Electronic Supporting Information for

Computational Studies of Complexation of Nitrous Oxide by Borane-Phosphine Frustrated Lewis Pairs

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Table S1. Comparisons of core distances (Å) and angles (deg) from experiment and theory using different ONIOM model chemistries

Notes: The compounds are listed with their numbers from the paper from Neu, Otten and Stephan, *Chem Sci*., 2011, **2**, 170-176. Four distances and three angles involving the core atoms were used as the database. In the leftmost column, "onimpw1k631pgd" is shorthand for the ONIOM(MPW1K/6-31+G(d):MPW1K/3-21G) approach; with this in mind, the other designations are self-explanatory. The three rightmost columns give RMS deviations of the values for a particular model chemistry from experiment. "RMS A-B" is the RMS error for the four distances only, "RMS A-B-C" is the RMS error for the three angles only, and "RMS F", is the RMS error for all seven parameters, scaled to account for the differences in magnitude of the values. Specifically, each term in the "RMS F" calculation is (theory value-experimental value/experimental value), so technically the "RMS F" value is the RMS of the normalized errors.

At the bottom of the RMS columns are averages for each ONIOM model chemistry. It can be seen that the ONIOM(M06-2X) approaches give better agreement than the ONIOM(MPW1K) approaches when predicting bond distances, but worse agreement when predicting bond angles. The bottom of the "RMS F" column gives average deviations and the standard deviation of the last significant figure in parenthesis. One sees that the ONIOM models overall differ little.

	P–N	N–N	N–O	B–O	P–N–N	N–N–O	N–O–B	RMS A-B	RMS A-B-C	RMS F
$(F_5C_6)_3BONNPtBu_3$, 1	**1.709**	**1.257**	**1.336**	**1.543**	**117.0**	**109.1**	**114.4**			
onimpw1k631pgd	1.691	1.249	1.274	1.536	113.9	112.4	117.2	0.038	3.8	0.028
onimpw1k6311pgd	1.683	1.244	1.268	1.536	116.4	112.5	117.6	0.043	3.3	0.028
onim062X631pgd	1.706	1.250	1.287	1.530	110.2	113.7	110.9	0.030	6.3	0.035
onim062X6311pgd	1.705	1.246	1.283	1.530	110.4	114.0	110.9	0.032	6.3	0.036
$(F_5C_6)_2(H_5C_6)BONNPtBu_3$, 2	**1.711**	**1.260**	**1.327**	**1.548**	**112.9**	**111.7**	**111.6**			
onimpw1k631pgd	1.685	1.253	1.267	1.554	114.9	112.8	117.2	0.038	4.3	0.030
onimpw1k6311pgd	1.681	1.249	1.261	1.557	115.3	113.0	117.5	0.043	4.6	0.032
onim062X631pgd	1.703	1.260	1.279	1.559	111.4	113.5	114.5	0.029	2.6	0.020
onim062X6311pgd	1.702	1.256	1.274	1.560	111.7	113.8	114.7	0.032	2.8	0.022
$(p\text{-}HC_6F_4)_3BONNPtBu_3$, 5	**1.709**	**1.255**	**1.327**	**1.533**	**115.3**	**109.5**	**114.9**			
onimpw1k631pgd	1.685	1.249	1.271	1.537	115.6	112.3	117.3	0.035	2.6	0.023
onimpw1k6311pgd	1.681	1.245	1.265	1.539	116.1	112.6	117.4	0.040	2.9	0.025
onim062X631pgd	1.704	1.252	1.284	1.533	110.0	113.8	110.7	0.025	5.7	0.032
onim062X6311pgd	1.703	1.247	1.280	1.533	110.3	114.1	110.8	0.028	5.6	0.032
$(p\text{-}HC_6F_4)_3BONNPCy_3$, 8	**1.715**	**1.260**	**1.335**	**1.551**	**111.1**	**111.1**	**110.3**			
onimpw1k631pgd	1.686	1.246	1.275	1.529	112.7	113.0	114.0	0.041	3.2	0.027
onimpw1k6311pgd	1.682	1.246	1.267	1.536	112.9	113.4	114.8	0.045	3.8	0.030
onim062X631pgd	1.703	1.251	1.288	1.533	111.6	113.2	112.4	0.030	2.1	0.019
onim062X6311pgd	1.702	1.247	1.284	1.533	111.9	113.5	112.6	0.033	2.4	0.021
$Ph_3CONNPtBu_3^+$, 10	**1.722**	**1.242**	**1.375**	**1.496**	**116.0**	**108.5**	**110.7**			
onimpw1k631pgd	1.712	1.230	1.318	1.462	115.7	110.3	112.4	0.039	1.8	0.022
onimpw1k6311pgd	1.708	1.225	1.313	1.462	116.4	110.6	112.8	0.043	2.1	0.024
onim062X631pgd	1.731	1.236	1.330	1.477	111.9	111.5	111.0	0.029	3.6	0.023
onim062X6311pgd	1.730	1.232	1.328	1.476	112.1	111.8	111.1	0.030	3.6	0.024
								0.038	3.1	0.026(3)
								0.043	3.3	0.028(3)
								0.029	4.1	0.026(7)
								0.031	4.2	0.027(7)

Table S2. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(F_5C_6)_3B$–ONN–P(*t*-Bu)$_3$

O	-0.291323	-0.556222	-0.125698		C	3.859309	1.581093	1.609915
N	0.942833	-0.915363	-0.064079		C	2.732326	-0.384952	2.655659
N	1.749105	0.024562	-0.236357		C	5.199939	-0.498069	2.063797
B	-1.217922	-1.769333	-0.021156		C	3.040315	-3.098218	1.017024
P	3.351744	-0.539223	-0.083979		C	2.453304	-2.911696	-1.408349
C	-0.585038	-2.747004	1.123734		C	4.892887	-2.809200	-0.639789
C	-1.316165	-2.461039	-1.486596		C	3.708932	-0.310898	-2.797226
C	-2.639097	-1.112016	0.364651		C	3.616476	1.841059	-1.575020
C	3.820163	0.035754	1.630317		C	5.692558	0.425716	-1.376578
C	3.438611	-2.397625	-0.301073		H	3.993141	1.920900	2.642531
C	4.156659	0.389676	-1.488365		H	4.700139	1.955896	1.021598
C	-0.217622	-4.081525	1.027305		H	2.921698	1.995922	1.226338
C	-0.234057	-2.129672	2.320962		H	2.921619	0.185402	3.572311
C	0.413086	-4.771573	2.059584		H	1.714678	-0.152300	2.327425
C	0.438776	-2.762902	3.345807		H	2.783856	-1.440241	2.918494
C	0.742066	-4.109656	3.224223		H	5.435547	-0.062632	3.041701
F	-0.358453	-4.757795	-0.123712		H	5.204548	-1.584849	2.174211
F	-0.487909	-0.787756	2.477440		H	5.990972	-0.207678	1.365238
F	0.771930	-6.075040	1.892155		H	3.006109	-4.175944	0.816135
F	0.860549	-2.062478	4.439206		H	3.759271	-2.928306	1.821065
F	1.403706	-4.753671	4.224169		H	2.046948	-2.775841	1.327237
C	-0.678112	-2.108455	-2.665705		H	2.997532	-3.593903	-2.070395
C	-2.215784	-3.514307	-1.577959		H	1.628301	-3.461360	-0.943053
C	-0.907379	-2.771277	-3.865934		H	1.994426	-2.131745	-2.011204
C	-2.482618	-4.190795	-2.751969		H	4.933189	-3.904074	-0.626611
C	-1.817836	-3.808914	-3.907527		H	5.195461	-2.476010	-1.634785
F	0.243160	-1.116173	-2.705356		H	5.612471	-2.437560	0.097233
F	-2.852645	-3.905870	-0.429340		H	4.143050	0.248340	-3.633181
F	-0.240075	-2.399373	-4.994833		H	4.050624	-1.345318	-2.867367
F	-3.371610	-5.220152	-2.791831		H	2.617600	-0.283297	-2.899127
F	-2.056329	-4.463752	-5.076476		H	3.919622	2.234078	-2.552091
C	-3.411050	-1.352700	1.493479		H	2.526414	1.855226	-1.507023
C	-3.142324	-0.180430	-0.535553		H	4.037435	2.490404	-0.808390
C	-4.620511	-0.706242	1.717240		H	6.081067	0.937288	-2.264630
C	-4.342637	0.481920	-0.343094		H	6.010975	0.996974	-0.498887
C	-5.084003	0.211984	0.794424		H	6.142196	-0.568931	-1.335785
F	-3.009683	-2.227633	2.422250					
F	-2.428019	0.105720	-1.668652					
F	-5.347262	-0.970553	2.838696					
F	-4.799435	1.388820	-1.251049					
F	-6.266238	0.853153	1.002560					

Table S3. Optimized (ONI(M06-2X)) Cartesian coordinates of the *ct* conformer of $(F_5C_6)_3B–ONN–P(t\text{-}Bu)_3$

O	-0.003489	0.085489	0.318231		C	3.934791	2.935919	1.998153
N	1.275967	0.030190	0.317723		C	3.343438	0.688595	2.847961
N	1.885579	1.124078	0.191631		C	5.681170	1.115682	1.969071
B	-0.939654	1.285382	0.053491		C	3.874674	-1.747547	0.744380
P	3.576964	0.958572	0.075776		C	3.178588	-1.296233	-1.620358
C	-0.362821	2.342671	-1.045109		C	5.541734	-0.822398	-0.890879
C	-1.355515	1.951796	1.469167		C	3.624075	1.613437	-2.607591
C	-2.240750	0.479609	-0.505720		C	3.095019	3.487228	-1.047626
C	4.183566	1.426215	1.778839		C	5.465481	2.639907	-1.215428
C	4.061039	-0.776249	-0.446883		H	4.153772	3.151286	3.049887
C	3.979229	2.228492	-1.231669		H	4.589580	3.558263	1.385335
C	-0.448396	3.732655	-1.020369		H	2.888320	3.193846	1.806301
C	0.227039	1.823542	-2.191200		H	3.678509	1.055043	3.825466
C	-0.024400	4.536500	-2.077368		H	2.279762	0.910751	2.750209
C	0.668684	2.585717	-3.252139		H	3.482689	-0.391232	2.832966
C	0.536204	3.961617	-3.197627		H	5.978801	1.505375	2.949318
F	-0.922881	4.392257	0.041017		H	5.874980	0.040063	1.967338
F	0.442842	0.462580	-2.283928		H	6.308572	1.594074	1.210693
F	-0.140191	5.890141	-1.991900		H	4.110686	-2.753479	0.380287
F	1.290660	2.001443	-4.319284		H	4.556755	-1.525804	1.567373
F	0.993859	4.733025	-4.221309		H	2.839601	-1.736760	1.093658
C	-0.827955	1.700486	2.723565		H	3.565890	-0.972692	-2.585898
C	-2.458906	2.796233	1.436097		H	3.221775	-2.390322	-1.592825
C	-1.344322	2.266678	3.883302		H	2.133627	-0.997633	-1.539903
C	-3.005110	3.377690	2.564003		H	5.779335	-1.868726	-1.116402
C	-2.436709	3.107070	3.799303		H	5.711035	-0.241784	-1.800565
F	0.230263	0.880005	2.875822		H	6.229208	-0.480465	-0.112821
F	-3.029377	3.066169	0.219950		H	3.587994	2.420434	-3.346467
F	-0.779976	1.993241	5.093525		H	4.380116	0.894673	-2.931912
F	-4.082416	4.205144	2.481850		H	2.646017	1.128614	-2.610834
F	-2.955129	3.670559	4.924531		H	3.188764	4.084592	-1.961985
C	-2.916804	0.663888	-1.705954		H	2.048938	3.213137	-0.907431
C	-2.750572	-0.507900	0.332215		H	3.417629	4.103568	-0.209458
C	-4.022908	-0.097903	-2.064518		H	5.628166	3.322578	-2.057538
C	-3.850304	-1.282842	0.005342		H	5.726539	3.174846	-0.298512
C	-4.487363	-1.074130	-1.205614		H	6.142010	1.789555	-1.335662
F	-2.523153	1.595049	-2.583347					
F	-2.161052	-0.733661	1.546852					
F	-4.647529	0.115341	-3.256466					
F	-4.311460	-2.241254	0.856688					
F	-5.568092	-1.828385	-1.545279					

Table S4. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(4\text{-H-}F_4C_6)_3B\text{–ONN–P}(t\text{-Bu})_3$

O	-0.287681	-0.545211	-0.122097		C	3.865965	1.586083	1.597034
N	0.943687	-0.904896	-0.060034		C	2.733114	-0.371484	2.653453
N	1.753921	0.032240	-0.238264		C	5.200963	-0.493172	2.063727
B	-1.212649	-1.763166	-0.019315		C	3.030845	-3.092374	1.031971
P	3.351355	-0.541854	-0.083927		C	2.441958	-2.915784	-1.396611
C	-0.573163	-2.738440	1.125080		C	4.881933	-2.823131	-0.628308
C	-1.314145	-2.450020	-1.487485		C	3.709582	-0.334262	-2.797207
C	-2.638426	-1.113676	0.365825		C	3.629199	1.826543	-1.590858
C	3.822944	0.041008	1.626376		C	5.697875	0.402535	-1.382086
C	3.429977	-2.401670	-0.291104		H	4.000937	1.931932	2.627563
C	4.161824	0.373269	-1.493625		H	4.707310	1.955659	1.005818
C	-0.202819	-4.072210	1.020832		H	2.928922	2.000289	1.211312
C	-0.232404	-2.122003	2.327234		H	2.919826	0.207625	3.565260
C	0.416131	-4.762331	2.062305		H	1.715342	-0.144506	2.321540
C	0.431434	-2.767481	3.352459		H	2.784612	-1.424731	2.924593
C	0.736314	-4.113464	3.236051		H	5.435292	-0.056417	3.041436
F	-0.324077	-4.734473	-0.143373		H	5.203466	-1.579823	2.175090
F	-0.486994	-0.777432	2.480472		H	5.993728	-0.205068	1.366098
F	0.770496	-6.067464	1.877206		H	2.987637	-4.170696	0.836980
F	0.839433	-2.057248	4.448543		H	3.754800	-2.923101	1.832011
H	1.242585	-4.634626	4.034089		H	2.041352	-2.763506	1.346759
C	-0.679048	-2.091444	-2.667608		H	2.989791	-3.579602	-2.074341
C	-2.218306	-3.501078	-1.574546		H	1.629067	-3.484398	-0.932845
C	-0.925066	-2.750930	-3.868268		H	1.965367	-2.134525	-1.983962
C	-2.491683	-4.165345	-2.756248		H	4.914593	-3.918290	-0.611543
C	-1.838418	-3.784316	-3.917230		H	5.187345	-2.495665	-1.624334
F	0.251042	-1.103048	-2.699622		H	5.603885	-2.453901	0.107759
F	-2.843861	-3.894664	-0.417782		H	4.145203	0.217208	-3.637664
F	-0.254154	-2.363669	-4.993399		H	4.046345	-1.370758	-2.859997
F	-3.389613	-5.191226	-2.780865		H	2.618259	-0.303829	-2.897800
H	-2.039221	-4.294641	-4.846605		H	3.933924	2.211310	-2.570821
C	-3.420293	-1.388003	1.481174		H	2.539240	1.845579	-1.522309
C	-3.135317	-0.168949	-0.525348		H	4.053244	2.479243	-0.828667
C	-4.637732	-0.749820	1.697221		H	6.089295	0.907581	-2.272712
C	-4.345191	0.478265	-0.326616		H	6.018275	0.976782	-0.507007
C	-5.102159	0.185010	0.793320		H	6.143009	-0.593954	-1.335355
F	-3.017269	-2.282899	2.392583					
F	-2.406943	0.136396	-1.646890					
F	-5.366992	-1.053934	2.810560					
F	-4.786961	1.398608	-1.232812					
H	-6.045869	0.681796	0.958079					

Table S5. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(4\text{-H-}F_4C_6)_3B$–ONN–PCy_3

O	0.189548	-0.576597	-0.002793		C	2.666413	2.205440	3.961226
N	1.455775	-0.346915	0.057245		C	1.834587	3.471666	3.703721
N	1.755503	0.838798	-0.206296		H	3.006147	4.031645	0.480989
B	-0.160022	-2.025391	0.355444		H	1.563392	3.113484	0.952203
P	3.422812	1.124497	-0.005991		H	3.331714	0.443376	2.916347
C	0.768833	-2.430282	1.639612		H	1.745973	1.027654	2.399917
C	0.086626	-2.970638	-0.940220		H	3.473147	4.603929	2.851688
C	-1.741049	-1.934458	0.666837		H	1.874253	5.173720	2.340821
C	3.409633	2.147498	1.527843		H	3.676402	2.488882	4.286465
C	4.429666	-0.421875	0.026690		H	2.213921	1.584923	4.736952
C	3.942701	1.947372	-1.572942		H	1.778655	4.082219	4.610904
C	1.634371	-3.509621	1.778792		H	0.813094	3.182722	3.426300
C	0.816859	-1.498284	2.674164		H	5.471714	-0.067126	-0.019461
C	2.499595	-3.636651	2.862470		C	4.249710	-1.299951	1.286552
C	1.676850	-1.597705	3.750299		C	4.116006	-1.211512	-1.280117
C	2.531685	-2.680295	3.854159		C	5.051944	-2.613778	1.163290
F	1.739370	-4.450442	0.823290		C	4.914099	-2.529410	-1.340675
F	0.026712	-0.373443	2.595999		C	4.643508	-3.394000	-0.098596
F	3.390942	-4.675752	2.889950		H	4.594436	-0.759937	2.172747
F	1.719235	-0.594483	4.683702		H	3.187350	-1.528134	1.401034
H	3.215292	-2.767397	4.684847		H	4.367937	-0.606863	-2.158997
C	0.630938	-2.635651	-2.170422		H	3.047228	-1.431280	-1.325686
C	-0.366164	-4.277034	-0.805960		H	6.125246	-2.383842	1.118130
C	0.722827	-3.552935	-3.212993		H	4.870782	-3.233413	2.044992
C	-0.298412	-5.206108	-1.828431		H	5.988130	-2.306210	-1.398271
C	0.250310	-4.838945	-3.046509		H	4.630821	-3.063573	-2.253967
F	1.137377	-1.398419	-2.398780		H	5.216793	-4.325264	-0.159270
F	-0.880355	-4.649252	0.410676		H	3.583463	-3.663878	-0.040613
F	1.284521	-3.167250	-4.397130		H	4.850642	1.390560	-1.842026
F	-0.759179	-6.475614	-1.639808		C	2.882362	1.708404	-2.680010
H	0.312052	-5.554008	-3.852365		C	4.339962	3.436942	-1.537975
C	-2.388938	-2.251444	1.854166		C	3.499308	2.083988	-4.042632
C	-2.539319	-1.472637	-0.373548		C	4.988035	3.795183	-2.894222
C	-3.766139	-2.116223	1.996010		C	3.988425	3.547297	-4.043433
C	-3.912925	-1.330316	-0.251181		H	2.524822	0.672875	-2.687124
C	-4.531027	-1.655187	0.942798		H	2.011590	2.338555	-2.466174
F	-1.695845	-2.699122	2.909676		H	5.030831	3.649452	-0.712992
F	-1.951544	-1.144315	-1.568516		H	3.444928	4.053906	-1.412023
F	-4.353869	-2.440825	3.184891		H	4.345881	1.415115	-4.250113
F	-4.650891	-0.871875	-1.304305		H	2.755255	1.932586	-4.831079
H	-5.599746	-1.549523	1.049286		H	5.882276	3.176229	-3.044289
H	4.443086	2.416123	1.785599		H	5.302807	4.843918	-2.884265
C	2.564933	3.426089	1.272346		H	4.454192	3.788585	-5.004498
C	2.757475	1.340363	2.685914		H	3.125048	4.212572	-3.913730
C	2.466776	4.278116	2.556276					

Table S6. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(H_5C_6)(F_5C_6)_2B–ONN–P(t\text{-}Bu)_3$

O	0.032607	-0.118206	-0.191234		C	3.299803	2.855760	2.079269
N	1.304926	-0.092797	-0.067598		C	2.906459	0.477825	2.687200
N	1.801911	1.054721	-0.219919		C	5.251891	1.265559	2.199321
B	-0.589539	-1.547570	-0.173809		C	4.011835	-1.665648	0.591161
P	3.492162	1.034075	-0.009679		C	3.485803	-1.192831	-1.777324
C	0.346575	-2.457142	0.820697		C	5.721645	-0.475253	-0.821079
C	-0.654075	-2.057807	-1.695646		C	3.886585	1.954496	-2.599138
C	-2.079190	-1.272196	0.411761		C	2.964265	3.613180	-1.014165
C	3.768162	1.409337	1.802429		C	5.402092	2.969576	-0.850641
C	4.209412	-0.617579	-0.530856		H	3.329221	3.006118	3.163856
C	3.980457	2.446930	-1.135203		H	3.958900	3.596262	1.621548
C	0.990177	-3.664794	0.572200		H	2.271104	3.010966	1.738291
C	0.629059	-1.891281	2.060659		H	2.951186	0.872081	3.708908
C	1.860538	-4.256136	1.490054		H	1.855366	0.450628	2.391933
C	1.508195	-2.425637	2.976892		H	3.290307	-0.538478	2.722222
C	2.130176	-3.630425	2.688731		H	5.344972	1.570091	3.248239
F	0.814990	-4.334946	-0.569295		H	5.592964	0.230072	2.124626
F	0.051276	-0.682723	2.381874		H	5.910702	1.902858	1.602828
F	2.467989	-5.438505	1.189375		H	4.333464	-2.633922	0.189079
F	1.817235	-1.752517	4.126379		H	4.616052	-1.453606	1.475674
F	3.007085	-4.175794	3.576253		H	2.957217	-1.741287	0.862547
C	-0.127333	-1.323478	-2.772101		H	4.019547	-2.110111	-2.053031
C	-1.298613	-3.271406	-1.995053		H	2.453421	-1.463641	-1.543293
C	-0.215762	-1.795543	-4.086079		H	3.492607	-0.528197	-2.639687
C	-1.396006	-3.744997	-3.300631		H	6.114363	-1.480339	-1.012161
C	-0.847491	-3.008185	-4.353794		H	5.915139	0.131656	-1.708524
H	0.327840	-0.353602	-2.585344		H	6.272375	-0.055434	0.026184
H	-1.724502	-3.854557	-1.183669		H	4.070364	2.817767	-3.247759
H	0.192972	-1.207356	-4.900403		H	4.630892	1.192873	-2.836435
H	-1.898115	-4.684545	-3.501254		H	2.883211	1.573156	-2.817658
H	-0.922720	-3.372433	-5.371675		H	3.161823	4.296746	-1.847621
C	-2.670185	-1.826982	1.540193		H	1.940408	3.240000	-1.087753
C	-2.860224	-0.365284	-0.298472		H	3.077188	4.174497	-0.088323
C	-3.964626	-1.514312	1.939192		H	5.630295	3.739240	-1.596981
C	-4.150596	-0.028476	0.073735		H	5.467345	3.435887	0.136073
C	-4.703869	-0.611457	1.201095		H	6.163952	2.188958	-0.926790
F	-2.004202	-2.707021	2.301413					
F	-2.346074	0.235974	-1.412408					
F	-4.502422	-2.089154	3.052395					
F	-4.880011	0.867139	-0.649733					
F	-5.972020	-0.291167	1.580211					

Table S7. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(4\text{-F-H}_4C_6)_3B–ONN–P(t\text{-Bu})_3$

O	-0.277070	-0.575424	-0.211863		C	3.834920	1.700909	1.426098
N	0.947753	-0.922021	-0.124816		C	2.573687	-0.165240	2.447991
N	1.762184	-0.020394	-0.476055		C	5.078272	-0.389863	2.061299
B	-1.280941	-1.785926	-0.003446		C	3.015396	-3.046594	1.030547
P	3.362371	-0.525360	-0.197759		C	2.649761	-2.991356	-1.411314
C	-0.643527	-2.764980	1.122608		C	5.003979	-2.785534	-0.492727
C	-1.434016	-2.485628	-1.451115		C	4.012086	-0.393827	-2.894377
C	-2.641684	-1.062748	0.464405		C	3.685005	1.785806	-1.766828
C	3.752900	0.159709	1.496547		C	5.786382	0.458399	-1.311376
C	3.523712	-2.391875	-0.277278		H	3.898341	2.070367	2.455970
C	4.269620	0.362458	-1.569340		H	4.722865	2.045354	0.891896
C	-0.317652	-4.117049	0.917090		H	2.936149	2.121823	0.964912
C	-0.337768	-2.223644	2.389961		H	2.832135	0.242184	3.432456
C	0.288377	-4.888347	1.915458		H	1.656850	0.322748	2.104667
C	0.283989	-2.974688	3.385545		H	2.371922	-1.229862	2.558570
C	0.594230	-4.305507	3.132879		H	5.268068	0.112613	3.016833
H	-0.539428	-4.575608	-0.043124		H	5.030797	-1.463280	2.253538
H	-0.603241	-1.189300	2.591474		H	5.924711	-0.183572	1.398941
H	0.528906	-5.931558	1.755075		H	3.062529	-4.132003	0.884157
H	0.513139	-2.554419	4.356949		H	3.629935	-2.800334	1.898405
F	1.207643	-5.050532	4.109346		H	1.970654	-2.785712	1.213240
C	-0.715195	-2.101532	-2.598534		H	2.868054	-4.065753	-1.437220
C	-2.343984	-3.552812	-1.600032		H	1.587528	-2.868431	-1.186973
C	-0.873060	-2.763480	-3.820532		H	2.858995	-2.581114	-2.398247
C	-2.505657	-4.222166	-2.809499		H	5.062170	-3.877735	-0.425820
C	-1.760702	-3.820880	-3.910324		H	5.369941	-2.493236	-1.479865
H	-0.028143	-1.260366	-2.546981		H	5.664789	-2.367640	0.272945
H	-2.943075	-3.851479	-0.744233		H	4.458077	0.196319	-3.702277
H	-0.323650	-2.461839	-4.702913		H	4.470538	-1.383818	-2.909244
H	-3.205325	-5.040711	-2.916518		H	2.937923	-0.482633	-3.090321
F	-1.913104	-4.478061	-5.106072		H	4.070038	2.162454	-2.721186
C	-3.502323	-1.594148	1.440583		H	2.593707	1.751894	-1.804982
C	-3.038278	0.137228	-0.157235		H	3.996419	2.477023	-0.985198
C	-4.703556	-0.963046	1.778228		H	6.243220	0.945714	-2.180655
C	-4.226814	0.779034	0.177841		H	6.007472	1.071728	-0.433786
C	-5.050341	0.217000	1.143760		H	6.256243	-0.520688	-1.187598
H	-3.226775	-2.511733	1.954749					
H	-2.392362	0.570290	-0.913073					
H	-5.366630	-1.373428	2.528491					
H	-4.528548	1.702661	-0.298695					
F	-6.225343	0.845544	1.476302					

Table S8. Optimized (ONI(M06-2X)) Cartesian coordinates of the *ct* conformer of (4-F-H_4C_6)$_3$B–ONN–P(*t*-Bu)$_3$

O	-0.051436	-0.257616	0.016428		C	3.332596	1.913933	2.995079
N	1.228453	-0.238848	0.153320		C	3.125880	-0.531155	2.666679
N	1.722886	0.917024	0.241250		C	5.372451	0.591654	2.325747
B	-0.917443	1.051898	-0.215595		C	4.203909	-1.602916	-0.196613
P	3.397912	1.034008	0.351860		C	3.338769	-0.314561	-2.116514
C	-0.296231	1.828975	-1.500683		C	5.633072	0.226651	-1.174481
C	-0.996261	1.909901	1.151873		C	3.364512	2.892505	-1.682368
C	-2.364844	0.412986	-0.547332		C	2.516855	3.691614	0.510862
C	3.847065	0.732075	2.140924		C	5.011142	3.370426	0.179093
C	4.188115	-0.189224	-0.825138		H	3.470163	1.639360	4.047409
C	3.613155	2.817270	-0.158033		H	3.899346	2.828618	2.811864
C	-0.180541	3.225422	-1.632001		H	2.266087	2.101700	2.824374
C	0.104427	1.057381	-2.611543		H	3.352765	-0.610532	3.736054
C	0.298119	3.819868	-2.804197		H	2.043481	-0.436980	2.555545
C	0.607067	1.635777	-3.776727		H	3.450679	-1.449707	2.181828
C	0.693522	3.018734	-3.862033		H	5.572561	0.501198	3.399742
H	-0.464571	3.865991	-0.801601		H	5.765027	-0.302917	1.836317
H	0.001651	-0.022802	-2.557380		H	5.914891	1.466448	1.954767
H	0.370903	4.895689	-2.901421		H	4.575925	-2.292584	-0.963009
H	0.907670	1.034056	-4.625380		H	4.869401	-1.672674	0.665850
F	1.178370	3.596793	-5.009475		H	3.190726	-1.906851	0.080970
C	-0.381377	1.541145	2.362566		H	3.855107	-1.030929	-2.766509
C	-1.798258	3.068545	1.186684		H	2.347876	-0.711171	-1.884825
C	-0.501927	2.311475	3.522444		H	3.215770	0.619922	-2.660093
C	-1.919493	3.853592	2.332136		H	6.067491	-0.567754	-1.792389
C	-1.257225	3.472374	3.488846		H	5.661672	1.152875	-1.752624
H	0.186390	0.615176	2.411010		H	6.259166	0.341665	-0.284182
H	-2.361330	3.343357	0.299401		H	3.341052	3.950955	-1.962784
H	-0.032025	2.013996	4.451680		H	4.157093	2.409555	-2.258210
H	-2.534989	4.743562	2.345671		H	2.390594	2.464231	-1.939711
F	-1.366108	4.242043	4.620433		H	2.463503	4.626150	-0.059128
C	-3.178462	0.835473	-1.612143		H	1.541491	3.197566	0.462293
C	-2.881374	-0.589939	0.296245		H	2.753647	3.939708	1.544693
C	-4.448426	0.288447	-1.823397		H	5.064918	4.392269	-0.213655
C	-4.138508	-1.148842	0.089620		H	5.177432	3.421951	1.258640
C	-4.912117	-0.698173	-0.971536		H	5.817501	2.790600	-0.279582
H	-2.814353	1.596574	-2.297337					
H	-2.275249	-0.936007	1.126802					
H	-5.075227	0.615490	-2.642616					
H	-4.531429	-1.922101	0.736642					
F	-6.155830	-1.243448	-1.177657					

Table S9. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(H_5C_6)_3B–ONN–P(t\text{-}Bu)_3$

O	0.906106	-0.006166	-1.131524	C	-3.563622	-1.967126	-2.111851
N	-0.209538	0.000486	-0.517808	C	-1.901098	-2.644796	-0.411098
N	-1.210878	0.182038	-1.271990	C	-4.305518	-2.178932	0.280399
B	2.153796	-0.001227	-0.146330	C	-1.737856	-0.710828	2.181996
P	-2.652015	0.034129	-0.385265	C	-1.451064	1.671305	1.599897
C	1.761004	-0.915022	1.137593	C	-3.771903	0.772867	2.083822
C	2.419902	1.548418	0.223199	C	-3.377205	2.669249	-0.870178
C	3.338915	-0.622435	-1.043152	C	-3.508033	1.150044	-2.820087
C	-3.145697	-1.750161	-0.640434	C	-5.258682	0.989500	-1.005524
C	-2.407788	0.461755	1.424239	H	-3.681969	-3.046553	-2.260526
C	-3.763736	1.231723	-1.292200	H	-4.517333	-1.489826	-2.347222
C	1.732218	-0.457186	2.466766	H	-2.788676	-1.608754	-2.796446
C	1.371485	-2.254149	0.914955	H	-2.218662	-3.683778	-0.558933
C	1.328790	-1.288537	3.519927	H	-1.123251	-2.415554	-1.145191
C	0.948976	-3.082502	1.954482	H	-1.464473	-2.555507	0.582791
C	0.923438	-2.597963	3.267308	H	-4.575368	-3.209115	0.020442
H	2.030139	0.567322	2.677521	H	-4.020803	-2.164442	1.334004
H	1.413454	-2.643106	-0.099647	H	-5.193127	-1.553513	0.142803
H	1.326215	-0.908737	4.536201	H	-1.550163	-0.365418	3.205238
H	0.657715	-4.107832	1.749686	H	-2.370055	-1.599017	2.239734
H	0.607736	-3.241076	4.081027	H	-0.769416	-0.957190	1.740399
C	1.603581	2.618078	-0.191412	H	-1.431682	1.899065	2.672478
C	3.539407	1.871373	1.018183	H	-0.435959	1.408781	1.292972
C	1.875574	3.937494	0.190206	H	-1.766250	2.569108	1.069910
C	3.813412	3.181111	1.405756	H	-3.589104	0.910801	3.155438
C	2.976252	4.222920	0.995160	H	-4.215725	1.695080	1.701145
H	0.749097	2.422199	-0.836131	H	-4.489934	-0.044939	1.969015
H	4.207543	1.070013	1.323759	H	-3.957790	3.361842	-1.489270
H	1.232517	4.742330	-0.150178	H	-3.610065	2.876738	0.175420
H	4.682236	3.395642	2.018257	H	-2.313585	2.856422	-1.054050
H	3.188944	5.243874	1.290413	H	-3.986502	2.025155	-3.274312
C	4.326861	-1.476500	-0.521438	H	-2.436508	1.171747	-3.031887
C	3.443201	-0.268645	-2.402571	H	-3.945589	0.259582	-3.268883
C	5.375245	-1.950189	-1.318532	H	-5.830416	1.760546	-1.535192
C	4.478266	-0.745403	-3.204574	H	-5.587693	0.016572	-1.380325
C	5.452590	-1.588083	-2.662391	H	-5.500732	1.060217	0.057993
H	4.268358	-1.783310	0.520802				
H	2.690593	0.388332	-2.826274				
H	6.126226	-2.605475	-0.890578				
H	4.532008	-0.459682	-4.249527				
H	6.261872	-1.956972	-3.282154				

Table S10. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C2(F5)

N	-0.044214	-0.058078	0.035123		C	1.743155	-2.271175	-2.687792
N	1.187426	-0.076172	-0.066462		C	3.423423	-0.527908	-2.164493
O	1.977180	0.919083	-0.146577		C	3.913062	-2.948170	-1.576219
B	-0.748670	1.337404	0.181842		C	4.397065	-0.558594	0.978421
P	1.997681	-1.672850	0.011841		C	2.450682	-0.507255	2.511496
C	-0.478067	2.317590	-1.078101		C	3.659758	-2.707521	2.055354
C	-0.163555	1.827887	1.613809		C	0.119846	-2.737945	1.787370
C	-2.336568	1.006492	0.189388		C	-0.530258	-2.939353	-0.629107
C	2.817820	-1.860028	-1.655479		C	1.311878	-4.371088	0.270521
C	3.170129	-1.377179	1.445864		H	2.216382	-2.236985	-3.675330
C	0.673002	-2.960909	0.358224		H	1.382246	-3.287196	-2.524782
C	0.056407	2.001856	-2.315062		H	0.908056	-1.562501	-2.690527
C	-0.945226	3.616989	-0.935685		H	3.860185	-0.750177	-3.144967
C	0.150437	2.922282	-3.351224		H	2.642949	0.222967	-2.280623
C	-0.874824	4.562645	-1.939907		H	4.205401	-0.133703	-1.519206
C	-0.318707	4.206679	-3.159554		H	4.319702	-3.075249	-2.586062
F	0.527320	0.758695	-2.575128		H	4.735643	-2.653344	-0.920875
F	-1.504084	3.969405	0.263963		H	3.523678	-3.915402	-1.247777
F	0.696719	2.560482	-4.546518		H	4.993472	-0.343139	1.872291
F	-1.340287	5.828049	-1.753766		H	5.028202	-1.108871	0.278128
F	-0.239609	5.122020	-4.163960		H	4.065126	0.382043	0.536862
C	-0.456560	1.101977	2.762969		H	3.154510	-0.365269	3.339914
C	0.779854	2.834491	1.759065		H	2.216189	0.472552	2.084916
C	0.136432	1.343143	3.989762		H	1.543619	-0.960620	2.911667
C	1.392845	3.106581	2.976008		H	4.398164	-2.457633	2.825350
C	1.071163	2.358170	4.092328		H	2.855067	-3.266998	2.536000
F	-1.313916	0.064200	2.693022		H	4.152205	-3.344503	1.312753
F	1.162566	3.599681	0.699519		H	-0.652890	-3.497716	1.948876
F	-0.167309	0.575131	5.074715		H	0.883155	-2.881528	2.554374
F	2.321249	4.098486	3.076132		H	-0.347531	-1.756199	1.897537
F	1.679155	2.608500	5.284478		H	-1.334549	-3.495351	-0.133159
C	-2.877482	0.196707	-0.802773		H	-0.894295	-1.937015	-0.844714
C	-3.231834	1.509210	1.120759		H	-0.300455	-3.460308	-1.557577
C	-4.224538	-0.120813	-0.872729		H	0.536032	-5.088542	0.561800
C	-4.588273	1.219221	1.077493		H	1.611113	-4.609823	-0.753672
C	-5.083441	0.401996	0.077731		H	2.164425	-4.508204	0.938709
F	-2.066038	-0.319414	-1.747984					
F	-2.800309	2.307202	2.141457					
F	-4.703497	-0.929653	-1.859451					
F	-5.437105	1.726144	2.013797					
F	-6.411846	0.108474	0.030101					

Table S11. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C3(F5)

N	-0.319691	0.031199	-0.465961		C	-1.786441	-2.057788	2.135644
N	0.857315	0.022527	-1.155439		C	-3.386566	-1.212962	0.457733
O	1.390673	1.088003	-1.325616		C	-2.621493	-3.577723	0.314714
B	-0.675156	1.549379	0.174934		C	-2.428363	-1.611302	-2.646610
P	-0.675714	-1.680186	-0.469328		C	-0.030770	-1.546788	-3.267325
C	-0.783084	2.676045	-1.012772		C	-0.994552	-3.696043	-2.468819
C	0.581634	1.838011	1.185230		C	1.999540	-2.703588	-0.898594
C	-2.152064	1.726780	0.847236		C	1.475750	-1.681312	1.309331
C	-2.146131	-2.132981	0.634136		C	0.605870	-3.984846	0.675375
C	-1.035878	-2.161680	-2.259650		H	-2.700995	-2.303714	2.688013
C	0.886211	-2.547050	0.168820		H	-1.012636	-2.760417	2.441136
C	-0.972717	2.517099	-2.374243		H	-1.482116	-1.051493	2.412034
C	-0.839346	3.993003	-0.566243		H	-4.282969	-1.828279	0.591423
C	-1.160707	3.578167	-3.250631		H	-3.383536	-0.453630	1.238270
C	-1.021114	5.079674	-1.398882		H	-3.446883	-0.715595	-0.504642
C	-1.177707	4.867416	-2.759318		H	-3.337169	-3.842197	1.101157
F	-1.020849	1.282737	-2.919729		H	-3.152441	-3.618512	-0.638260
F	-0.712325	4.231363	0.779360		H	-1.828817	-4.324017	0.321823
F	-1.339972	3.345571	-4.581014		H	-2.578171	-1.818900	-3.712129
F	-1.054190	6.346483	-0.902165		H	-3.239613	-2.090379	-2.094103
F	-1.361001	5.922460	-3.598853		H	-2.462429	-0.527678	-2.504412
C	0.721030	1.198470	2.409999		H	-0.335036	-1.913020	-4.255303
C	1.644267	2.686261	0.868385		H	-0.089090	-0.461515	-3.275627
C	1.811255	1.327900	3.252445		H	0.997261	-1.855526	-3.087319
C	2.750772	2.856215	1.689945		H	-1.250899	-3.875032	-3.519371
C	2.840788	2.170963	2.885326		H	0.006339	-4.100192	-2.304357
F	-0.234819	0.348917	2.844935		H	-1.706615	-4.247146	-1.858724
F	1.668458	3.406508	-0.286894		H	2.865673	-3.133253	-0.381253
F	1.866131	0.630091	4.421328		H	1.716062	-3.393075	-1.696016
F	3.758492	3.691842	1.316314		H	2.285132	-1.745079	-1.325106
F	3.928167	2.321308	3.687445		H	2.269759	-2.261275	1.792648
C	-3.285331	1.653037	0.035434		H	1.922355	-0.770514	0.898884
C	-2.394773	2.235649	2.120569		H	0.745578	-1.388228	2.063747
C	-4.568591	1.950253	0.450342		H	1.567068	-4.392553	1.007460
C	-3.671582	2.551637	2.575369		H	-0.078081	-4.030028	1.520177
C	-4.762186	2.400351	1.744367		H	0.234592	-4.630537	-0.125740
F	-3.165959	1.199555	-1.229733					
F	-1.390264	2.490981	3.005482					
F	-5.626508	1.794625	-0.391852					
F	-3.847478	3.022473	3.839327					
F	-6.012212	2.697530	2.186105					

Table S12. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C5(F5)

N	0.052356	0.065796	0.022581		C	2.703064	-0.263338	2.945230
N	1.321365	0.046285	0.043877		C	0.681185	-1.690792	2.731722
B	-0.561498	1.576498	-0.035314		C	2.971036	-2.759849	2.697223
O	-0.674950	-0.924328	0.155964		C	0.697199	-3.657424	0.137626
P	2.262207	-1.290352	0.407246		C	1.139742	-2.345125	-1.921207
C	-0.006223	2.344121	-1.344920		C	2.992192	-3.723913	-0.831481
C	0.024183	2.125850	1.374873		C	3.847895	-0.481628	-1.705154
C	-2.153565	1.451469	-0.177682		C	4.031479	0.934266	0.310360
C	2.148875	-1.529931	2.256266		C	5.123294	-1.330120	0.329568
C	1.770969	-2.809177	-0.583010		H	2.452600	-0.325777	4.010573
C	3.893046	-0.540591	-0.156858		H	3.789592	-0.195793	2.857647
C	0.589907	1.842214	-2.491474		H	2.243004	0.642007	2.536094
C	-0.264689	3.709647	-1.351297		H	0.719402	-1.770531	3.825305
C	0.943449	2.649515	-3.566873		H	0.046430	-0.838879	2.484782
C	0.063062	4.544079	-2.401260		H	0.208088	-2.590781	2.344741
C	0.677892	4.002928	-3.520140		H	2.928245	-2.816913	3.791230
F	0.863515	0.528084	-2.621231		H	2.560629	-3.690610	2.298538
F	-0.872603	4.250924	-0.248064		H	4.021591	-2.681071	2.404634
F	1.542953	2.104370	-4.662169		H	0.430844	-4.472087	-0.545802
F	-0.203656	5.877214	-2.353556		H	1.066462	-4.107400	1.061506
F	1.013240	4.805133	-4.566391		H	-0.192816	-3.060120	0.331786
C	-0.475581	1.671976	2.591089		H	0.869152	-3.251764	-2.475269
C	1.169379	2.904818	1.455683		H	0.228120	-1.768388	-1.742244
C	0.081798	2.003329	3.815776		H	1.812533	-1.753999	-2.539112
C	1.754406	3.262029	2.662267		H	2.634976	-4.609717	-1.368804
C	1.197637	2.820136	3.848137		H	3.758672	-3.249293	-1.445133
F	-1.489917	0.795616	2.595993		H	3.443275	-4.061329	0.108368
F	1.824530	3.316947	0.323297		H	4.716906	0.096110	-2.037797
F	-0.439482	1.511472	4.973132		H	3.906630	-1.467418	-2.168812
F	2.878271	4.030663	2.685845		H	2.940699	0.028972	-2.042297
F	1.765559	3.155396	5.037946		H	4.899646	1.343257	-0.220025
C	-2.685081	0.697115	-1.220079		H	3.153424	1.529002	0.054781
C	-3.059653	2.114193	0.633244		H	4.230632	1.023466	1.377452
C	-4.047871	0.576561	-1.435018		H	6.009677	-0.886592	-0.138238
C	-4.430499	2.017704	0.441156		H	5.244287	-1.241721	1.413723
C	-4.921859	1.242724	-0.592728		H	5.092215	-2.388161	0.058885
F	-1.854238	0.075468	-2.068887					
F	-2.626566	2.903412	1.660439					
F	-4.529990	-0.177928	-2.461036					
F	-5.294291	2.678700	1.259893					
F	-6.264077	1.138757	-0.788276					

Table S13. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C7(F5)

O	0.010147	-0.029835	0.305262		C	0.439498	-1.810935	-2.466717
N	1.393832	-0.038377	0.210608		C	2.522255	-0.465316	-2.489052
N	2.124682	0.893055	0.233953		C	2.712636	-2.973001	-2.486890
B	-0.638156	1.202851	0.944280		C	4.581204	-1.080958	-0.013174
P	1.847314	-1.782128	-0.075136		C	3.411352	-1.255177	2.178745
C	-0.638509	2.487619	-0.033344		C	4.002452	-3.353244	0.841055
C	0.177099	1.364006	2.337824		C	0.810143	-3.239914	2.154624
C	-2.173978	0.706608	1.100043		C	-0.887608	-2.605081	0.470037
C	1.897204	-1.776744	-1.947228		C	0.836818	-4.372529	-0.085908
C	3.513434	-1.888071	0.764684		H	0.483272	-1.706742	-3.556908
C	0.603131	-3.016797	0.635790		H	-0.065469	-2.751013	-2.238086
C	-0.318819	2.520178	-1.378793		H	-0.138203	-0.971779	-2.064760
C	-1.113460	3.673348	0.508297		H	2.547206	-0.571760	-3.579994
C	-0.436203	3.669977	-2.150599		H	1.896657	0.395157	-2.254630
C	-1.248370	4.837848	-0.221994		H	3.539871	-0.290732	-2.144541
C	-0.902373	4.830839	-1.565426		H	2.648330	-2.943624	-3.580597
F	0.128112	1.411362	-2.010504		H	3.768812	-2.891172	-2.214457
F	-1.469089	3.675010	1.830910		H	2.330565	-3.939535	-2.154973
F	-0.100709	3.652891	-3.471420		H	5.503247	-1.121463	0.578069
F	-1.713130	5.982644	0.349016		H	4.792305	-1.518744	-0.991774
F	-1.027873	5.967006	-2.304657		H	4.275394	-0.038966	-0.118349
C	0.203742	0.279334	3.205106		H	4.405063	-1.327889	2.635994
C	1.125473	2.344196	2.585904		H	3.156123	-0.194551	2.099786
C	1.165077	0.100420	4.179574		H	2.699495	-1.746254	2.843596
C	2.063836	2.234585	3.608055		H	5.003339	-3.335449	1.287485
C	2.099360	1.097866	4.394725		H	3.371488	-3.984876	1.465777
F	-0.685907	-0.725709	3.054279		H	4.087989	-3.803189	-0.153233
F	1.222068	3.443712	1.787566		H	0.055800	-3.977409	2.454988
F	1.242769	-1.091367	4.847954		H	1.787614	-3.647984	2.408858
F	2.984192	3.217276	3.808538		H	0.614030	-2.339499	2.735481
F	3.055215	0.949330	5.352157		H	-1.473524	-3.522521	0.601781
C	-2.837368	0.076764	0.051075		H	-1.152267	-1.894674	1.251316
C	-2.903297	0.884549	2.266413		H	-1.136967	-2.146626	-0.483445
C	-4.148639	-0.363455	0.147582		H	0.212354	-5.115462	0.422488
C	-4.220119	0.466497	2.391450		H	0.520512	-4.334561	-1.130050
C	-4.842702	-0.158837	1.326642		H	1.873749	-4.715586	-0.031931
F	-2.204227	-0.147968	-1.117074					
F	-2.328419	1.468105	3.358716					
F	-4.751958	-0.989315	-0.901930					
F	-4.902480	0.654579	3.554546					
F	-6.132118	-0.579353	1.440188					

Table S14. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C2(F)

N	-0.062400	-0.051818	-0.061366		C	1.667337	-2.347778	-2.672529
N	1.171673	-0.067137	-0.146117		C	3.392183	-0.598922	-2.249046
O	1.977706	0.919604	-0.217940		C	3.865081	-3.002297	-1.624124
B	-0.824837	1.330783	0.153528		C	4.439363	-0.505414	0.825817
P	2.005954	-1.652603	-0.006279		C	2.553342	-0.404364	2.435899
C	-0.505325	2.400273	-1.014913		C	3.761158	-2.612851	2.002693
C	-0.263773	1.733800	1.627650		C	0.250547	-2.673160	1.895669
C	-2.401311	0.962690	0.127824		C	-0.552303	-2.978457	-0.426356
C	2.776344	-1.907495	-1.691029		C	1.382156	-4.358312	0.361826
C	3.233014	-1.306982	1.371060		H	2.095434	-2.338438	-3.680430
C	0.728764	-2.956499	0.450625		H	1.320455	-3.361682	-2.465092
C	0.035909	2.057696	-2.265162		H	0.816920	-1.656388	-2.655804
C	-0.862932	3.748279	-0.827450		H	3.657264	-0.798088	-3.293256
C	0.222976	3.004015	-3.274047		H	2.694325	0.238428	-2.195745
C	-0.677786	4.705970	-1.822885		H	4.297907	-0.312528	-1.716131
C	-0.134364	4.321664	-3.039164		H	4.257875	-3.138866	-2.638555
H	0.321216	1.023848	-2.461407		H	4.697538	-2.707635	-0.981133
H	-1.296304	4.049116	0.121801		H	3.472691	-3.963297	-1.282464
H	0.641397	2.735417	-4.235192		H	5.060061	-0.244440	1.690468
H	-0.952781	5.741504	-1.671350		H	5.053950	-1.088351	0.136255
F	0.052651	5.258703	-4.025976		H	4.087084	0.410685	0.350642
C	-0.698811	1.041779	2.778991		H	3.301821	-0.206913	3.212364
C	0.792442	2.650173	1.794444		H	2.262118	0.549328	1.987374
C	-0.101901	1.239575	4.025783		H	1.683396	-0.854219	2.911436
C	1.388807	2.862305	3.038419		H	4.517844	-2.326117	2.741669
C	0.941754	2.146655	4.138202		H	2.983643	-3.172065	2.525791
H	-1.527863	0.341820	2.692059		H	4.243124	-3.263620	1.265045
H	1.155770	3.187454	0.926722		H	-0.550276	-3.386922	2.117357
H	-0.441164	0.713150	4.908823		H	1.037837	-2.809968	2.637658
H	2.198537	3.569590	3.163768		H	-0.162538	-1.661443	1.967704
F	1.538080	2.339202	5.359988		H	-1.195116	-3.754783	0.005778
C	-2.923825	0.076687	-0.834176		H	-1.067226	-2.020083	-0.375809
C	-3.326109	1.571066	0.994601		H	-0.360328	-3.247742	-1.462855
C	-4.286635	-0.208410	-0.913770		H	0.667328	-5.073220	0.785394
C	-4.693483	1.299440	0.923616		H	1.556286	-4.645068	-0.679338
C	-5.158380	0.406315	-0.027325		H	2.316295	-4.445735	0.920052
H	-2.246869	-0.385490	-1.551456					
H	-2.965492	2.266830	1.745686					
H	-4.683856	-0.888399	-1.656164					
H	-5.399744	1.770372	1.594856					
F	-6.501046	0.125727	-0.097623					

Table S15. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C3(F)

N	-0.090256	-0.091221	0.292908		C	0.170640	-3.088933	2.124945
N	1.068137	-0.376759	0.967222		C	-1.872827	-1.677567	2.296983
O	1.843497	0.533292	1.097926		C	-1.948172	-3.873056	1.063161
B	-0.551837	1.563440	0.208300		C	-3.408486	-1.180701	-0.578084
P	-0.634956	-1.656899	-0.194878		C	-1.826484	-0.381158	-2.405082
C	0.144745	2.201378	-1.112526		C	-2.394001	-2.804044	-2.139732
C	-0.055111	2.314593	1.577198		C	0.916393	-1.907731	-2.547045
C	-2.188226	1.691057	0.228085		C	2.188643	-2.353806	-0.478066
C	-1.089300	-2.621072	1.357011		C	0.526909	-4.034155	-1.245764
C	-2.104737	-1.496135	-1.357128		H	-0.171965	-3.530885	3.067719
C	0.785287	-2.509890	-1.125008		H	0.722958	-3.856531	1.578818
C	1.297603	1.658186	-1.715547		H	0.834470	-2.251303	2.341449
C	-0.337590	3.399926	-1.683158		H	-2.088174	-2.230357	3.218653
C	1.901556	2.235145	-2.833364		H	-1.273568	-0.802011	2.548195
C	0.261155	3.995093	-2.793882		H	-2.815444	-1.334434	1.869173
C	1.371686	3.398451	-3.367121		H	-2.117538	-4.376279	2.022404
H	1.753477	0.771430	-1.286515		H	-2.924417	-3.621807	0.648171
H	-1.201665	3.885810	-1.241149		H	-1.445787	-4.581017	0.400310
H	2.787303	1.804290	-3.281783		H	-4.173438	-0.934525	-1.322020
H	-0.122645	4.914569	-3.216135		H	-3.756530	-2.049200	-0.015701
F	1.958051	3.967821	-4.468182		H	-3.311926	-0.329730	0.087444
C	0.008996	1.736584	2.860956		H	-2.793188	-0.000506	-2.748886
C	0.185025	3.701416	1.522757		H	-1.258351	0.457063	-2.001000
C	0.252728	2.484294	4.012493		H	-1.290820	-0.778226	-3.267302
C	0.434432	4.463715	2.663207		H	-3.296146	-2.607665	-2.731298
C	0.456480	3.849594	3.903154		H	-1.597910	-3.065503	-2.836501
H	-0.100561	0.661191	2.978499		H	-2.602656	-3.654939	-1.487341
H	0.191425	4.199989	0.561897		H	1.861423	-2.270620	-2.967281
H	0.301451	2.017861	4.987788		H	0.116185	-2.228607	-3.213558
H	0.615910	5.528428	2.596628		H	0.951443	-0.814006	-2.525514
F	0.695475	4.592821	5.031777		H	2.859410	-3.001669	-1.055570
C	-2.993544	2.036305	-0.876224		H	2.562512	-1.331897	-0.548368
C	-2.876607	1.490826	1.445639		H	2.220533	-2.658101	0.566235
C	-4.386749	2.104270	-0.794793		H	1.282582	-4.435329	-1.931227
C	-4.265768	1.537371	1.540866		H	0.654477	-4.536739	-0.284498
C	-5.012065	1.832754	0.409704		H	-0.453912	-4.284515	-1.648586
H	-2.530551	2.244694	-1.835138					
H	-2.303581	1.315136	2.347974					
H	-4.988545	2.367913	-1.655062					
H	-4.773809	1.371946	2.482173					
F	-6.379474	1.875328	0.490651					

Table S16. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C5(F)

N	0.060222	-0.034268	0.038299	C	3.155243	-0.020750	2.607058
N	1.326777	0.008344	-0.098169	C	1.190955	-1.513025	2.699408
B	-0.653818	1.461849	0.034444	C	3.511051	-2.516560	2.455154
O	-0.577382	-1.074700	0.247082	C	1.019923	-3.696502	0.263341
P	2.419848	-1.215244	0.198378	C	1.170321	-2.520454	-1.907270
C	-0.179320	2.201938	-1.322775	C	3.215798	-3.694366	-0.924534
C	0.006407	2.074945	1.388939	C	3.756638	-0.495768	-2.152877
C	-2.254697	1.315816	0.064705	C	3.930746	1.115128	-0.310306
C	2.589222	-1.346800	2.052510	C	5.242136	-1.039022	-0.169067
C	1.963939	-2.842865	-0.616044	H	3.075008	-0.060641	3.699633
C	3.908939	-0.406309	-0.614674	H	4.208758	0.116304	2.351527
C	0.292697	1.556605	-2.480388	H	2.569350	0.836620	2.258085
C	-0.342267	3.599075	-1.401814	H	1.350679	-1.577171	3.782669
C	0.609975	2.263737	-3.642822	H	0.573449	-0.631428	2.509604
C	-0.022599	4.317425	-2.551782	H	0.660097	-2.404504	2.373747
C	0.455945	3.639923	-3.662933	H	3.612402	-2.497817	3.546662
H	0.409256	0.474268	-2.486736	H	3.093459	-3.486482	2.176163
H	-0.730434	4.131268	-0.538361	H	4.511200	-2.423168	2.023303
H	0.966769	1.760301	-4.532058	H	0.745865	-4.577962	-0.328314
H	-0.146310	5.391205	-2.600945	H	1.500152	-4.046563	1.178997
F	0.776783	4.340076	-4.798595	H	0.114925	-3.135868	0.498249
C	-0.448397	1.680376	2.662774	H	0.915889	-3.473429	-2.385542
C	1.152810	2.890558	1.345720	H	0.239071	-2.012234	-1.639850
C	0.212465	2.069298	3.831891	H	1.727778	-1.917061	-2.623002
C	1.811250	3.298151	2.505986	H	2.873474	-4.638406	-1.363976
C	1.334320	2.876907	3.739163	H	3.887829	-3.218172	-1.639461
H	-1.334970	1.053055	2.737496	H	3.775900	-3.932458	-0.013992
H	1.529823	3.210587	0.380727	H	4.586310	0.067490	-2.594539
H	-0.138534	1.762476	4.808679	H	3.802658	-1.515075	-2.537602
H	2.685491	3.935497	2.467802	H	2.822925	-0.015163	-2.466259
F	1.986999	3.261462	4.883004	H	4.764216	1.538394	-0.883246
C	-2.953134	0.421931	-0.770120	H	2.993547	1.572186	-0.634554
C	-3.030558	2.199077	0.836441	H	4.087785	1.344114	0.742084
C	-4.345020	0.394970	-0.814771	H	6.044849	-0.573612	-0.752385
C	-4.425904	2.186770	0.795318	H	5.442072	-0.837631	0.887020
C	-5.068589	1.279119	-0.027822	H	5.283045	-2.118087	-0.339432
H	-2.398836	-0.268671	-1.399341				
H	-2.532802	2.913110	1.484230				
H	-4.877183	-0.296730	-1.454437				
H	-5.015100	2.870917	1.391618				
F	-6.439943	1.253502	-0.071429				

Table S17. Optimized (ONI(M06-2X)) Cartesian coordinates of isomer C7(F)

O	0.186664	0.021878	-0.505418		C	1.259486	-2.467533	-2.331709
N	1.511427	0.117266	-0.124094		C	3.157888	-0.880532	-2.298777
N	2.197071	1.078558	-0.086504		C	3.539856	-3.268364	-1.564427
B	-0.733439	1.235787	-0.068393		C	4.694005	-0.669050	0.610625
P	2.064912	-1.609000	0.194371		C	3.092244	-0.394536	2.502145
C	-0.479802	2.504932	-1.031744		C	4.022332	-2.691800	1.918822
C	-0.380028	1.496968	1.498349		C	0.590066	-2.443709	2.453236
C	-2.225959	0.661145	-0.319986		C	-0.670238	-2.543720	0.332583
C	2.540736	-2.090679	-1.552961		C	1.177186	-4.205805	0.746123
C	3.514296	-1.347469	1.349619		H	1.536777	-2.587932	-3.384965
C	0.742005	-2.730214	0.941421		H	0.824117	-3.407188	-1.987304
C	0.168721	2.403693	-2.273464		H	0.520800	-1.663933	-2.247438
C	-0.992515	3.768366	-0.683872		H	3.443375	-1.237224	-3.294904
C	0.309227	3.501318	-3.123698		H	2.426071	-0.077977	-2.422153
C	-0.858392	4.874593	-1.521404		H	4.045196	-0.475829	-1.813790
C	-0.206233	4.727755	-2.735876		H	3.718061	-3.543914	-2.610454
H	0.574716	1.441072	-2.579882		H	4.500388	-2.988390	-1.124511
H	-1.506125	3.885408	0.266159		H	3.153601	-4.149250	-1.045883
H	0.811565	3.420471	-4.078963		H	5.478344	-0.496976	1.356632
H	-1.252804	5.844547	-1.248179		H	5.113263	-1.304587	-0.172636
F	-0.066736	5.813034	-3.566540		H	4.382465	0.292856	0.200987
C	-0.899702	0.685541	2.527597		H	3.989522	-0.205511	3.103200
C	0.582286	2.455649	1.878866		H	2.733892	0.562736	2.116201
C	-0.460176	0.794278	3.851421		H	2.331008	-0.816657	3.155906
C	1.029238	2.575087	3.195336		H	4.901067	-2.469632	2.535436
C	0.508751	1.733751	4.167652		H	3.286666	-3.184173	2.555858
H	-1.671693	-0.044595	2.288814		H	4.332755	-3.381859	1.127665
H	0.992088	3.107997	1.115646		H	-0.253587	-3.048569	2.805778
H	-0.870238	0.172885	4.637940		H	1.468382	-2.727096	3.034506
H	1.770093	3.312380	3.476822		H	0.346827	-1.393099	2.632974
F	0.951948	1.837594	5.462352		H	-1.302153	-3.314253	0.790498
C	-2.521097	-0.214047	-1.384608		H	-1.076019	-1.559833	0.561381
C	-3.313632	1.092269	0.461816		H	-0.703260	-2.668917	-0.747473
C	-3.819394	-0.656172	-1.637826		H	0.461214	-4.827659	1.296171
C	-4.618486	0.662936	0.215084		H	1.133748	-4.503507	-0.304083
C	-4.856341	-0.213586	-0.830356		H	2.175119	-4.415825	1.139389
H	-1.715333	-0.547910	-2.034522					
H	-3.133038	1.777040	1.284633					
H	-4.040960	-1.328498	-2.456606					
H	-5.449008	0.999877	0.821425					
F	-6.135103	-0.650786	-1.073248					

Table S18. Optimized (ONI(M06-2X)) Cartesian coordinates of $(F_5C_6)_3B/P(t\text{-}Bu)_3$

B	-1.720691	0.107499	-0.044407		C	2.732672	2.137423	-1.787106
P	2.075211	0.032282	0.036911		C	4.312208	0.216875	-1.878327
C	-1.628012	1.651425	0.187479		C	1.947325	0.008590	-2.743188
C	-1.699394	-0.865102	1.180182		C	2.603415	0.553099	2.800787
C	-1.634201	-0.467728	-1.496250		C	4.273542	1.572084	1.262439
C	2.839243	0.599404	-1.614778		C	1.909894	2.454052	1.398351
C	2.787616	1.170487	1.389566		C	2.617519	-2.628839	-0.866477
C	2.750970	-1.716426	0.381090		C	4.213637	-1.824837	0.865279
C	-0.885330	2.500254	-0.629086		C	1.812136	-2.354343	1.443789
C	-2.145326	2.224033	1.349264		H	3.045373	2.376960	-2.811877
C	-0.574032	3.798316	-0.269627		H	1.711205	2.496207	-1.662875
C	-1.902893	3.537117	1.706132		H	3.390188	2.680541	-1.107075
C	-1.092064	4.321440	0.899881		H	4.609629	0.635107	-2.849281
F	-0.368832	2.070135	-1.784406		H	4.979515	0.625601	-1.115345
F	-2.904555	1.463969	2.188169		H	4.458505	-0.863131	-1.924677
F	0.284615	4.521093	-1.039059		H	2.338513	0.347556	-3.711462
F	-2.425087	4.057226	2.847201		H	1.926667	-1.083690	-2.749314
F	-0.808430	5.595362	1.262187		H	0.925726	0.384734	-2.630704
C	-1.011382	-0.589178	2.358947		H	2.888958	1.317671	3.535109
C	-2.225586	-2.151990	1.070078		H	1.567449	0.278446	2.998328
C	-0.757433	-1.551830	3.317989		H	3.243365	-0.314939	2.964106
C	-2.041254	-3.119148	2.040122		H	4.536859	2.200365	2.123862
C	-1.281819	-2.820800	3.161196		H	4.930914	0.698989	1.266985
F	-0.491356	0.620739	2.587872		H	4.471055	2.150242	0.358717
F	-2.933860	-2.491292	-0.043973		H	2.271047	3.118925	2.193978
F	0.053762	-1.255233	4.369482		H	1.941789	3.004825	0.455443
F	-2.569914	-4.361998	1.894837		H	0.873069	2.181156	1.618089
F	-1.054000	-3.773721	4.096395		H	2.876666	-3.649926	-0.557387
C	-0.942896	-1.634535	-1.812354		H	1.598981	-2.651212	-1.253435
C	-2.099123	0.276413	-2.580485		H	3.300968	-2.344365	-1.667584
C	-0.628888	-1.987429	-3.111532		H	4.457604	-2.887947	0.993506
C	-1.854104	-0.083044	-3.892402		H	4.913135	-1.402613	0.139458
C	-1.093585	-1.211852	-4.156677		H	4.370367	-1.331503	1.825449
F	-0.478855	-2.443632	-0.854927		H	2.151824	-3.379933	1.639476
F	-2.807230	1.418616	-2.352871		H	1.803762	-1.812900	2.392596
F	0.181799	-3.056090	-3.340441		H	0.793164	-2.396075	1.046764
F	-2.324720	0.669183	-4.920967					
F	-0.806653	-1.549079	-5.436712					

Table S19. Optimized (ONI(M06-2X)) Cartesian coordinates of $(4\text{-F-}H_4C_6)_3B/P(t\text{-Bu})_3$

B	-1.498489	0.095833	-0.038184		C	2.734984	2.239710	-1.643383
P	2.111875	0.034578	0.036497		C	4.352109	0.359792	-1.869226
C	-1.482256	1.644547	0.189658		C	1.995584	0.169089	-2.748949
C	-1.544454	-0.875071	1.188786		C	2.607982	0.383227	2.811980
C	-1.480555	-0.481182	-1.493180		C	4.303357	1.505828	1.374643
C	2.873652	0.697539	-1.579954		C	1.943267	2.381171	1.538123
C	2.816418	1.097812	1.452700		C	2.639702	-2.548088	-1.024559
C	2.792916	-1.728707	0.281925		C	4.259064	-1.875295	0.743244
C	-0.827417	2.505170	-0.713047		C	1.865906	-2.437539	1.308988
C	-2.049938	2.228967	1.342204		H	2.984549	2.560794	-2.662752
C	-0.710893	3.871065	-0.467916		H	1.712464	2.556569	-1.422047
C	-1.954257	3.595649	1.588507		H	3.414427	2.747685	-0.956728
C	-1.274729	4.399865	0.684424		H	4.645084	0.847467	-2.809052
H	-0.375485	2.085376	-1.606980		H	5.013365	0.722202	-1.077716
H	-2.574214	1.598549	2.051970		H	4.512045	-0.713230	-1.990019
H	-0.188413	4.527753	-1.151146		H	2.353908	0.617027	-3.685099
H	-2.392492	4.046052	2.468798		H	2.036862	-0.915430	-2.853404
F	-1.162810	5.738889	0.931697		H	0.945955	0.450603	-2.602930
C	-0.944027	-0.526045	2.414328		H	2.825474	1.103961	3.610570
C	-2.115360	-2.162317	1.093172		H	1.576283	0.040825	2.927248
C	-0.881533	-1.420974	3.479475		H	3.275875	-0.470357	2.940572
C	-2.073723	-3.058551	2.157401		H	4.558108	2.074338	2.279545
C	-1.446146	-2.680402	3.336034		H	4.961009	0.634038	1.324660
H	-0.491479	0.455807	2.518149		H	4.509382	2.144968	0.514036
H	-2.599279	-2.459589	0.169319		H	2.264675	2.964933	2.410681
H	-0.400469	-1.159575	4.412928		H	2.031755	3.013830	0.654564
H	-2.514468	-4.043828	2.087692		H	0.884781	2.121741	1.658291
F	-1.387157	-3.563822	4.376572		H	2.837654	-3.601542	-0.788890
C	-0.874221	-1.720732	-1.776178		H	1.626724	-2.468756	-1.427563
C	-1.997171	0.248922	-2.585111		H	3.347626	-2.239052	-1.795580
C	-0.754481	-2.195927	-3.079730		H	4.504279	-2.944944	0.794781
C	-1.898015	-0.224612	-3.890303		H	4.953533	-1.400661	0.044959
C	-1.266520	-1.438212	-4.123373		H	4.421507	-1.450956	1.735806
H	-0.462165	-2.304193	-0.958026		H	2.176328	-3.487264	1.393441
H	-2.484143	1.200614	-2.402853		H	1.911273	-1.988777	2.301618
H	-0.268708	-3.137973	-3.298067		H	0.822081	-2.404687	0.975112
H	-2.297023	0.331298	-4.727901					
F	-1.150973	-1.897713	-5.404831					

Table S20. Optimized (ONI(M06-2X)) Cartesian coordinates of $(3\text{-F-}H_4C_6)_3B/P(t\text{-Bu})_3$

B	-0.721372	0.000826	-0.000117		C	2.320184	-2.262676	-1.665357
P	1.726775	-0.002579	0.000344		C	1.630291	-0.206869	-2.823511
C	-1.155411	1.492768	-0.472162		C	3.941842	-0.386358	-1.885879
C	-1.158969	-0.335579	1.527214		C	2.325199	2.569286	-1.122826
C	-1.159476	-1.152721	-1.055665		C	1.632552	2.544910	1.235467
C	2.455000	-0.720603	-1.616617		C	3.943991	1.820187	0.614560
C	2.457730	1.755567	0.188240		C	2.319394	-0.316735	2.790533
C	2.452891	-1.045618	1.430363		C	1.625414	-2.345933	1.588676
C	-0.881817	2.011739	-1.758156		C	3.938907	-1.448938	1.276224
C	-1.951140	2.304211	0.360032		H	2.646547	-2.586680	-2.661576
C	-1.331225	3.269036	-2.164798		H	2.949524	-2.766669	-0.931421
C	-2.393455	3.552984	-0.051009		H	1.282965	-2.571920	-1.538245
C	-2.088278	4.059603	-1.302312		H	2.048082	-0.658403	-3.732111
H	-0.319066	1.412104	-2.465067		H	0.585380	-0.517566	-2.738285
H	-2.255943	1.963711	1.339740		H	1.680404	0.877251	-2.933286
H	-1.097679	3.630516	-3.159346		H	4.229880	-0.904902	-2.809542
F	-3.158108	4.301516	0.805260		H	4.105707	0.679903	-2.044440
H	-2.451552	5.036230	-1.590780		H	4.602303	-0.730520	-1.088804
C	-0.885350	0.516980	2.620905		H	2.653454	3.593363	-0.904854
C	-1.959059	-1.459481	1.811080		H	2.954190	2.184840	-1.926090
C	-1.338866	0.240963	3.911783		H	1.288220	2.615975	-1.454770
C	-2.405523	-1.727457	3.096709		H	2.050516	3.557519	1.298073
C	-2.100330	-0.898925	4.162519		H	0.587937	2.626259	0.922931
H	-0.319490	1.427511	2.457448		H	1.682136	2.098739	2.229595
H	-2.263993	-2.136074	1.024988		H	4.232867	2.879156	0.627626
H	-1.105161	0.920201	4.723138		H	4.105890	1.424544	1.617646
F	-3.173936	-2.841200	3.314040		H	4.605211	1.301478	-0.080911
H	-2.466739	-1.136993	5.151499		H	2.644489	-1.018436	3.568945
C	-0.887908	-2.526514	-0.863658		H	2.950730	0.569449	2.860342
C	-1.957631	-0.835660	-2.172173		H	1.282702	-0.049885	2.995214
C	-1.340966	-3.505845	-1.748901		H	2.042252	-2.908093	2.433797
C	-2.403451	-1.814524	-3.047966		H	0.581079	-2.114427	1.815620
C	-2.099669	-3.152109	-2.863039		H	1.674087	-2.982886	0.704488
H	-0.324232	-2.840458	0.007930		H	4.225160	-1.990809	2.186964
H	-2.261371	0.183694	-2.365156		H	4.102308	-2.119169	0.431863
H	-1.108822	-4.548417	-1.566021		H	4.601009	-0.587726	1.177090
F	-3.170132	-1.445071	-4.122185					
H	-2.465378	-3.889194	-3.564512					

Table S21. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of (3-F-H_4C_6)$_3$B–ONN–P(*t*-Bu)$_3$

O	0.997294	0.027384	-0.985924		C	-3.391929	-1.313220	-2.900341
N	-0.187785	-0.102978	-0.511134		C	-2.016802	-2.578505	-1.279505
N	-1.091325	0.314789	-1.282075		C	-4.462796	-2.107037	-0.765728
B	2.097138	-0.053290	0.159472		C	-2.070321	-1.383445	1.735450
P	-2.635929	0.069332	-0.606458		C	-1.634148	1.036340	1.875629
C	1.626193	-1.276217	1.123681		C	-4.031732	0.196694	1.821007
C	2.009269	1.402756	0.871350		C	-3.184955	2.800491	-0.386673
C	3.468259	-0.314606	-0.638278		C	-3.088482	1.899108	-2.696898
C	-3.169758	-1.544962	-1.387974		C	-5.077228	1.365163	-1.235759
C	-2.603063	-0.009954	1.263139		H	-3.555352	-2.293520	-3.361896
C	-3.547842	1.568386	-1.253835		H	-4.271432	-0.697617	-3.099945
C	1.520146	-1.231543	2.525195		H	-2.508930	-0.858430	-3.360322
C	1.158816	-2.443988	0.485907		H	-2.347523	-3.477377	-1.813199
C	0.982676	-2.303696	3.250355		H	-1.117001	-2.204798	-1.775947
C	0.573816	-3.466134	1.206856		H	-1.754342	-2.876165	-0.265032
C	0.488463	-3.427221	2.592663		H	-4.742754	-3.004219	-1.329924
H	1.844132	-0.342751	3.059091		H	-4.321749	-2.399851	0.276690
H	1.209427	-2.530629	-0.594158		H	-5.292901	-1.396329	-0.828190
H	0.925109	-2.249863	4.331487		H	-1.976016	-1.335606	2.826607
F	0.002750	-4.521924	0.527968		H	-2.741634	-2.209513	1.490280
H	0.036515	-4.252442	3.126331		H	-1.074597	-1.569239	1.328228
C	2.846826	1.796910	1.937047		H	-1.820519	1.036094	2.956821
C	0.981479	2.293426	0.522775		H	-0.601333	0.724065	1.710293
C	2.612661	2.975941	2.648875		H	-1.747272	2.057441	1.511447
C	0.726108	3.427057	1.269145		H	-3.983807	0.017881	2.901126
C	1.522403	3.796055	2.337512		H	-4.390232	1.217187	1.669062
H	3.685949	1.163044	2.215309		H	-4.756256	-0.505416	1.397472
H	0.328337	2.098229	-0.314982		H	-3.669177	3.668543	-0.848498
H	3.267692	3.254003	3.466230		H	-3.562910	2.715573	0.633761
F	-0.413040	4.151434	0.953935		H	-2.109130	3.001954	-0.349261
H	1.299036	4.689357	2.904358		H	-3.499651	2.883761	-2.946171
C	4.320424	-1.407251	-0.402738		H	-1.998910	1.936585	-2.755799
C	3.842418	0.603059	-1.635833		H	-3.461241	1.183951	-3.429347
C	5.500485	-1.572506	-1.136425		H	-5.541605	2.295888	-1.581547
C	5.005893	0.423130	-2.361108		H	-5.386899	0.567050	-1.915748
C	5.848123	-0.655607	-2.124602		H	-5.461280	1.148410	-0.235588
H	4.055688	-2.136514	0.357961					
H	3.219539	1.464113	-1.848254					
H	6.148376	-2.418785	-0.940076					
F	5.345645	1.329343	-3.335950					
H	6.752705	-0.760755	-2.708206					

Table S22. Optimized (ONI(M06-2X)) Cartesian coordinates of $(2\text{-F-}H_4C_6)_3B/P(t\text{-Bu})_3$

B	1.843231	0.009491	-0.011513		C	-2.289467	1.672709	2.252543
P	-1.704066	-0.007891	0.009860		C	-1.523048	2.753967	0.186263
C	1.953635	-1.069345	-1.144292		C	-3.907939	1.923850	0.379525
C	1.970965	-0.431839	1.487809		C	-2.315885	1.087423	-2.564181
C	1.944191	1.530388	-0.379744		C	-1.519152	-1.232098	-2.472042
C	-2.433247	1.608160	0.710746		C	-3.908755	-0.681206	-1.838087
C	-2.439287	-0.217554	-1.736821		C	-2.276176	-2.791177	0.350142
C	-2.416225	-1.424683	1.067868		C	-1.490052	-1.541425	2.310906
C	2.605669	-0.804714	-2.365029		C	-3.885465	-1.299976	1.525802
C	1.411261	-2.346328	-1.005009		H	-2.573993	2.685181	2.568887
C	2.693477	-1.763888	-3.372170		H	-2.941186	0.966795	2.769046
C	1.459620	-3.314753	-1.994491		H	-1.254923	1.504042	2.546468
C	2.108399	-3.019441	-3.190785		H	-1.900624	3.708471	0.576787
H	3.049243	0.173725	-2.518169		H	-0.500912	2.604842	0.549046
F	0.763091	-2.676776	0.170366		H	-1.501066	2.813757	-0.903302
H	3.203473	-1.531867	-4.298498		H	-4.175279	2.870902	0.867902
H	0.993430	-4.274610	-1.818451		H	-4.078808	2.043446	-0.690967
H	2.156984	-3.764242	-3.975343		H	-4.581274	1.148141	0.753808
C	2.646065	-1.610650	1.862636		H	-2.602752	0.851596	-3.597734
C	1.421899	0.315612	2.528645		H	-2.975708	1.879437	-2.207733
C	2.749022	-2.003841	3.195614		H	-1.285637	1.439223	-2.570580
C	1.484908	-0.058281	3.861263		H	-1.898293	-1.373668	-3.492975
C	2.156305	-1.231117	4.197281		H	-0.502419	-0.830082	-2.526755
H	3.096391	-2.223147	1.088277		H	-1.483483	-2.206276	-1.981104
F	0.751498	1.487489	2.232220		H	-4.180021	-0.735861	-2.901302
H	3.276979	-2.913184	3.453238		H	-4.065017	-1.670036	-1.405300
H	1.012075	0.564223	4.608680		H	-4.589599	0.022014	-1.351113
H	2.216989	-1.539127	5.233661		H	-2.547967	-3.572976	1.072033
C	2.605907	2.455618	0.451961		H	-2.938274	-2.888355	-0.511189
C	1.382201	2.049065	-1.545352		H	-1.244502	-2.956452	0.043926
C	2.684614	3.808338	0.126397		H	-1.858156	-2.357326	2.947236
C	1.420672	3.391208	-1.887050		H	-0.471832	-1.779269	1.987194
C	2.079895	4.279665	-1.041290		H	-1.461958	-0.627564	2.906871
H	3.064679	2.098111	1.368038		H	-4.142733	-2.196879	2.105697
F	0.723641	1.196022	-2.411057		H	-4.050192	-0.432695	2.166436
H	3.202558	4.494914	0.783860		H	-4.570262	-1.238527	0.675774
H	0.939143	3.719279	-2.798329					
H	2.121671	5.332209	-1.292448					

Table S23. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of (2-F-H_4C_6)$_3$B–ONN–P(*t*-Bu)$_3$

O	0.832814	0.024942	-1.053723		C	-3.697585	-1.530960	-2.419288
N	-0.302859	-0.049664	-0.479843		C	-2.325923	-2.662527	-0.672325
N	-1.276074	0.178679	-1.242343		C	-4.705626	-1.961326	-0.154814
B	1.985134	-0.084001	-0.028358		C	-2.064333	-1.104832	2.072555
P	-2.740958	0.087863	-0.392206		C	-1.457273	1.271791	1.889358
C	1.540987	-1.179511	1.094793		C	-3.897870	0.617148	2.099671
C	2.234773	1.377483	0.629618		C	-3.056205	2.822976	-0.504754
C	3.260607	-0.562185	-0.886503		C	-3.327613	1.648862	-2.664971
C	-3.413223	-1.578653	-0.900838		C	-5.167317	1.479411	-0.951016
C	-2.536601	0.238115	1.466786		H	-3.939387	-2.549484	-2.742275
C	-3.641400	1.541213	-1.149723		H	-4.553673	-0.893099	-2.651596
C	1.613132	-1.007262	2.488137		H	-2.816938	-1.189225	-2.972472
C	0.989728	-2.390984	0.672405		H	-2.634197	-3.549772	-1.237953
C	1.172794	-1.993063	3.381599		H	-1.333658	-2.366307	-1.023501
C	0.545980	-3.390468	1.523713		H	-2.245076	-2.948250	0.376059
C	0.641553	-3.189121	2.902332		H	-5.056667	-2.917312	-0.560990
H	2.015066	-0.076568	2.879530		H	-4.533128	-2.096919	0.915516
F	0.835172	-2.600049	-0.690740		H	-5.499395	-1.221431	-0.296964
H	1.247658	-1.823796	4.449410		H	-1.845972	-0.920654	3.131100
H	0.140051	-4.302212	1.103835		H	-2.826618	-1.885019	2.016856
H	0.305626	-3.958192	3.587142		H	-1.138245	-1.441502	1.601706
C	3.410017	1.588908	1.380060		H	-1.592625	1.429942	2.966390
C	1.386379	2.478501	0.542196		H	-0.462708	0.855665	1.719717
C	3.690743	2.800789	2.012961		H	-1.516866	2.228911	1.381007
C	1.634255	3.700022	1.153852		H	-3.779320	0.552214	3.187231
C	2.796675	3.866619	1.900564		H	-4.191537	1.641080	1.857232
H	4.122454	0.769909	1.455926		H	-4.703177	-0.064548	1.808634
F	0.193669	2.395266	-0.178042		H	-3.475236	3.681459	-1.041067
H	4.606596	2.916602	2.579993		H	-3.329037	2.919295	0.547999
H	0.920341	4.503357	1.026198		H	-1.964997	2.848472	-0.603839
H	3.003998	4.815531	2.379477		H	-3.685652	2.631033	-2.994112
C	3.993218	-1.740134	-0.682114		H	-2.252164	1.576948	-2.839997
C	3.693034	0.263399	-1.922517		H	-3.840708	0.890542	-3.254952
C	5.099237	-2.062723	-1.477642		H	-5.597147	2.396606	-1.370467
C	4.780364	-0.027143	-2.731371		H	-5.602971	0.631969	-1.489195
C	5.492152	-1.205825	-2.504500		H	-5.458003	1.420010	0.100606
H	3.694197	-2.415094	0.115887					
F	2.998053	1.429599	-2.151961					
H	5.647943	-2.979292	-1.296361					
H	5.054429	0.662745	-3.518309					
H	6.345465	-1.448671	-3.126104					

Table S24. Optimized (ONI(M06-2X)) Cartesian coordinates of $(H_5C_6)_3B/P(t\text{-}Bu)_3$

B	2.080233	-0.011546	-0.002092		C	-2.070847	0.714894	-2.694575
P	-1.521809	0.009240	0.001637		C	-3.709915	1.679360	-1.086855
C	2.078067	-0.819649	-1.345656		C	-1.335227	2.523371	-1.196156
C	2.081361	-0.771485	1.369410		C	-2.086042	-2.675034	0.741232
C	2.096947	1.555928	-0.030032		C	-3.727596	-1.752223	-0.887850
C	-2.234307	1.256261	-1.251652		C	-1.361092	-2.287060	-1.578427
C	-2.248847	-1.694520	-0.447837		C	-2.059894	1.995440	1.959738
C	-2.235092	0.476684	1.706230		C	-3.714572	0.134685	1.986208
C	1.461162	-0.303573	-2.501851		C	-1.344016	-0.212266	2.777981
C	2.623817	-2.118665	-1.425576		H	-2.285846	1.536000	-3.390562
C	1.356501	-1.058087	-3.670853		H	-1.050493	0.366835	-2.874689
C	2.537729	-2.871709	-2.596269		H	-2.762812	-0.100153	-2.914601
C	1.892117	-2.346737	-3.717589		H	-3.971880	2.361390	-1.907487
H	1.034069	0.694981	-2.466389		H	-4.385428	0.820829	-1.129453
H	3.118020	-2.536729	-0.554853		H	-3.882187	2.209670	-0.148428
H	0.856434	-0.645546	-4.540023		H	-1.664987	3.219118	-1.979126
H	2.966045	-3.866404	-2.634487		H	-1.388012	3.039767	-0.237473
H	1.811273	-2.936333	-4.623312		H	-0.285450	2.263349	-1.375188
C	1.455187	-2.025754	1.504996		H	-2.312829	-3.686231	0.379476
C	2.640998	-0.196293	2.530106		H	-1.063006	-2.666609	1.125867
C	1.355581	-2.660840	2.743364		H	-2.770283	-2.451672	1.561723
C	2.560465	-0.834002	3.767903		H	-3.998362	-2.801758	-1.067787
C	1.905822	-2.062368	3.878448		H	-4.395550	-1.355639	-0.118626
H	1.017273	-2.490235	0.625641		H	-3.901112	-1.202328	-1.814756
H	3.142131	0.762978	2.453387		H	-1.697208	-3.312100	-1.783880
H	0.848225	-3.615752	2.824218		H	-1.419584	-1.717528	-2.506262
H	2.999998	-0.374068	4.645219		H	-0.308625	-2.315966	-1.272993
H	1.828989	-2.552010	4.842183		H	-2.277481	2.189181	3.018030
C	1.482779	2.307172	0.990896		H	-1.036082	2.317198	1.752475
C	2.659280	2.267238	-1.111252		H	-2.744540	2.599154	1.361268
C	1.397899	3.698196	0.921890		H	-3.974912	0.502823	2.988175
C	2.593542	3.658759	-1.177653		H	-4.384637	0.609802	1.264715
C	1.951029	4.375812	-0.166394		H	-3.896459	-0.941553	1.971462
H	1.042994	1.782758	1.834871		H	-1.671109	0.123295	3.771105
H	3.150866	1.715615	-1.905860		H	-1.408242	-1.300128	2.748153
H	0.899728	4.251203	1.710431		H	-0.290982	0.060977	2.642728
H	3.035259	4.183711	-2.016529					
H	1.885748	5.456040	-0.224019					

Table S25. Optimized (ONI(M06-2X)) Cartesian coordinates of $(F_3C)_3B–P(t\text{-}Bu)_3$

B	-1.075316	0.000102	-0.000300
P	1.024164	0.000144	-0.000237
C	-1.753253	1.235623	-0.879392
C	-1.753006	-1.379440	-0.630009
C	-1.753272	0.144203	1.509111
C	1.688948	-0.724381	-1.631491
C	1.690142	1.774917	0.188530
C	1.689191	-1.050665	1.442789
F	-3.039543	0.983078	-1.175637
F	-1.762023	2.436909	-0.232821
F	-1.173434	1.510934	-2.087864
F	-3.040546	-1.507484	-0.266799
F	-1.175758	-2.563319	-0.259275
F	-1.757398	-1.423715	-1.993711
F	-3.040695	0.523283	1.438143
F	-1.758258	-1.014992	2.228789
F	-1.175905	1.056473	2.349487
C	1.519348	-2.263093	-1.651418
C	0.891103	-0.191864	-2.846439
C	3.182874	-0.412280	-1.879960
C	1.522744	2.561904	-1.134073
C	0.891491	2.561578	1.256003
C	3.183613	1.832623	0.584998
C	1.518998	-0.299208	2.785615
C	0.892014	-2.369511	1.589615
C	3.183172	-1.421632	1.296159
H	1.786376	-2.602202	-2.658976
H	2.185220	-2.762672	-0.946413
H	0.492528	-2.561909	-1.450033
H	1.314581	-0.673893	-3.735768
H	-0.158221	-0.462103	-2.772588
H	0.968109	0.885756	-2.970463
H	3.470093	-0.951461	-2.791023
H	3.355631	0.649523	-2.061054
H	3.834078	-0.749556	-1.072929
H	1.791300	3.603537	-0.923525
H	2.188460	2.200262	-1.918862
H	0.496141	2.538460	-1.494374
H	1.316938	3.571859	1.285156
H	-0.156988	2.634970	0.982471
H	0.964866	2.129155	2.251024
H	3.471899	2.890901	0.573304
H	3.354786	1.458590	1.595357
H	3.835084	1.301242	-0.109506
H	1.788178	-1.001830	3.582694
H	2.182556	0.562825	2.865862
H	0.491441	0.021928	2.944384
H	1.317495	-2.899112	2.450473
H	-0.156923	-2.170767	1.789047
H	0.967394	-3.015095	0.717859
H	3.471162	-1.939653	2.219154
H	3.355317	-2.110475	0.467829
H	3.834018	-0.554105	1.182920

Table S26. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(F_3C)_3B–ONN–P(t\text{-}Bu)_3$

O	0.005243	-0.108881	-0.316471		H	3.410895	2.583927	3.243756
N	1.289421	-0.068390	-0.105042		H	4.084810	3.347183	1.797385
N	1.801950	1.014929	-0.464129		H	2.362504	2.860710	1.843733
B	-0.613591	-1.404198	0.143868		H	3.080361	0.258702	3.493660
P	3.491654	0.999545	-0.165362		H	1.756564	0.512698	2.349505
C	-0.096251	-1.773996	1.652373		H	2.839907	-0.831694	2.115477
C	-0.224060	-2.603902	-0.889957		H	5.326620	1.073536	3.124678
C	-2.214441	-1.128542	0.141269		H	5.490329	-0.160392	1.871725
C	3.746665	1.167348	1.677721		H	5.918959	1.531963	1.519977
C	4.197338	-0.589634	-0.858505		H	4.369288	-2.664963	-0.392892
C	3.998449	2.528249	-1.111145		H	4.505293	-1.661480	1.054884
F	-0.883287	-2.654379	2.290796		H	2.906879	-1.949292	0.296275
F	1.167893	-2.318008	1.702975		H	4.014543	-1.822050	-2.594820
F	-0.029612	-0.674300	2.459658		H	2.454074	-1.323960	-1.953015
F	-0.559726	-3.828701	-0.445753		H	3.436321	-0.182532	-2.915283
F	1.138440	-2.672415	-1.123410		H	6.091013	-1.404687	-1.444462
F	-0.771984	-2.465479	-2.113686		H	5.913182	0.285544	-1.927908
F	-2.943456	-2.262001	0.242932		H	6.266332	-0.128948	-0.231224
F	-2.605680	-0.330841	1.166020		H	4.122815	3.174885	-3.152258
F	-2.627389	-0.509634	-0.988897		H	4.647441	1.498025	-2.955537
C	3.378595	2.591924	2.148351		H	2.906399	1.908411	-2.903686
C	2.799322	0.206923	2.434749		H	3.194809	4.462945	-1.573676
C	5.217881	0.881209	2.051203		H	1.964066	3.323373	-0.971485
C	3.969761	-1.776462	0.110972		H	3.103085	4.108151	0.153046
C	3.463576	-0.974310	-2.169831		H	5.660202	3.858100	-1.382931
C	5.711321	-0.427863	-1.125142		H	5.496350	3.312489	0.289390
C	3.913796	2.236293	-2.627428		H	6.177594	2.223023	-0.941922
C	2.990105	3.675547	-0.839446					
C	5.424332	2.992583	-0.753134					

Table S27. Optimized (ONI(M06-2X)) Cartesian coordinates of *bic*-(FC(F_4C_6)$_3$)B–P(*t*-Bu)$_3$

B	0.000419	0.025012	0.184755		P	-0.965173	-0.976882	1.792999
C	1.678708	0.082559	0.198537		C	-0.377567	-0.129540	3.489819
C	-0.393721	1.640500	0.086013		C	-2.925773	-0.873503	1.497902
C	-0.331766	-0.504023	-1.374052		C	-0.566131	-2.865580	1.986859
C	2.652865	-0.387254	1.061474		C	0.510177	1.110193	3.198671
C	2.202938	0.801627	-0.903856		C	-1.505098	0.389500	4.415067
C	4.023494	-0.235274	0.862558		C	0.470669	-1.056711	4.404929
C	3.551873	0.968258	-1.135689		C	-3.243061	0.015684	0.265645
C	4.476773	0.430643	-0.247252		C	-3.601359	-2.245605	1.219286
F	2.333430	-0.973837	2.229995		C	-3.756372	-0.270149	2.656872
F	4.893894	-0.740203	1.777627		C	-0.894550	-3.739012	0.743114
F	4.053372	1.644982	-2.202735		C	0.939645	-3.203093	2.177287
F	5.807864	0.587085	-0.468444		C	-1.368775	-3.413196	3.217755
C	-1.216058	2.466150	0.829253		H	0.967024	1.406595	4.150633
C	0.260939	2.283838	-0.991302		H	1.309011	0.904710	2.495892
C	-1.407164	3.818758	0.568307		H	-0.089400	1.939724	2.842760
C	0.093736	3.623407	-1.277983		H	-1.004253	0.825076	5.287528
C	-0.749837	4.398970	-0.489077		H	-2.083335	1.178467	3.947049
F	-1.915603	2.001508	1.897883		H	-2.156584	-0.408507	4.775235
F	-2.238113	4.550683	1.357520		H	0.589738	-0.520906	5.353419
F	0.714792	4.255700	-2.308283		H	-0.012612	-2.006279	4.625270
F	-0.918425	5.718505	-0.766570		H	1.462638	-1.215125	3.999174
C	-1.139570	-1.494004	-1.904880		H	-4.304178	-0.130879	0.030489
C	0.343786	0.258870	-2.358195		H	-3.093318	1.063807	0.496488
C	-1.252739	-1.775565	-3.264681		H	-2.667247	-0.254452	-0.611781
C	0.259795	0.006803	-3.711225		H	-4.681292	-2.059680	1.227914
C	-0.539336	-1.034064	-4.171293		H	-3.348133	-2.620373	0.234865
F	-1.957880	-2.226079	-1.126510		H	-3.393233	-2.992865	1.982297
F	-2.077855	-2.775514	-3.676072		H	-4.799949	-0.286000	2.321538
F	0.921606	0.729850	-4.653154		H	-3.696826	-0.862428	3.571606
F	-0.626577	-1.292205	-5.502065		H	-3.494611	0.764365	2.849326
C	1.170181	1.402376	-1.824591		H	-0.593667	-4.759016	1.007684
F	1.761607	2.128315	-2.851561		H	-1.937608	-3.765214	0.466200
					H	-0.298412	-3.427083	-0.116598
					H	0.993602	-4.295341	2.248255
					H	1.517934	-2.895901	1.303758
					H	1.390172	-2.793048	3.068417
					H	-0.679058	-3.826921	3.959272
					H	-1.981317	-2.653124	3.716155
					H	-2.032037	-4.223199	2.900486

Table S28. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of *bic*-(FC(F_4C_6)$_3$)B–ONN–P(*t*-Bu)$_3$

N	-0.010590	0.173410	-0.357804	P	-2.268697	1.239125	-0.376973
O	1.281876	0.235675	-0.510281	C	-2.784285	1.715400	-2.110086
N	-0.568862	1.270609	-0.550263	C	-2.928478	-0.427465	0.163276
B	1.920989	-1.051054	-0.095187	C	-2.557653	2.590002	0.888095
C	1.422018	-2.373645	-0.912146	C	-2.349241	3.176042	-2.369038
C	1.691821	-1.429328	1.477135	C	-2.005595	0.840251	-3.125403
C	3.526751	-1.056238	-0.273072	C	-4.301632	1.580252	-2.341268
C	0.536826	-2.527908	-1.957846	C	-2.898899	-1.421112	-1.022089
C	2.064898	-3.538769	-0.448619	C	-2.088983	-1.083568	1.296698
C	0.242324	-3.773395	-2.505042	C	-4.395807	-0.263197	0.631345
C	1.801804	-4.780937	-0.981340	C	-2.326907	2.018513	2.308056
C	0.874110	-4.895506	-2.016007	C	-1.519532	3.726927	0.709779
F	-0.111452	-1.465302	-2.501449	C	-3.985769	3.165265	0.790953
F	-0.664532	-3.876342	-3.517411	H	-2.528938	3.385347	-3.429290
F	2.400288	-5.923101	-0.549664	H	-2.929728	3.892034	-1.784190
F	0.595669	-6.119297	-2.544803	H	-1.281600	3.305066	-2.166703
C	1.021788	-0.768976	2.485065	H	-2.193029	1.260112	-4.120048
C	2.310654	-2.646843	1.815244	H	-0.929884	0.869222	-2.934746
C	0.902033	-1.299202	3.765599	H	-2.326367	-0.199448	-3.131578
C	2.225261	-3.183969	3.080387	H	-4.516365	1.941399	-3.353608
C	1.503259	-2.503617	4.060569	H	-4.632935	0.540729	-2.283411
F	0.436499	0.434594	2.268723	H	-4.885478	2.181556	-1.637935
F	0.190313	-0.627536	4.715405	H	-3.160205	-2.406753	-0.619688
F	2.806421	-4.361198	3.434130	H	-3.634373	-1.170133	-1.790041
F	1.395684	-3.029877	5.312071	H	-1.906217	-1.482654	-1.470426
C	4.386239	-0.088150	-0.753736	H	-2.689843	-1.912755	1.688748
C	4.081960	-2.277714	0.153935	H	-1.158975	-1.479504	0.886511
C	5.760671	-0.313822	-0.813140	H	-1.838672	-0.416668	2.119006
C	5.437544	-2.514443	0.101971	H	-4.794344	-1.268943	0.806401
C	6.279518	-1.518044	-0.387524	H	-4.469556	0.291405	1.569099
F	3.928595	1.095184	-1.177367	H	-5.025654	0.219881	-0.121592
F	6.591495	0.654331	-1.291388	H	-2.418559	2.854899	3.009742
F	6.009587	-3.681324	0.506728	H	-3.070249	1.269330	2.585759
F	7.622978	-1.737805	-0.445156	H	-1.324183	1.595953	2.411271
C	3.071670	-3.298556	0.668860	H	-1.640808	4.403073	1.563506
F	3.685805	-4.479760	1.067997	H	-0.501810	3.330368	0.710543
				H	-1.672879	4.302776	-0.201345
				H	-4.099428	3.904059	1.592567
				H	-4.155225	3.677738	-0.159339
				H	-4.756482	2.401455	0.926759

Table S29. Optimized (ONI(M06-2X)) Cartesian coordinates of (*bic*-HC(4-F-$H_3C_6)_3$)B–P(*t*-Bu)$_3$

B	0.085304	0.107007	-0.095417		P	-0.833706	-0.996074	1.555587
C	1.739025	0.044952	-0.133688		C	-2.757109	-1.045042	1.435128
C	-0.248120	1.728360	-0.115587		C	-0.254265	-2.832956	1.632381
C	-0.362669	-0.405135	-1.604449		C	-0.423265	-0.231390	3.277014
C	2.713441	-0.529388	0.692570		C	-3.306182	-2.058482	0.390623
C	2.244924	0.760873	-1.248951		C	-3.460280	-1.363038	2.780179
C	4.085281	-0.446367	0.420778		C	-3.298553	0.317878	0.932823
C	3.598406	0.858079	-1.534290		C	1.168466	-3.029212	2.229738
C	4.515212	0.238666	-0.696354		C	-1.207621	-3.757118	2.433576
H	2.429630	-1.034399	1.598504		C	-0.127052	-3.416226	0.201867
H	4.812190	-0.902994	1.079037		C	-1.238016	1.049252	3.617403
H	3.952583	1.412304	-2.394343		C	-0.617745	-1.213628	4.461137
F	5.853029	0.327095	-0.977050		C	1.046834	0.258996	3.309844
C	-1.038036	2.572174	0.675636		H	-4.372360	-2.194166	0.607656
C	0.409803	2.364936	-1.199248		H	-3.233308	-1.643238	-0.613875
C	-1.140858	3.950736	0.448016		H	-2.837094	-3.039646	0.412191
C	0.319103	3.726713	-1.444033		H	-4.540576	-1.308274	2.597619
C	-0.452997	4.517576	-0.604474		H	-3.234499	-2.364557	3.148586
H	-1.627519	2.169077	1.479661		H	-3.225910	-0.641696	3.561252
H	-1.758836	4.575051	1.079260		H	-4.357703	0.180127	0.682052
H	0.834279	4.182531	-2.280152		H	-3.243788	1.099698	1.689603
F	-0.541417	5.864280	-0.838841		H	-2.768515	0.649296	0.034513
C	-1.182256	-1.435786	-2.081752		H	1.267442	-4.093134	2.475739
C	0.257324	0.381838	-2.608739		H	1.927135	-2.800487	1.482200
C	-1.413684	-1.652490	-3.446396		H	1.368812	-2.460640	3.135179
C	0.044396	0.182461	-3.964278		H	-0.804582	-4.774646	2.359067
C	-0.805802	-0.834554	-4.375700		H	-1.259440	-3.495356	3.491179
H	-1.641524	-2.126335	-1.397217		H	-2.217803	-3.777486	2.027948
H	-2.054094	-2.457155	-3.781969		H	0.397181	-4.376626	0.282521
H	0.532926	0.801192	-4.706413		H	-1.092861	-3.612204	-0.262506
F	-1.024080	-1.031850	-5.713538		H	0.456149	-2.754766	-0.446302
C	1.207700	1.453453	-2.111212		H	-1.127347	1.220927	4.694666
H	1.666816	2.004263	-2.935818		H	-0.812941	1.913946	3.109116
					H	-2.302065	0.987957	3.400145
					H	-0.302986	-0.685777	5.369802
					H	-1.657634	-1.515077	4.593577
					H	-0.002185	-2.107553	4.375262
					H	1.172272	0.865655	4.215332
					H	1.764574	-0.558698	3.365627
					H	1.277258	0.881178	2.439466

Table S30. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of *bic*-(HC(4-F-H_3C_6)$_3$)B–ONN–P(*t*-Bu)$_3$

N	0.009152	0.219264	-0.275127		P	-2.254799	1.251743	-0.317116
O	1.291409	0.295636	-0.350388		C	-2.675620	1.590306	-2.106974
N	-0.556002	1.343694	-0.326104		C	-2.909644	-0.398764	0.286683
B	1.933444	-1.058024	-0.029056		C	-2.695421	2.679200	0.810218
C	1.400914	-2.287234	-0.933766		C	-2.326892	3.055544	-2.452043
C	1.699808	-1.487416	1.511622		C	-1.765286	0.712519	-3.000785
C	3.528971	-1.067489	-0.219142		C	-4.160855	1.332382	-2.428347
C	0.540530	-2.316352	-2.034524		C	-2.753462	-1.487980	-0.801398
C	2.003437	-3.501844	-0.536157		C	-2.124611	-0.927249	1.515577
C	0.236360	-3.522012	-2.683881		C	-4.407891	-0.262618	0.649698
C	1.710648	-4.700359	-1.169870		C	-2.495205	2.230624	2.277345
C	0.813861	-4.695406	-2.234362		C	-1.723037	3.866657	0.587291
H	0.120395	-1.388576	-2.418034		C	-4.147578	3.158433	0.610279
H	-0.425641	-3.555425	-3.539428		H	-2.430897	3.167896	-3.537195
H	2.168021	-5.634388	-0.868187		H	-3.005182	3.766628	-1.976284
F	0.514834	-5.880558	-2.860945		H	-1.292812	3.286725	-2.178954
C	1.078084	-0.805541	2.561347		H	-1.999388	0.955283	-4.043448
C	2.287632	-2.739810	1.789644		H	-0.711378	0.945334	-2.822477
C	0.997476	-1.374550	3.840298		H	-1.920209	-0.356089	-2.857961
C	2.216297	-3.312420	3.050688		H	-4.330821	1.619012	-3.472592
C	1.557801	-2.619575	4.062961		H	-4.427290	0.278386	-2.324944
H	0.658729	0.185550	2.393268		H	-4.828986	1.931540	-1.802047
H	0.520929	-0.858562	4.663529		H	-3.115848	-2.425170	-0.363200
H	2.663572	-4.273703	3.271005		H	-3.348843	-1.288346	-1.694296
F	1.476639	-3.182939	5.313033		H	-1.701498	-1.635605	-1.063190
C	4.411365	-0.075512	-0.650466		H	-2.615989	-1.858650	1.822038
C	4.059369	-2.330122	0.132533		H	-1.092307	-1.160465	1.249094
C	5.787151	-0.332391	-0.733121		H	-2.128186	-0.252021	2.369715
C	5.418550	-2.592054	0.053538		H	-4.773222	-1.266808	0.892572
C	6.269248	-1.580134	-0.382412		H	-4.560176	0.365763	1.530314
H	4.032711	0.905250	-0.924068		H	-5.012135	0.123811	-0.176186
H	6.484196	0.425427	-1.065432		H	-2.641891	3.110709	2.912632
H	5.834660	-3.555561	0.320246		H	-3.215075	1.471122	2.585745
F	7.617151	-1.834291	-0.462995		H	-1.477287	1.860282	2.441265
C	3.021323	-3.364301	0.599871		H	-1.883609	4.570515	1.411617
H	3.483434	-4.321410	0.855875		H	-0.685111	3.526966	0.599371
					H	-1.914202	4.395203	-0.345124
					H	-4.337376	3.957237	1.336611
					H	-4.300833	3.575619	-0.388236
					H	-4.881387	2.366704	0.780912

Table S31. Optimized (ONI(M06-2X)) Cartesian coordinates of $(H_5C_6)_3C^+/BF_4^-$ in PCM dichloromethane solvent

C	0.288001	-0.049368	-0.108170
C	1.705281	-0.006137	0.210553
C	-0.434540	1.181405	-0.304294
C	-0.376890	-1.319728	-0.240978
C	2.220437	0.999983	1.055616
C	2.584288	-0.975035	-0.332197
C	3.577079	1.023500	1.363115
C	3.940642	-0.926854	-0.038339
C	4.436559	0.066562	0.813575
H	1.545723	1.726001	1.495993
H	2.192366	-1.724916	-1.008779
H	3.964324	1.781306	2.031668
H	4.613121	-1.654551	-0.473542
H	5.493528	0.095302	1.048338
C	-1.830622	1.248454	-0.095761
C	0.242442	2.328538	-0.809485
C	-2.543219	2.386843	-0.454255
C	-0.469679	3.475994	-1.113916
C	-1.863444	3.500542	-0.952000
H	-2.352055	0.401835	0.335675
H	1.305104	2.270935	-1.009018
H	-3.622282	2.355847	-0.412759
H	0.044197	4.339043	-1.516787
H	-2.418401	4.387072	-1.233988
C	0.091900	-2.440457	0.494360
C	-1.531495	-1.463385	-1.062692
C	-0.577772	-3.652389	0.422069
C	-2.198756	-2.681282	-1.109619
C	-1.723521	-3.772142	-0.377507
H	0.943307	-2.328775	1.155622
H	-1.891131	-0.646479	-1.684236
H	-0.228277	-4.496889	1.001775
H	-3.097822	-2.732529	-1.705147
H	-2.249036	-4.718807	-0.419869
F	-3.017094	0.487493	-2.862160
B	-4.365072	0.124313	-2.589355
F	-4.865456	0.907071	-1.527975
F	-5.138700	0.306178	-3.734337
F	-4.377006	-1.242893	-2.211687

Table S32. Optimized (ONI(M06-2X)) Cartesian coordinates of the *tt* conformer of $(H_5C_6)_3C$–ONN–P(*t*-Bu)$_3$/BF_4^- in PCM dichloromethane solvent

O	0.028943	-0.057512	-0.090460		C	3.256439	3.319458	1.865464
N	1.372573	-0.034327	0.011065		C	2.450000	1.120605	2.641343
N	1.819517	1.087123	-0.224995		C	4.974452	1.588419	2.458788
C	-0.470755	-1.425769	-0.167229		C	3.918982	-1.437257	1.128143
P	3.526693	1.159664	0.082381		C	3.693845	-1.306085	-1.334420
C	0.334293	-2.305600	0.791120		C	5.797154	-0.441087	-0.240712
C	-0.394937	-1.863508	-1.630839		C	4.076196	1.702546	-2.580405
C	-1.927593	-1.333305	0.281987		C	3.112408	3.592670	-1.254517
C	3.580918	1.809495	1.833252		C	5.514602	2.900525	-0.886856
C	4.261218	-0.557137	-0.099290		H	3.230275	3.601738	2.925194
C	4.091303	2.388743	-1.195750		H	4.023307	3.924457	1.380123
C	1.078374	-3.418413	0.396893		H	2.265206	3.505014	1.443984
C	0.355358	-1.908287	2.139136		H	2.589733	1.408132	3.689459
C	1.813102	-4.144126	1.345403		H	1.485294	1.510095	2.298184
C	1.102797	-2.616301	3.074482		H	2.455218	0.030276	2.582551
C	1.830958	-3.745473	2.678692		H	4.955453	2.044537	3.454710
H	1.092232	-3.725013	-0.643125		H	5.229977	0.535249	2.578993
H	-0.216179	-1.035534	2.439226		H	5.761400	2.084049	1.880917
H	2.379014	-5.012126	1.029050		H	4.362801	-2.422379	0.943124
H	1.114658	-2.295240	4.109227		H	4.332449	-1.053955	2.061184
H	2.406395	-4.303489	3.407326		H	2.840317	-1.569932	1.224572
C	0.138908	-1.027263	-2.620633		H	4.208483	-2.273714	-1.368071
C	-0.886612	-3.123691	-2.007826		H	2.624771	-1.498104	-1.224430
C	0.203394	-1.457022	-3.951248		H	3.876659	-0.795493	-2.278237
C	-0.818277	-3.549400	-3.332043		H	6.200498	-1.459550	-0.223094
C	-0.267564	-2.716981	-4.310623		H	6.083044	0.013543	-1.192419
H	0.489387	-0.032291	-2.372531		H	6.258388	0.117126	0.578905
H	-1.327408	-3.775687	-1.262529		H	4.307252	2.470479	-3.325659
H	0.616597	-0.794812	-4.702439		H	4.833517	0.920678	-2.662571
H	-1.199712	-4.527062	-3.600494		H	3.087542	1.291474	-2.814138
H	-0.216329	-3.046700	-5.340951		H	3.271278	4.073106	-2.227080
C	-2.605746	-2.477649	0.726991		H	2.057029	3.320455	-1.166569
C	-2.598595	-0.105191	0.242461		H	3.345511	4.329688	-0.486573
C	-3.953735	-2.402738	1.081960		H	5.776947	3.619486	-1.671361
C	-3.944149	-0.038104	0.611690		H	5.556369	3.425713	0.070762
C	-4.629756	-1.182481	1.018472		H	6.264147	2.106203	-0.892819
H	-2.080724	-3.423566	0.821603		F	-1.725074	2.758823	0.128219
H	-2.076368	0.806110	-0.021626		B	-0.601194	3.605006	0.267965
H	-4.467898	-3.294024	1.421175		F	-1.011706	4.881993	0.653766
H	-4.447759	0.921050	0.587347		F	0.264036	3.070440	1.269209
H	-5.674299	-1.124239	1.300195		F	0.084600	3.666401	-0.963965

Table S33. Optimized (ONI(M06-2X)) Cartesian coordinates of the transition state ONN···P(*t*-Bu)$_3$ and the complex ONN–P(*t*-Bu)$_3$

transition state					complex			
O	-2.645929	-1.672827	0.546457		O	-0.168722	0.428546	0.351435
N	-2.933527	-0.703635	-0.156438		N	1.042051	0.325014	0.274670
N	-2.459112	0.240130	-0.636779		N	1.663907	1.416566	-0.171475
P	-0.155801	0.103133	-0.014839		P	3.312377	1.285586	-0.193489
C	0.346235	1.566065	-1.097669		C	3.959597	1.644910	1.530114
C	0.475455	0.358392	1.749071		C	3.872015	-0.402477	-0.792380
C	0.574182	-1.489393	-0.720057		C	3.769339	2.649051	-1.392818
C	0.069620	1.196398	-2.575962		C	3.698039	3.134099	1.851723
C	-0.600613	2.762429	-0.805245		C	3.126658	0.845092	2.561623
C	1.805786	2.042763	-0.959973		C	5.459432	1.343075	1.710106
C	0.106208	1.789364	2.205185		C	3.754042	-1.434400	0.355949
C	-0.289238	-0.611857	2.692634		C	2.906248	-0.905542	-1.894806
C	1.994334	0.166647	1.945220		C	5.321663	-0.404784	-1.320332
C	0.531481	-2.604665	0.351244		C	3.419938	2.169774	-2.821661
C	-0.387802	-1.986993	-1.832187		C	2.872806	3.889035	-1.139104
C	2.016805	-1.386326	-1.257183		C	5.254658	3.052690	-1.336883
H	0.236740	2.093139	-3.184931		H	3.910919	3.287530	2.916032
H	0.732175	0.411793	-2.944429		H	4.346290	3.801407	1.280550
H	-0.971743	0.883042	-2.703070		H	2.649681	3.388567	1.664915
H	-0.409313	3.534662	-1.561094		H	3.418158	1.192035	3.560093
H	-1.644456	2.448048	-0.880280		H	2.058495	1.032122	2.423192
H	-0.430239	3.205824	0.174941		H	3.300374	-0.228412	2.510768
H	1.981553	2.844370	-1.689317		H	5.751627	1.650627	2.721762
H	1.997279	2.452240	0.035807		H	5.675317	0.276622	1.611370
H	2.523401	1.241006	-1.152588		H	6.079607	1.894704	0.997266
H	0.318409	1.868736	3.277902		H	3.959217	-2.424384	-0.068967
H	0.700677	2.547210	1.690334		H	4.477823	-1.257681	1.153903
H	-0.958261	1.994697	2.047216		H	2.735836	-1.419031	0.754793
H	-0.217848	-0.227769	3.717331		H	3.220056	-1.921558	-2.163117
H	-1.341225	-0.701686	2.405844		H	1.886148	-0.942588	-1.506689
H	0.145516	-1.611654	2.680243		H	2.924985	-0.294696	-2.795592
H	2.235349	0.353302	3.000406		H	5.586753	-1.439405	-1.570223
H	2.307061	-0.852615	1.707522		H	5.428348	0.194793	-2.227747
H	2.576382	0.861654	1.334438		H	6.035225	-0.044796	-0.572914
H	0.762403	-3.553906	-0.148150		H	3.560110	3.018112	-3.500754
H	1.270270	-2.455114	1.140923		H	4.067060	1.358817	-3.161164
H	-0.472100	-2.669335	0.781680		H	2.372109	1.855757	-2.867008
H	0.031392	-2.905664	-2.261437		H	2.954344	4.541490	-2.016174
H	-1.353919	-2.228360	-1.378373		H	1.837004	3.563328	-1.009146
H	-0.533458	-1.267180	-2.637302		H	3.187187	4.459286	-0.265726
H	2.336508	-2.383842	-1.585556		H	5.432167	3.802163	-2.117594
H	2.093212	-0.713099	-2.113641		H	5.512920	3.507169	-0.376966
H	2.709831	-1.045142	-0.481831		H	5.926099	2.208796	-1.519106

Table S34. Optimized (ONI(M06-2X)) Cartesian coordinates of $[(F_5C_6)_3]B–O(Me)NN–P(t\text{-}Bu)_3]Li$ ([MeO]Li) in PCM diethyl ether solvent

O	-0.311942	-0.186310	-0.364540		C	3.829367	-0.186696	-2.377670
N	1.239259	-0.293989	-0.666018		C	2.659375	1.981398	-2.214642
N	1.775835	0.574718	0.352796		C	5.150559	1.861345	-1.803654
B	-0.823774	-1.653093	-0.271015		C	3.207814	3.587475	0.589493
P	3.362978	0.819563	0.205969		C	2.992986	2.227234	2.634985
C	0.131930	-2.406851	0.793236		C	5.237127	2.483760	1.556004
C	-0.766313	-2.232564	-1.784971		C	4.221802	-0.766798	2.347798
C	-2.295363	-1.604867	0.418370		C	3.669061	-1.952456	0.243301
C	3.802521	1.147625	-1.588246		C	5.839899	-0.690807	0.444886
C	3.729883	2.308600	1.279515		H	3.874654	0.068058	-3.444220
C	4.343812	-0.675141	0.811506		H	4.714220	-0.782217	-2.144599
C	0.462063	-1.783610	1.982428		H	2.929304	-0.780155	-2.193186
C	0.658402	-3.681983	0.634971		H	2.877672	2.094205	-3.283699
C	1.361733	-2.286899	2.894776		H	1.728554	1.421575	-2.085948
C	1.563031	-4.229863	1.532271		H	2.566255	2.975839	-1.779223
C	1.946351	-3.514199	2.652920		H	5.324093	1.923536	-2.885320
F	-0.132373	-0.612001	2.310959		H	5.146097	2.881183	-1.410695
F	0.303761	-4.457064	-0.433469		H	5.987764	1.315889	-1.359246
F	1.696913	-1.554281	4.000215		H	3.310429	4.419130	1.296281
F	2.104435	-5.459300	1.303898		H	3.776977	3.837496	-0.307393
F	2.896718	-4.000783	3.498811		H	2.150967	3.477657	0.326692
C	0.377000	-2.722969	-2.413774		H	3.295218	1.374207	3.238881
C	-1.897837	-2.164234	-2.584853		H	3.222772	3.144287	3.191115
C	0.376064	-3.144800	-3.734424		H	1.911428	2.188643	2.490568
C	-1.932938	-2.577270	-3.906816		H	5.374917	3.432058	2.089281
C	-0.782791	-3.077711	-4.483059		H	5.628372	1.685525	2.189804
F	1.550123	-2.810297	-1.787599		H	5.827200	2.524763	0.637461
F	-3.061477	-1.622888	-2.090552		H	4.569747	-1.760405	2.659031
F	1.520194	-3.623183	-4.300848		H	4.837934	-0.022473	2.858764
F	-3.079066	-2.483385	-4.638130		H	3.187821	-0.664864	2.679400
F	-0.787397	-3.489473	-5.780091		H	3.991972	-2.165217	-0.776286
C	-2.861786	-0.555090	1.117584		H	3.969643	-2.800235	0.872086
C	-3.012833	-2.791101	0.428899		H	2.578946	-1.863722	0.225935
C	-4.073686	-0.662747	1.785849		H	6.281850	-1.595974	0.881388
C	-4.223849	-2.940877	1.075565		H	5.995891	-0.737135	-0.634952
C	-4.758463	-1.860291	1.760807		H	6.381107	0.172477	0.841434
F	-2.253047	0.645180	1.194447		C	-0.951510	0.635399	-1.360574
F	-2.483350	-3.872453	-0.225850		H	-0.553544	0.364088	-2.335805
F	-4.577938	0.404910	2.466773		H	-2.027688	0.465781	-1.324548
F	-4.893544	-4.125663	1.055314		H	-0.709251	1.674115	-1.141079
F	-5.947666	-1.986062	2.410120		Li	0.185939	1.027838	1.325141

Table S35. Optimized (ONI(M06-2X)) Cartesian coordinates of $[(F_5C_6)_3]B–ON(Me)N–P(t\text{-}Bu)_3]Li$ ([MeN1]Li) in PCM diethyl ether solvent

O	-0.079734	0.752009	0.174176	C	5.116118	2.359231	1.176462
N	1.096149	0.772152	1.002874	C	4.347286	0.043971	1.155642
N	1.876554	1.843090	0.510533	C	5.822032	0.885672	-0.719018
B	-1.029967	-0.350991	0.047380	C	2.913547	-0.816675	-1.665471
P	3.044746	1.756906	-0.601614	C	1.232422	0.807299	-2.544210
C	-0.220568	-1.729218	-0.365335	C	3.627511	0.919565	-3.306405
C	-2.043034	0.139219	-1.134106	C	1.939705	3.802378	-2.093396
C	-1.998093	-0.563790	1.359454	C	2.944877	4.485897	0.061947
C	4.655359	1.236097	0.219750	C	4.443595	3.908481	-1.878897
C	2.712516	0.652962	-2.093649	H	5.922489	1.961056	1.804697
C	3.137726	3.544882	-1.148156	H	5.506618	3.225739	0.640880
C	-0.041904	-2.279840	-1.626878	H	4.291252	2.674522	1.823881
C	0.544432	-2.332691	0.606072	H	5.281828	-0.285751	1.624206
C	0.860944	-3.301955	-1.888465	H	3.692414	0.410097	1.957200
C	1.482589	-3.323743	0.404901	H	3.905033	-0.815800	0.644530
C	1.640623	-3.823775	-0.873119	H	6.714328	0.700223	-0.107848
F	-0.678630	-1.785436	-2.694928	H	5.629455	-0.014211	-1.306969
F	0.465945	-1.864744	1.938544	H	6.048583	1.708227	-1.403527
F	1.044208	-3.737555	-3.164872	H	2.628525	-1.452249	-2.511978
F	2.286421	-3.732096	1.434928	H	3.951483	-1.045474	-1.414951
F	2.575805	-4.775881	-1.130830	H	2.266789	-1.063634	-0.818390
C	-2.133173	1.387361	-1.737184	H	1.142788	1.539109	-3.349594
C	-2.993756	-0.790728	-1.525066	H	0.867410	-0.152911	-2.923027
C	-3.113620	1.676529	-2.680967	H	0.589256	1.105891	-1.715160
C	-3.984137	-0.537936	-2.454019	H	3.385243	0.169737	-4.070417
C	-4.040541	0.717366	-3.035634	H	3.439188	1.903247	-3.742290
F	-1.272777	2.377271	-1.475920	H	4.690585	0.832617	-3.070920
F	-2.945868	-2.042455	-0.957039	H	1.869551	4.884331	-2.253660
F	-3.164119	2.911959	-3.258793	H	2.083257	3.331916	-3.068071
F	-4.893222	-1.492322	-2.803615	H	1.001142	3.448068	-1.654313
F	-5.004548	1.000057	-3.956872	H	3.823693	4.521952	0.706508
C	-2.393855	-1.754653	1.948158	H	2.766923	5.494875	-0.327432
C	-2.545850	0.587122	1.910100	H	2.081597	4.150381	0.639900
C	-3.244587	-1.805355	3.042917	H	4.355735	4.946158	-2.223206
C	-3.399820	0.577769	3.000759	H	5.312177	3.852494	-1.218383
C	-3.748740	-0.633129	3.571393	H	4.628673	3.280186	-2.753189
F	-1.938011	-2.930219	1.500191	C	0.604725	1.253608	2.314209
F	-2.243254	1.813629	1.373229	H	0.009820	0.470683	2.792849
F	-3.584173	-3.003318	3.600341	H	1.465909	1.514872	2.933487
F	-3.899483	1.738091	3.513912	H	-0.020132	2.134343	2.166981
F	-4.584520	-0.667529	4.646551	Li	1.928328	-0.762099	2.091809

Table S36. Optimized (ONI(M06-2X)) Cartesian coordinates of $[(F_5C_6)_3]B–ON(Me)N–P(t\text{-}Bu)_3]^-$ anion ([MeN1]$^-$) in PCM diethyl ether solvent

O	-0.288357	1.000014	0.045920		C	4.713967	1.987329	1.523223
N	0.959887	1.009471	0.763315		C	3.824221	-0.286050	1.048850
N	1.694213	2.098515	0.246318		C	5.669861	0.685148	-0.384314
B	-1.072586	-0.232258	0.019635		C	2.813408	-0.623110	-1.868833
P	3.025431	1.845826	-0.635290		C	1.265659	1.149285	-2.691749
C	-0.112925	-1.513692	-0.325942		C	3.725677	1.132973	-3.357514
C	-2.218515	-0.016199	-1.126061		C	2.408757	4.084615	-2.098686
C	-1.949688	-0.457810	1.405345		C	3.222033	4.533036	0.183250
C	4.371342	1.008647	0.377316		C	4.870725	3.833710	-1.586105
C	2.719993	0.873138	-2.219411		H	5.359260	1.467395	2.240658
C	3.446454	3.623865	-1.046965		H	5.254002	2.864174	1.157123
C	0.039529	-2.117355	-1.562057		H	3.799785	2.312352	2.031469
C	0.753955	-1.963106	0.658942		H	4.402968	-0.462397	1.963864
C	0.975329	-3.111251	-1.808521		H	2.761287	-0.201903	1.303024
C	1.727029	-2.920047	0.443118		H	3.950842	-1.162015	0.409307
C	1.829042	-3.511589	-0.803538		H	6.390056	0.259714	0.327388
F	-0.659855	-1.704730	-2.632871		H	5.509795	-0.052303	-1.174220
F	0.688965	-1.444964	1.928206		H	6.119808	1.577566	-0.828358
F	1.120884	-3.620753	-3.069019		H	2.457074	-1.200545	-2.730482
F	2.612707	-3.256839	1.428397		H	3.838834	-0.933979	-1.658693
F	2.789375	-4.451968	-1.042045		H	2.186249	-0.849297	-1.006785
C	-2.459240	1.106957	-1.905107		H	1.233377	1.966486	-3.417670
C	-3.091023	-1.077034	-1.311677		H	0.867743	0.244087	-3.168489
C	-3.518841	1.163650	-2.804962		H	0.610982	1.392172	-1.847619
C	-4.154684	-1.056433	-2.194031		H	3.485179	0.448568	-4.181835
C	-4.369239	0.085950	-2.945822		H	3.666447	2.152435	-3.744665
F	-1.672387	2.182504	-1.863588		H	4.756763	0.935683	-3.044495
F	-2.885948	-2.228579	-0.587411		H	2.520055	5.166558	-2.236901
F	-3.723414	2.286641	-3.557270		H	2.553304	3.603483	-3.066866
F	-4.985166	-2.131255	-2.337985		H	1.400025	3.867630	-1.733121
F	-5.411607	0.140560	-3.826163		H	4.013792	4.431364	0.926655
C	-2.137746	-1.627334	2.125608		H	3.210683	5.573104	-0.164466
C	-2.637799	0.651792	1.877228		H	2.262487	4.269407	0.634594
C	-2.921969	-1.688908	3.268641		H	4.964899	4.879895	-1.903417
C	-3.431344	0.628341	3.013886		H	5.619378	3.653678	-0.808719
C	-3.569253	-0.554420	3.716371		H	5.096405	3.196018	-2.444980
F	-1.556073	-2.773448	1.754617		C	0.620844	1.375228	2.142718
F	-2.565009	1.845123	1.206962		H	0.021298	0.592355	2.596387
F	-3.062961	-2.863983	3.952594		H	1.555554	1.474290	2.695173
F	-4.081699	1.750295	3.443913		H	0.079999	2.328342	2.149223
F	-4.344499	-0.600684	4.839051					

Table S37. Optimized (ONI(M06-2X)) Cartesian coordinates of $[(F_5C_6)_3]B–ONN(Me)–P(t\text{-}Bu)_3]Li$ ([MeN2]Li) in PCM diethyl ether solvent

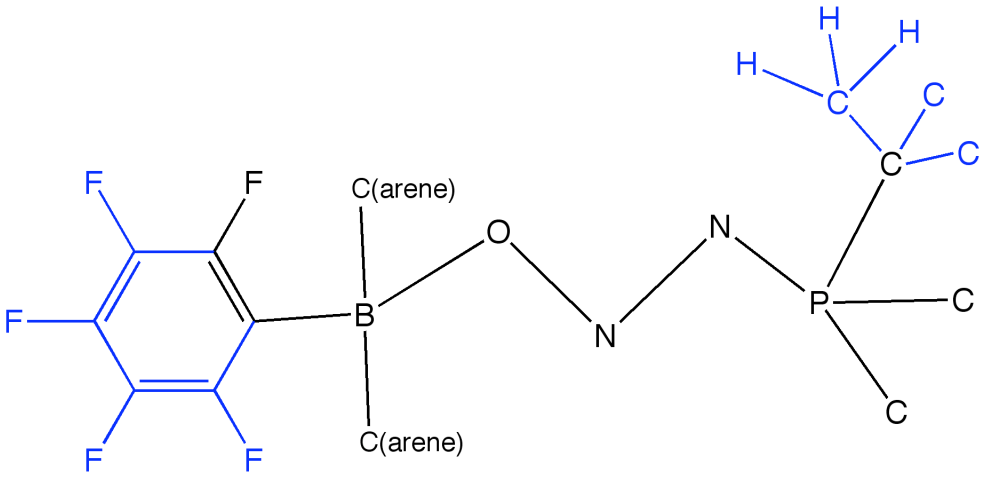
O	0.196541	-0.221789	-0.092738		C	4.618924	2.366580	-2.431031
N	1.591976	-0.564581	-0.395740		C	3.617931	3.561740	-0.429908
N	2.146467	0.785202	-0.536915		C	5.947306	2.600242	-0.357587
B	-0.629908	-1.398190	0.098744		C	3.726118	1.975729	2.270435
P	3.813960	0.734774	-0.249020		C	3.121315	-0.448496	2.217956
C	0.011779	-2.203368	1.392079		C	5.525996	0.264887	1.983164
C	-0.818734	-2.333437	-1.221551		C	4.240360	-2.038841	-0.316609
C	-2.111266	-0.785115	0.423824		C	3.808069	-0.895549	-2.478893
C	4.510658	2.358858	-0.884373		C	6.063609	-0.657973	-1.344018
C	4.069144	0.621740	1.610285		H	4.996793	3.354076	-2.718741
C	4.540617	-0.749902	-1.120599		H	5.329877	1.622598	-2.792976
C	0.544918	-3.480487	1.479772		H	3.661640	2.213891	-2.928662
C	0.191115	-1.439316	2.527566		H	3.392356	4.189543	-1.297340
C	1.208481	-3.945140	2.608837		H	2.671261	3.254607	0.018953
C	0.855477	-1.839444	3.666149		H	4.154763	4.175132	0.298387
C	1.369277	-3.121890	3.708200		H	6.318100	3.510508	-0.842674
F	0.485662	-4.324795	0.445107		H	5.967990	2.771542	0.719219
F	-0.247296	-0.099417	2.541034		H	6.630392	1.784878	-0.604471
F	1.724749	-5.206567	2.632315		H	3.838426	1.847097	3.352434
F	1.074727	-0.964707	4.693332		H	4.387342	2.783690	1.955788
F	2.045839	-3.556965	4.807257		H	2.691864	2.274835	2.075312
C	-0.421119	-2.085848	-2.526888		H	3.634239	-1.409465	2.323262
C	-1.588324	-3.470924	-1.030442		H	2.795355	-0.129136	3.214471
C	-0.743187	-2.948846	-3.568931		H	2.270764	-0.623421	1.545425
C	-1.931787	-4.349369	-2.039684		H	5.573907	0.222686	3.077922
C	-1.495969	-4.080052	-3.326095		H	5.812253	-0.717821	1.605075
F	0.290638	-1.008868	-2.860759		H	6.255317	1.001252	1.642874
F	-2.047313	-3.736400	0.238697		H	4.539848	-2.884257	-0.947433
F	-0.321961	-2.677186	-4.840163		H	4.816058	-2.092871	0.609662
F	-2.685782	-5.459876	-1.794290		H	3.171313	-2.105687	-0.102057
F	-1.816477	-4.925755	-4.347227		H	4.204331	-1.793696	-2.967963
C	-2.944732	-1.064158	1.494819		H	2.733115	-1.020498	-2.300307
C	-2.594263	0.140788	-0.491666		H	3.983535	-0.047897	-3.145603
C	-4.174844	-0.444614	1.667439		H	6.378166	-1.603614	-1.801043
C	-3.816602	0.778210	-0.353380		H	6.340033	0.145634	-2.029358
C	-4.611640	0.480048	0.738871		H	6.618745	-0.537261	-0.409474
F	-2.574079	-1.925222	2.447288		C	1.593212	1.463906	-1.736993
F	-1.856297	0.462021	-1.606577		H	0.512535	1.339577	-1.677905
F	-4.950843	-0.737018	2.750671		H	1.827763	2.525940	-1.742521
F	-4.240387	1.693925	-1.271927		H	1.927863	1.005299	-2.668820
F	-5.815548	1.098374	0.897871		Li	0.452411	1.070699	1.175227

Table S38. Optimized (ONI(M06-2X)) Cartesian coordinates of $[(F_5C_6)_3]B–ONN(Me)–P(t\text{-}Bu)_3]^-$ anion ([MeN2]$^-$) in PCM diethyl ether solvent

O	0.373476	-0.301411	-0.134246		C	5.186563	1.366107	-2.533175
N	1.607855	-0.660337	-0.859582		C	4.059812	3.326342	-1.577615
N	2.272929	0.582303	-1.008718		C	6.020360	2.388275	-0.384132
B	-0.485074	-1.456568	-0.038271		C	3.062364	2.795807	1.521993
P	3.718648	0.743818	-0.233048		C	2.275301	0.529381	2.136312
C	0.354300	-2.581326	0.829947		C	4.700849	1.151311	2.458062
C	-1.038089	-2.058819	-1.470070		C	3.929848	-1.852019	0.804641
C	-1.853119	-0.935105	0.695121		C	4.243912	-1.633671	-1.630901
C	4.757597	1.993929	-1.187296		C	6.077046	-0.903486	-0.045578
C	3.472990	1.306544	1.541239		H	5.676761	2.147814	-3.126113
C	4.552880	-0.942717	-0.278870		H	5.894784	0.547003	-2.407302
C	0.967861	-3.736470	0.375444		H	4.314257	1.004898	-3.088154
C	0.689061	-2.209061	2.120259		H	4.857878	4.010750	-1.891394
C	1.865000	-4.466963	1.141671		H	3.389485	3.189633	-2.425745
C	1.604650	-2.886274	2.903422		H	3.510462	3.797758	-0.764157
C	2.194007	-4.035166	2.411079		H	6.683846	2.942916	-1.058928
F	0.748477	-4.194641	-0.865330		H	5.765484	3.050821	0.447312
F	0.142641	-1.073767	2.671184		H	6.573589	1.534355	0.006259
F	2.457999	-5.592554	0.636974		H	2.781069	3.075746	2.543614
F	1.970787	-2.396774	4.128367		H	3.878644	3.450699	1.208431
F	3.108198	-4.720725	3.161531		H	2.190829	2.955501	0.877345
C	-1.007678	-1.463443	-2.723732		H	2.573912	-0.444443	2.527414
C	-1.748924	-3.246058	-1.391100		H	1.886615	1.111160	2.982266
C	-1.621034	-2.041533	-3.829738		H	1.470673	0.386823	1.402269
C	-2.373253	-3.850282	-2.466891		H	4.420402	1.519064	3.453868
C	-2.301814	-3.235697	-3.704208		H	4.996080	0.105483	2.565318
F	-0.392250	-0.305979	-2.943611		H	5.563481	1.729171	2.117207
F	-1.866583	-3.866738	-0.168153		H	4.322464	-2.864699	0.646522
F	-1.558927	-1.428033	-5.052410		H	4.191566	-1.542768	1.819120
F	-3.056614	-5.027086	-2.330500		H	2.846423	-1.843579	0.654770
F	-2.908478	-3.802860	-4.789971		H	4.675979	-2.641211	-1.581271
C	-2.489364	-1.449534	1.815534		H	3.156544	-1.702938	-1.749116
C	-2.474492	0.151894	0.095828		H	4.684113	-1.119072	-2.485209
C	-3.654230	-0.901135	2.332486		H	6.418544	-1.945097	-0.013486
C	-3.638920	0.724226	0.584422		H	6.619599	-0.403535	-0.850707
C	-4.228833	0.193340	1.716336		H	6.342229	-0.437790	0.908498
F	-2.004562	-2.516926	2.458169		C	1.543716	1.607668	-1.764075
F	-1.965739	0.694771	-1.058132		H	0.489231	1.356000	-1.672361
F	-4.240339	-1.435713	3.446292		H	1.674023	2.602833	-1.342051
F	-4.214755	1.796450	-0.038238		H	1.825563	1.615433	-2.823715
F	-5.375724	0.742757	2.215141					

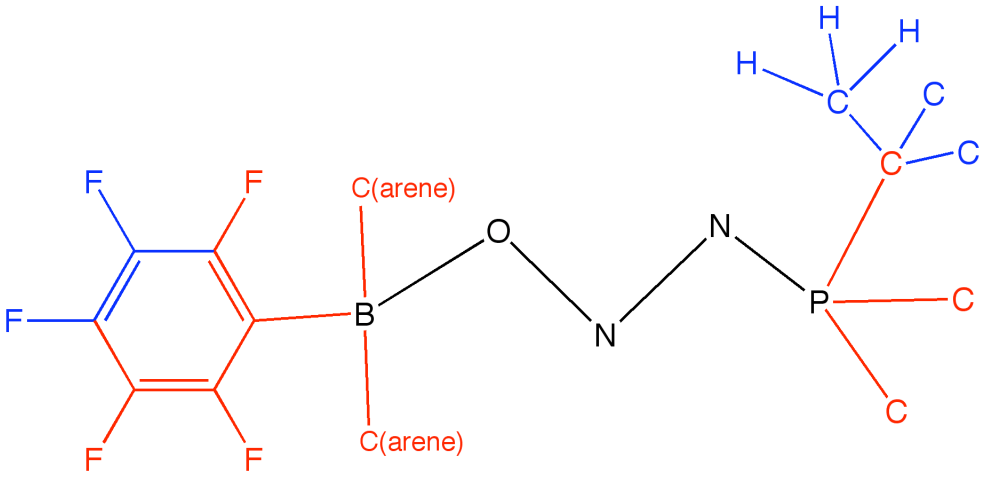
Graphic S1G. ONIOM layers for optimizations and OG2R3 calculations

(a)



For two-layer ONIOM optimizations, high layer atoms are shown in black. The entire molecule comprised the low layer, atoms specifically identified as the low layer are in blue. Atoms not shown are in the same layer as chemically identical ones shown.

(b)



For three-layer OG2R3 single energy calculations, high layer atoms are shown in black, middle layer atoms in red. The entire molecule comprised the low layer, atoms specifically identified as the low layer are in blue. Atoms not shown are in the same layer as chemically identical ones shown.