-2.118842	2.790843
5	1.293138	-3.202806	0.775079
5	1.148399	-3.030819	-1.520181
5	0.011043	-1.553893	-3.185819
5	-0.757087	0.790498	-3.363656
5	-1.531703	2.567291	-2.019775
5	-2.030151	2.981789	0.420184
5	-3.665288	-0.202743	-0.508163
5	-3.013181	-1.502589	1.541146
5	-2.630703	-2.468007	-0.750778
7	2.534933	2.485663	0.775281
7	3.647627	0.196262	0.517733
7	2.922493	1.530978	-1.534177
7	2.119195	-2.971315	-0.411848
7	1.606024	-2.530657	1.993986
7	0.790677	-0.815354	3.365319
7	0.029806	1.578780	3.221861
7	-1.062829	3.071690	1.539862
7	-1.263133	3.321598	-0.808802
7	-0.402861	2.132767	-2.893798
7	0.306123	-0.171666	-3.525121
7	1.237427	-2.114083	-2.621076
7	-2.541823	-2.603779	0.668606
7	-3.584896	-0.314841	0.964818
7	-3.240144	-1.270415	-1.370742

1	-0.879277	0.408447	1.152571
9	1.018944	-0.470244	0.143994
1	-1.161973	-0.792059	-0.517886
7	-0.441003	0.396445	-0.208113

H₂PF@ C₃₀B₁₅N₁₅

6	-1.023440	-3.309726	0.269352
6	-1.663574	-2.086339	2.284363
6	-2.016924	-2.694982	1.028408
6	-0.951416	-3.157653	-1.154148
6	2.560450	-2.654522	-0.253138
6	2.036350	-2.100876	2.147185
6	-1.836845	0.225269	2.987689
6	-2.450761	-0.937624	2.513044
6	-1.909969	-2.428405	-1.842066
6	-1.504077	-1.465504	-2.801643
6	-2.282444	-0.280842	-2.668176
6	-2.872401	1.644095	1.261270
6	-2.083069	1.493053	2.407568
6	1.761356	-0.952871	3.001207
6	1.058223	3.234761	1.103338
6	2.001964	2.345309	1.784218
6	2.077120	2.815709	-1.097359
6	1.611372	1.550549	2.860627
6	2.512255	0.905707	-2.408846
6	1.761572	2.185075	-2.285041
6	-2.481087	2.559482	0.233137
6	-2.833840	2.041550	-1.026957
6	-1.938041	2.100449	-2.094251
6	-1.683737	0.966515	-2.901337
6	1.969138	-0.203173	-3.023927
6	2.165146	-1.571510	-2.499312
6	2.918593	-1.772519	-1.341964
6	2.367280	0.279738	2.809265
6	2.838986	-1.959597	0.992883
6	1.075427	3.465803	-0.263359
5	-3.488240	0.681609	-0.760967
5	-2.999846	-1.753999	-1.008329
5	-3.318506	-0.774070	1.267913
5	-0.469524	3.163556	1.535169
5	-0.418783	3.482248	-0.750922
5	0.286623	2.205437	-2.765538

5	0.467649	-0.142091	-3.494349
5	0.818552	-2.306203	-2.617855
5	1.242178	-3.361807	-0.364201
5	0.694066	-2.853603	1.993364
5	0.241924	-1.016360	3.387154
5	0.118394	1.483567	3.221826
5	3.301482	0.397849	1.617936
5	3.092475	1.904634	-0.377378
5	3.572272	-0.530109	-0.705963
7	-3.576798	0.521444	0.710469
7	-3.261725	-0.431391	-1.626557
7	-3.080001	-1.959121	0.404734
7	-0.190702	-1.432232	-3.272688
7	-0.339406	1.043397	-3.382920
7	-0.756873	2.894850	-2.017537
7	-1.346316	3.382438	0.385845
7	-0.909788	2.302998	2.585911
7	-0.523717	0.195098	3.519717
7	-0.379432	-2.208162	2.799922
7	0.295688	-3.482404	0.766959
7	0.392748	-3.205757	-1.569624
7	3.380457	0.769072	-1.274873
7	3.085068	1.744332	1.041002
7	3.548954	-0.731131	0.757269
1	0.948855	-0.516676	-0.698494
9	-0.829210	-0.270622	0.099776
1	0.941939	0.041876	0.880548
15	0.559986	0.184104	-0.059661

HNF₂@ C₃₀B₁₅N₁₅

6	0.296882	-3.412559	0.568097
6	-0.703488	-2.328783	2.503992
6	-0.842045	-3.144171	1.325197
6	0.273576	-3.371909	-0.876748
6	3.385056	-1.571375	-0.186083
6	2.739869	-1.033298	2.199942
6	-1.703902	-0.193536	3.039210
6	-1.866364	-1.530772	2.694996
6	-0.907355	-3.095326	-1.546395
6	-0.920590	-2.146010	-2.619006
6	-2.069170	-1.324645	-2.528615
6	-3.236298	0.602821	1.292876
6	-2.431929	0.858315	2.393084
6	2.071239	0.011039	2.972932

6	-0.182278	3.499987	0.818585
6	1.038240	3.055819	1.505375
6	0.874758	3.269496	-1.390296
6	0.994304	2.269441	2.656366
6	1.954657	1.538576	-2.574196
6	0.789918	2.466966	-2.511183
6	-3.249713	1.517874	0.164090
6	-3.410361	0.792519	-1.018692
6	-2.620517	1.078003	-2.154186
6	-1.986267	0.053249	-2.875130
6	1.853850	0.262373	-3.083134
6	2.559259	-0.893127	-2.481182
6	3.357371	-0.711402	-1.355757
6	2.158111	1.356063	2.657837
6	3.403872	-0.713016	0.991349
6	-0.280814	3.600756	-0.562862
5	-3.506889	-0.688178	-0.621821
5	-2.158575	-2.808730	-0.712728
5	-2.757350	-1.808187	1.494871
5	-1.579627	2.927239	1.331734
5	-1.696621	3.044440	-0.982663
5	-0.598643	1.927630	-2.930067
5	0.430210	-0.260432	-3.486521
5	1.572206	-2.069950	-2.478104
5	2.417793	-2.720013	-0.185809
5	1.768659	-2.229573	2.157694
5	0.689141	-0.550729	3.422411
5	-0.362947	1.711886	3.084511
5	2.945583	1.689737	1.407877
5	2.170231	2.850812	-0.663857
5	3.495521	0.733467	-0.836761
7	-3.483717	-0.742248	0.859684
7	-2.893492	-1.719391	-1.404862
7	-2.119273	-2.898872	0.712713
7	0.295960	-1.677848	-3.145346
7	-0.756907	0.563119	-3.411284
7	-1.811430	2.256504	-2.186832
7	-2.509435	2.719907	0.208738
7	-1.646315	2.057762	2.467914
7	-0.474473	0.299628	3.501211
7	0.531334	-1.938033	2.951855
7	1.596980	-3.080301	1.005672
7	1.537213	-2.991519	-1.357887
7	2.837327	1.829053	-1.485984
7	2.246243	2.821492	0.755745
7	3.590967	0.665383	0.630531

7	-0.479180	-0.454940	-0.058990
1	-0.638708	-0.587294	-1.070748
9	-0.575284	0.968981	0.042873
9	0.933440	-0.603191	0.028680

HPF₂@C₃₀B₁₅N₁₅

6	-0.232180	-3.425797	-0.454726
6	0.778125	-2.383830	-2.408335
6	0.913316	-3.159308	-1.202528
6	-0.232410	-3.339737	0.988315
6	-3.365755	-1.621622	0.194290
6	-2.693226	-1.145821	-2.197409
6	1.746733	-0.247480	-2.995169
6	1.928735	-1.569986	-2.606670
6	0.932441	-3.019826	1.666770
6	0.911012	-2.037493	2.709090
6	2.045309	-1.197451	2.610356
6	3.236254	0.632127	-1.251690
6	2.444684	0.837756	-2.371457
6	-2.032150	-0.113421	-2.992613
6	0.121481	3.483518	-0.915065
6	-1.079541	2.994841	-1.605986
6	-0.965736	3.301678	1.283685
6	-1.002771	2.173993	-2.730892
6	-2.031590	1.588058	2.504891
6	-0.883573	2.536216	2.430400
6	3.214761	1.581974	-0.152149
6	3.370290	0.897017	1.055147
6	2.557449	1.202510	2.168998
6	1.931196	0.188720	2.912094
6	-1.914962	0.330491	3.055161
6	-2.589060	-0.856516	2.479197
6	-3.372597	-0.725271	1.336642
6	-2.149121	1.238847	-2.721303
6	-3.382067	-0.800861	-1.009689
6	0.196333	3.629126	0.463868
5	3.500741	-0.593195	0.706522
5	2.191063	-2.735371	0.843578
5	2.805732	-1.792748	-1.385044
5	1.537212	2.921989	-1.388708
5	1.615507	3.113423	0.922370
5	0.508060	2.036930	2.887039
5	-0.488325	-0.152084	3.496325
5	-1.580240	-2.013706	2.528079

5	-2.377292	-2.750939	0.244789
5	-1.700596	-2.321343	-2.102858
5	-0.632874	-0.662288	-3.403201
5	0.371251	1.629524	-3.120668
5	-2.962296	1.596108	-1.494535
5	-2.241542	2.835795	0.551202
5	-3.529554	0.699819	0.770453
7	3.501933	-0.693805	-0.772732
7	2.894477	-1.611106	1.512196
7	2.175922	-2.870593	-0.578758
7	-0.322225	-1.576599	3.201945
7	0.684218	0.691353	3.413251
7	1.726045	2.365713	2.152312
7	2.452923	2.767607	-0.245778
7	1.638048	2.018995	-2.495856
7	0.515727	0.207376	-3.491034
7	-0.456580	-2.030983	-2.886934
7	-1.531209	-3.132335	-0.922194
7	-1.510367	-2.968869	1.438041
7	-2.902281	1.827518	1.394826
7	-2.294612	2.760832	-0.867767
7	-3.600576	0.584260	-0.695253
1	0.624456	-0.533439	1.108508
9	0.549489	0.985902	-0.054313
9	-0.929599	-0.613728	-0.013593
15	0.433595	-0.405729	-0.221816

H₂NF @C₃₀Al₁₅N₁₅

6	-2.827663	2.665390	-0.565408
6	-2.445699	2.284007	-1.870108
6	-2.940969	0.880488	-2.302006
6	-2.144485	0.020350	-3.119014
6	-2.598543	-2.236632	-1.919700
6	-2.464030	-2.867127	0.493754
6	-1.570876	-3.005848	1.616505
6	-1.488243	-2.071427	2.841734
6	-2.312441	-0.952431	2.982493
6	-1.932493	0.444618	3.210695
6	-2.608188	1.406396	2.354432
6	-1.910219	2.619585	1.842876
6	-1.991355	3.209931	0.474376
6	-1.982075	-3.096522	-0.924493
6	2.987573	-2.440246	0.483876
6	2.200244	-3.134484	-0.550206

6	2.003024	-2.687592	-1.942161
6	2.610313	-1.583611	-2.568410
6	2.813670	-1.022606	2.506896
6	2.502889	-2.306622	1.888956
6	2.042795	-0.381560	-3.218875
6	2.520768	0.875382	-2.745837
6	2.159810	-0.045713	3.276577
6	2.129815	1.430763	2.895794
6	2.766147	2.068921	1.813566
6	1.977594	3.097155	0.927602
6	2.286118	3.045758	-0.424612
6	1.521682	3.093442	-1.690166
6	1.637687	2.116422	-2.706737
6	-1.947849	-1.493833	-2.928036
7	-3.806627	0.903833	1.687910
7	-3.671765	-2.085187	0.575595
7	-3.998853	0.379957	-1.471298
7	-1.400336	2.948575	-2.500344
7	-0.912426	4.021461	0.167820
7	-0.757162	3.062817	2.459178
7	-0.728805	0.695226	3.877046
7	-0.258578	-2.162935	3.526983
7	-0.371137	-3.716348	1.493830
7	-0.819111	-3.751760	-1.218958
7	-0.786152	-1.983462	-3.523040
7	-1.057866	0.546368	-3.861372
7	3.743651	0.837068	-1.985331
7	3.898479	1.479539	1.165668
7	4.042495	-1.560490	0.107003
13	-4.098172	1.472874	0.014610
13	-3.829494	-0.920018	1.937226
13	-3.994084	-1.379481	-1.093660
13	4.060525	-0.950418	-1.608360
13	3.803370	1.971051	-0.597980
13	4.166006	-0.279160	1.441269
13	0.464406	-0.631083	4.115729
13	0.341751	2.074586	3.444816
13	0.344210	4.211674	1.510560
13	-0.269905	3.953621	-1.493360
13	-0.203307	2.057644	-3.510589
13	0.305499	-0.625387	-4.044132
13	0.181672	-3.194578	-2.626816
13	0.520049	-4.024649	-0.018708
13	0.951855	-3.175929	2.634838
7	0.930588	-0.002784	0.052498
1	0.524429	0.818782	0.506680

1	1.049021	-0.779866	0.710065
9	-0.171688	-0.467326	-0.807335

H₂PF@ C₃₀Al₁₅N₁₅

6	-2.888516	2.673562	-0.245817
6	-2.518791	2.448608	-1.592039
6	-2.985623	1.081797	-2.169077
6	-2.183116	0.321815	-3.082683
6	-2.584042	-2.057435	-2.123381
6	-2.421982	-2.961587	0.189775
6	-1.512966	-3.213085	1.285833
6	-1.426670	-2.420464	2.601109
6	-2.261707	-1.330001	2.872135
6	-1.903072	0.034041	3.255650
6	-2.602359	1.077867	2.514073
6	-1.934075	2.352882	2.133294
6	-2.047128	3.100286	0.845711
6	-1.951422	-3.022145	-1.244732
6	3.018244	-2.445841	0.173829
6	2.232995	-3.054048	-0.928591
6	2.011617	-2.455925	-2.246568
6	2.585765	-1.261174	-2.736325
6	2.851882	-1.253982	2.341049
6	2.536755	-2.461868	1.574173
6	1.988092	-0.003541	-3.229631
6	2.473462	1.204075	-2.637460
6	2.204108	-0.385263	3.229641
6	2.159020	1.126130	3.022846
6	2.773501	1.887552	2.009973
6	1.962786	2.998375	1.248695
6	2.254060	3.103404	-0.103787
6	1.470494	3.290574	-1.348103
6	1.586379	2.429886	-2.462633
6	-1.955884	-1.192195	-3.045833
7	-3.799777	0.635450	1.810826
7	-3.637422	-2.209579	0.370638
7	-4.016198	0.465815	-1.385526
7	-1.494662	3.198773	-2.160066
7	-0.984246	3.965030	0.625092
7	-0.774915	2.735116	2.786545
7	-0.692399	0.226340	3.934212
7	-0.186396	-2.566970	3.262413
7	-0.306391	-3.889817	1.064349

7	-0.782177	-3.630531	-1.630242
7	-0.781756	-1.599137	-3.687103
7	-1.118026	0.939689	-3.787808
7	3.704515	1.082887	-1.901979
7	3.906842	1.394675	1.288400
7	4.064362	-1.523577	-0.117625
13	-4.112356	1.386443	0.213258
13	-3.790780	-1.204087	1.851945
13	-3.994340	-1.324196	-1.207458
13	4.072334	-0.733632	-1.763579
13	3.788529	2.078646	-0.410524
13	4.177348	-0.384996	1.342587
13	0.521930	-1.098502	4.012024
13	0.353846	1.658948	3.635041
13	0.297514	3.974673	1.945422
13	-0.349750	4.049535	-1.035520
13	-0.274731	2.384819	-3.204823
13	0.263181	-0.177680	-4.119233
13	0.193386	-2.931252	-2.994347
13	0.569090	-4.041406	-0.483882
13	1.020002	-3.447734	2.239768
15	0.711438	-0.104899	0.123731
1	0.119180	-1.340915	-0.343868
1	-0.079942	-0.074474	1.338230
9	-0.396532	0.920157	-0.781201

HNF₂@C₃₀Al₁₅N₁₅

6	-2.711507	2.867453	-0.347052
6	-2.280811	2.629212	-1.670613
6	-2.827676	1.324542	-2.295781
6	-2.031215	0.518000	-3.172597
6	-2.691420	-1.828321	-2.299308
6	-2.736733	-2.771462	0.006837
6	-1.917289	-3.109013	1.145900
6	-1.846326	-2.343061	2.482138
6	-2.608751	-1.196122	2.724992
6	-2.159991	0.132163	3.147647
6	-2.730613	1.240524	2.393914
6	-1.939561	2.463484	2.078478
6	-1.910358	3.223245	0.796824
6	-2.188664	-2.850182	-1.400137
6	2.727279	-2.682461	0.324054
6	1.952753	-3.204114	-0.835831
6	1.860994	-2.581506	-2.148548

6	2.566961	-1.439144	-2.597290
6	2.548814	-1.536414	2.496523
6	2.193438	-2.708028	1.696504
6	2.094234	-0.140645	-3.099333
6	2.628342	1.023582	-2.464964
6	1.902220	-0.624691	3.342408
6	1.983794	0.884704	3.163941
6	2.711960	1.611437	2.202366
6	2.033572	2.787821	1.420877
6	2.405943	2.885643	0.087621
6	1.713818	3.152566	-1.192238
6	1.827513	2.308947	-2.322521
6	-1.936626	-1.010033	-3.167232
7	-3.914693	0.902650	1.608538
7	-3.900056	-1.926435	0.129397
7	-3.959314	0.791765	-1.594193
7	-1.164397	3.300152	-2.166026
7	-0.769206	3.998793	0.644484
7	-0.799912	2.754826	2.809079
7	-0.980465	0.216523	3.893160
7	-0.663929	-2.600454	3.206440
7	-0.756491	-3.875025	0.984750
7	-1.052473	-3.541175	-1.728689
7	-0.768884	-1.500135	-3.755633
7	-0.872349	1.059317	-3.783359
7	3.792171	0.796244	-1.654372
7	3.839853	1.038862	1.535162
7	3.848593	-1.834465	0.095479
13	-4.082316	1.698085	0.013602
13	-4.058993	-0.932309	1.620244
13	-4.092881	-0.999832	-1.450698
13	4.041063	-1.046767	-1.544746
13	3.885760	1.764627	-0.147770
13	3.995277	-0.755203	1.593893
13	0.121091	-1.200219	4.004878
13	0.194761	1.557217	3.665036
13	0.422729	3.906946	2.044143
13	-0.037341	4.086566	-0.976897
13	0.037243	2.474671	-3.227045
13	0.420873	-0.165497	-4.092057
13	0.060427	-2.910225	-3.020714
13	0.195094	-4.059084	-0.511754
13	0.537610	-3.540794	2.230507
7	1.968110	0.000496	-0.297968
1	1.583864	-0.917615	-0.395070
9	1.620520	0.716698	-1.300282

9	1.530648	0.534291	0.780035
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HPF₂@C₃₀Al₁₅N₁₅

6	2.850987	2.721776	-0.031062
6	2.451300	2.676602	1.327118
6	2.916378	1.408632	2.083056
6	2.095357	0.759689	3.070276
6	2.549787	-1.712966	2.442032
6	2.463585	-2.912441	0.269377
6	1.589986	-3.314735	-0.810973
6	1.537858	-2.726900	-2.231750
6	2.366650	-1.669683	-2.639392
6	2.004744	-0.373268	-3.213230
6	2.664243	0.775839	-2.581071
6	1.971037	2.073839	-2.377198
6	2.040717	2.987884	-1.190030
6	1.957543	-2.797322	1.686434
6	-2.983576	-2.466873	0.078337
6	-2.208665	-2.928870	1.275477
6	-2.023165	-2.170190	2.497725
6	-2.616686	-0.913610	2.789803
6	-2.815123	-1.580525	-2.223123
6	-2.472778	-2.657197	-1.284315
6	-2.038575	0.397247	3.123837
6	-2.544336	1.525043	2.396053
6	-2.122797	-0.831037	-3.180909
6	-2.092966	0.686824	-3.178709
6	-2.743330	1.564629	-2.286699
6	-1.959973	2.772754	-1.660894
6	-2.287538	3.057564	-0.342053
6	-1.538424	3.437604	0.878998
6	-1.673125	2.736921	2.098081
6	1.889093	-0.743691	3.229424
7	3.838494	0.449693	-1.782589
7	3.678192	-2.177859	0.021581
7	3.973662	0.708379	1.417058
7	1.407466	3.489125	1.768439
7	0.960857	3.857025	-1.108271
7	0.825470	2.356800	-3.098623
7	0.825914	-0.285841	-3.966919
7	0.319144	-2.990859	-2.895989
7	0.377795	-3.953571	-0.519079

7	0.788972	-3.377517	2.131205
7	0.701244	-1.085225	3.893152
7	1.005632	1.452475	3.659114
7	-3.757533	1.283577	1.666815
7	-3.886625	1.155396	-1.535699
7	-4.053602	-1.535090	0.230855
13	4.101844	1.404074	-0.291198
13	3.843859	-1.377105	-1.579537
13	3.980872	-1.089463	1.476503
13	-4.117425	-0.542333	1.768252
13	-3.831076	2.074054	0.054315
13	-4.184380	-0.620076	-1.380889
13	-0.385554	-1.604863	-3.784729
13	-0.262382	1.137009	-3.782599
13	-0.288262	3.664744	-2.443301
13	0.285458	4.165237	0.509459
13	0.171250	2.817649	2.894638
13	-0.361843	0.367572	4.123134
13	-0.225639	-2.529926	3.378551
13	-0.524853	-3.960780	1.017585
13	-0.914962	-3.691159	-1.774219
15	-0.816180	-0.130800	0.183122
1	-0.112968	-1.164419	0.908814
9	0.296280	1.095689	0.684786
9	0.061615	-0.405759	-1.276812