

Supporting Information

On the association of frustrated Lewis pairs in ionic liquids: a molecular dynamics simulation study

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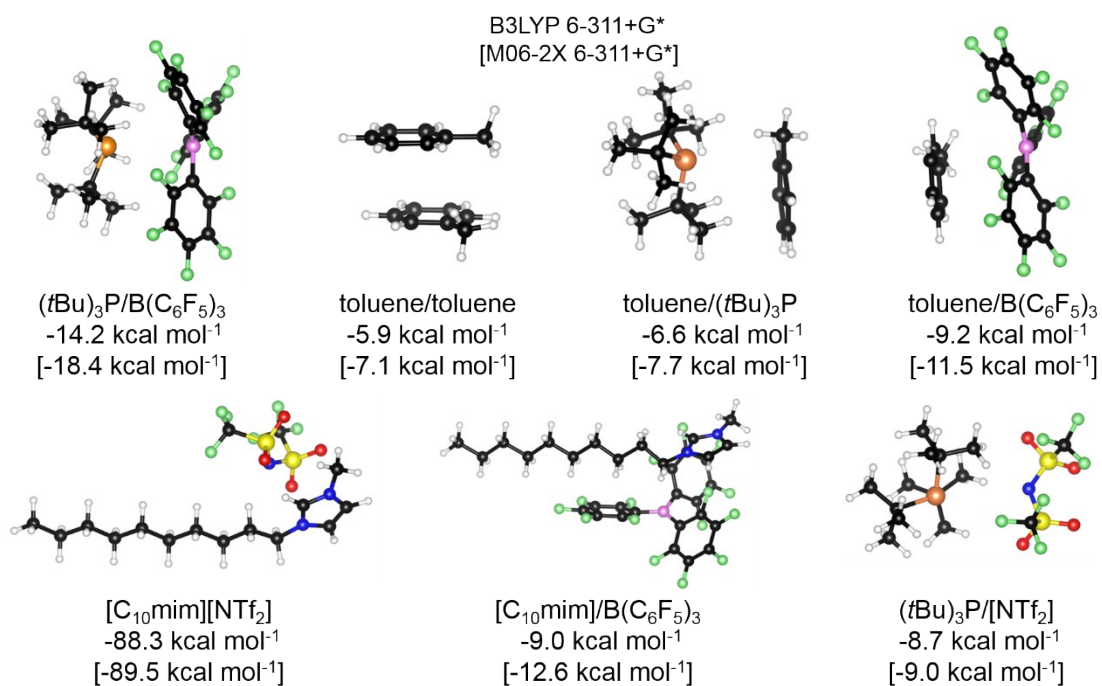


Figure S1. The DFT optimized structures and their interaction energies. Color legend: P brown, B pink, F green, N blue, O red, S yellow, C black, H white.

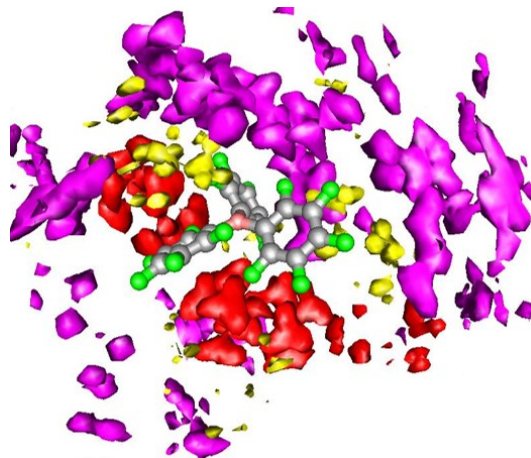


Figure S2. Computed SDFs for (tBu)₃P/B(C₆F₅)₃ in [C₆mim][CTf₃] with B(C₆F₅)₃ as the central molecule. Color legend: (tBu)₃P red, [C₆mim]⁺ pink, and [CTf₃]⁻ yellow. The isosurface values are 23.0 for [C₆mim]⁺, 45.0 for [CTf₃]⁻ and 100.0 for (tBu)₃P.

Cartesian coordinates (The DFT optimized structures at B3LYP-D3/6-31G* and their energies at B3LYP-D3/6-311+G* in hartree).

(*t*Bu)₃P

-815.086488805

P	-0.000234	0.000943	-0.721157
C	-0.395658	-1.753574	-0.004480
C	-1.321988	1.219343	-0.003365
C	1.717016	0.533957	-0.003918
C	-0.842097	2.669032	-0.215745
H	-1.675397	3.351299	-0.002257
H	-0.020901	2.947481	0.446860
H	-0.530171	2.845337	-1.250289
C	-1.715079	1.051770	1.473393
H	-2.440596	1.830245	1.748949
H	-2.189443	0.088108	1.670078
H	-0.858584	1.149062	2.144327
C	-2.581543	1.074988	-0.888283
H	-3.309798	1.847378	-0.606109
H	-2.334821	1.213639	-1.945942
H	-3.075521	0.109552	-0.783400
C	2.220688	1.697583	-0.889136
H	1.625249	2.604471	-0.788853
H	3.250827	1.948823	-0.602436
H	2.224422	1.412036	-1.946088
C	2.733176	-0.606137	-0.217108
H	3.740904	-0.222978	-0.009198
H	2.568268	-1.453780	0.450327
H	2.725764	-0.969029	-1.250030
C	1.772019	0.958185	1.473396
H	2.809942	1.196230	1.746018
H	1.176568	1.851737	1.672848
H	1.429167	0.168028	2.145098
C	-0.055210	-2.011057	1.472804
H	-0.371215	-3.026936	1.749304
H	1.016783	-1.945936	1.669596
H	-0.563474	-1.315220	2.144019
C	0.359856	-2.772347	-0.888625
H	1.442507	-2.718190	-0.779385
H	0.052887	-3.789257	-0.609088
H	0.119882	-2.626029	-1.946752
C	-1.891300	-2.063426	-0.216388
H	-2.542424	-1.494618	0.449673
H	-2.202564	-1.878503	-1.249669
H	-2.064041	-3.126995	-0.005508

B(C₆F₅)₃

-2209.01140634

B	-0.000612	0.001105	-0.000003
C	-1.513606	0.389522	0.000390
C	-2.475945	-0.354588	0.697824
C	-3.823955	-0.019526	0.717579
C	-4.258562	1.093625	0.001389
C	-3.342302	1.860067	-0.715542
C	-1.999446	1.504857	-0.696945
F	-2.110863	-1.430566	1.413442
F	-4.702156	-0.750038	1.411208
F	-5.548245	1.424406	0.001753
F	-3.761011	2.923244	-1.408662

F	-1.162219	2.271963	-1.413551
C	0.418970	-1.503490	0.000299
C	1.542727	-1.965906	0.699747
C	1.926075	-3.300927	0.718721
C	1.180307	-4.232763	0.000076
C	0.060028	-3.821408	-0.718720
C	-0.303292	-2.480701	-0.699345
F	2.290169	-1.112621	1.418196
F	-1.384141	-2.137535	-1.418406
F	-0.649558	-4.714719	-1.414740
F	1.538227	-5.515120	-0.000032
F	2.996003	-3.697717	1.414271
C	1.093019	1.116268	-0.001103
C	0.931332	2.322905	0.694995
C	1.897400	3.320976	0.714244
C	3.078934	3.137468	-0.000718
C	3.283422	1.959346	-0.715591
C	2.302437	0.975975	-0.696766
F	-0.182766	2.547602	1.409945
F	1.706188	4.448079	1.406339
F	4.012026	4.087101	-0.000688
F	4.413779	1.788072	-1.407591
F	2.546545	-0.133896	-1.411839

toluene

-271.650167723

C	-0.004393	0.913221	0.000000
C	-0.007715	0.194849	1.202180
C	-0.007715	-1.200207	1.205318
C	-0.007079	-1.903848	0.000000
C	-0.007715	-1.200207	-1.205318
C	-0.007715	0.194849	-1.202180
H	-0.012031	0.735787	2.145903
H	-0.012727	-1.737482	2.150048
H	-0.010453	-2.990315	0.000000
H	-0.012727	-1.737482	-2.150048
H	-0.012031	0.735787	-2.145903
C	0.029934	2.422703	0.000000
H	-0.464172	2.834779	0.886205
H	1.062706	2.795987	0.000000
H	-0.464172	2.834779	-0.886205

[C₁₀min]+

-659.263907193

N	-5.709815	0.866907	-0.000009
C	-4.379876	0.701103	0.000035
N	-4.109363	-0.608929	0.000011
C	-5.306779	-1.303128	-0.000017
C	-6.309578	-0.379849	-0.000037
C	-6.414134	2.154692	-0.000019
H	-3.653054	1.496466	0.000074
C	-2.765735	-1.241048	0.000043
H	-5.338016	-2.381558	-0.000033
H	-7.382038	-0.497734	-0.000073
H	-7.035361	2.228962	0.894616
H	-5.678855	2.959521	-0.000096
H	-7.035461	2.228889	-0.894590

C	-1.619798	-0.237100	0.000009
H	-2.721625	-1.881502	0.885841
H	-2.721616	-1.881572	-0.885703
C	-0.261627	-0.952572	0.000015
H	-1.688120	0.407725	-0.886213
H	-1.688103	0.407767	0.886202
C	0.916288	0.026909	0.000007
H	-0.194887	-1.606417	-0.880108
H	-0.194884	-1.606404	0.880148
C	2.276487	-0.676898	-0.000010
H	0.844367	0.682375	0.879702
H	0.844351	0.682385	-0.879678
C	3.457444	0.298162	0.000011
H	2.345464	-1.333740	-0.878915
H	2.345467	-1.333778	0.878867
C	4.818696	-0.403377	-0.000030
H	3.386456	0.955374	0.878850
H	3.386437	0.955436	-0.878781
C	6.001177	0.569441	0.000017
H	4.888134	-1.061069	-0.878643
H	4.888140	-1.061161	0.878514
C	7.363331	-0.131302	-0.000043
H	5.931565	1.227500	0.878658
H	5.931545	1.227611	-0.878540
C	8.538628	0.848568	0.000015
H	7.431141	-0.788468	-0.878280
H	7.431155	-0.788592	0.878100
H	9.498996	0.321961	-0.000035
H	8.512960	1.496216	0.884758
H	8.512939	1.496346	-0.884632

[NTf₂]-

-1827.64155887

N	0.033724	-0.879627	0.779233
S	-1.509528	-0.868148	0.314040
S	1.290052	-0.899007	-0.238092
O	-2.332126	-1.035166	1.516948
O	2.281799	-1.888040	0.201169
C	-1.851370	0.899837	-0.190755
C	2.075753	0.734116	0.208951
F	-3.169651	1.058397	-0.412947
F	-1.488959	1.752361	0.780848
F	-1.197601	1.233269	-1.309859
F	1.247562	1.758112	-0.050227
F	3.193810	0.908097	-0.520004
F	2.412679	0.781344	1.505054
O	-1.827114	-1.651218	-0.885435
O	0.996028	-0.775087	-1.672025

(tBu)₃P/B(C₆F₅)₃

-3024.12056353

P	-0.020673	0.061257	2.381006
C	-0.247598	1.863589	3.059798
C	1.629800	-0.621475	3.136185
C	-1.461149	-1.004671	3.122655
C	2.031939	-1.850661	2.290257
H	3.018059	-2.203499	2.620438

H	1.336904	-2.683727	2.384270
H	2.101518	-1.596392	1.230327
C	1.604816	-1.021900	4.621805
H	2.608756	-1.353884	4.920425
H	1.328001	-0.190157	5.272695
H	0.922223	-1.849387	4.821383
C	2.765892	0.404534	2.946778
H	3.717878	-0.082265	3.195473
H	2.841127	0.762048	1.919588
H	2.668967	1.270212	3.603838
C	-1.135399	-2.506494	2.987534
H	-0.361177	-2.837221	3.681669
H	-2.041741	-3.080184	3.220690
H	-0.827979	-2.779094	1.977624
C	-2.698382	-0.765087	2.228170
H	-3.507990	-1.431941	2.553517
H	-3.074227	0.255863	2.277550
H	-2.478121	-0.986140	1.181390
C	-1.843079	-0.738385	4.589466
H	-2.640408	-1.434556	4.884423
H	-1.005008	-0.892114	5.272000
H	-2.226347	0.271237	4.746819
C	0.125550	2.106440	4.532935
H	-0.085323	3.154290	4.787838
H	-0.451130	1.481079	5.217479
H	1.185223	1.936892	4.730884
C	-1.706157	2.325964	2.863886
H	-2.400313	1.841196	3.552099
H	-1.757990	3.404352	3.062110
H	-2.064783	2.164221	1.847104
C	0.607789	2.789057	2.165028
H	1.677545	2.604417	2.252673
H	0.338695	2.681694	1.111742
H	0.427169	3.832277	2.456701
B	0.013777	-0.038041	-1.447665
C	-1.111618	-1.128117	-1.458253
C	-0.983423	-2.344625	-0.775063
C	-1.998883	-3.287370	-0.695305
C	-3.202824	-3.049132	-1.352760
C	-3.369074	-1.872724	-2.078911
C	-2.335350	-0.944586	-2.117915
F	0.148186	-2.639781	-0.113378
F	-1.831636	-4.409983	0.012456
F	-4.186415	-3.945318	-1.294712
F	-4.515597	-1.647309	-2.728472
F	-2.557202	0.164630	-2.841638
C	1.520235	-0.467738	-1.450415
C	2.514296	0.281587	-0.807472
C	3.840323	-0.119341	-0.724556
C	4.232357	-1.306791	-1.336806
C	3.291370	-2.071587	-2.021244
C	1.969121	-1.645569	-2.064848
F	2.206532	1.433581	-0.188136
F	1.114135	-2.423700	-2.748001
F	3.666179	-3.202650	-2.627417
F	5.502006	-1.704381	-1.275011
F	4.734378	0.617493	-0.056073

C	-0.368033	1.480400	-1.509362
C	-1.509058	1.992104	-0.877668
C	-1.823997	3.343312	-0.845115
C	-0.996199	4.251580	-1.499498
C	0.130869	3.791871	-2.175660
C	0.422393	2.432932	-2.168318
F	-2.348825	1.175035	-0.220037
F	-2.903776	3.775373	-0.184316
F	-1.285575	5.551569	-1.485876
F	0.918434	4.657146	-2.822417
F	1.518345	2.054900	-2.846022

toluene/toluene

-543.309761428

C	-1.505816	0.771527	-0.781819
C	-1.182086	-0.478984	-1.322330
C	-1.554903	-1.655295	-0.677642
C	-2.258441	-1.604022	0.527394
C	-2.585485	-0.365670	1.078092
C	-2.213300	0.810620	0.424440
H	-0.611085	-0.528510	-2.245607
H	-1.282567	-2.614664	-1.108652
H	-2.544574	-2.521692	1.033883
H	-3.131883	-0.312116	2.016101
H	-2.474186	1.773999	0.856863
C	-1.098362	2.039285	-1.490476
H	-0.036730	2.010905	-1.758945
H	-1.667288	2.179739	-2.418395
H	-1.266158	2.919740	-0.862267
C	1.506131	0.771333	0.781491
C	2.214228	0.809624	-0.424446
C	2.585894	-0.367111	-1.077606
C	2.257684	-1.605114	-0.526781
C	1.553476	-1.655572	0.677883
C	1.181238	-0.478824	1.322119
H	2.476144	1.772671	-0.857024
H	3.132808	-0.314158	-2.015349
H	2.543372	-2.523113	-1.032926
H	1.280188	-2.614627	1.108989
H	0.609820	-0.527721	2.245169
C	1.099427	2.039531	1.489797
H	1.670479	2.181252	2.416233
H	1.265065	2.919573	0.860448
H	0.038487	2.010751	1.760789

toluene/(tBu)₃P

-1086.74720390

P	-1.027929	0.031380	0.269299
C	-0.463705	-1.427108	-0.870298
C	-1.251205	1.580455	-0.869150
C	-2.774893	-0.422130	0.965428
C	-2.070730	2.653040	-0.124821
H	-2.011371	3.594175	-0.687164
H	-3.128030	2.396559	-0.036884
H	-1.673566	2.843935	0.877428
C	-1.892323	1.357323	-2.248799

H	-1.983969	2.321666	-2.768201
H	-1.290074	0.706558	-2.885410
H	-2.894190	0.927452	-2.178330
C	0.154218	2.197687	-1.050728
H	0.065870	3.129351	-1.626205
H	0.597563	2.441695	-0.081245
H	0.851794	1.549060	-1.577721
C	-3.026298	0.511478	2.171812
H	-3.153152	1.556186	1.889906
H	-3.944976	0.196882	2.685123
H	-2.201833	0.454386	2.890150
C	-2.726174	-1.846244	1.554659
H	-3.640186	-2.018249	2.138078
H	-2.683395	-2.620812	0.786830
H	-1.874240	-1.978081	2.229657
C	-3.969981	-0.341277	0.000959
H	-4.883800	-0.655812	0.524691
H	-4.142875	0.673547	-0.363410
H	-3.846786	-0.995361	-0.865081
C	-1.527200	-2.056311	-1.784856
H	-1.059190	-2.837382	-2.400246
H	-2.332403	-2.532482	-1.220562
H	-1.976559	-1.327658	-2.463126
C	0.120136	-2.516798	0.057881
H	-0.626380	-2.983707	0.699698
H	0.563810	-3.309627	-0.559515
H	0.911024	-2.104671	0.690219
C	0.722070	-0.960601	-1.739501
H	0.424205	-0.277263	-2.537191
H	1.502544	-0.484800	-1.141391
H	1.170889	-1.840085	-2.219315
C	2.957395	0.702139	1.212240
C	3.481319	1.300312	0.060368
C	4.192786	0.552699	-0.879955
C	4.397081	-0.812572	-0.680533
C	3.885910	-1.421316	0.467135
C	3.175115	-0.669397	1.401623
H	3.327293	2.363999	-0.102660
H	4.588397	1.039403	-1.767409
H	4.949841	-1.396845	-1.410674
H	4.038708	-2.484116	0.634184
H	2.779152	-1.150682	2.292775
C	2.149393	1.493508	2.208880
H	2.294876	2.570737	2.077683
H	1.081037	1.275054	2.082727
H	2.421424	1.236964	3.239045

toluene/B(C₆F₅)₃

-2480.67625992

B	-0.192228	0.070387	-0.708275
C	1.345484	-0.080360	-0.910769
C	2.264906	0.842088	-0.382306
C	3.640097	0.653279	-0.428363
C	4.155362	-0.464928	-1.074799
C	3.288939	-1.382388	-1.666454
C	1.919515	-1.177556	-1.576083
F	1.849760	1.957775	0.230164

F	4.467670	1.534940	0.143996
F	5.471709	-0.655085	-1.136582
F	3.783774	-2.443245	-2.312268
F	1.140559	-2.086796	-2.181500
C	-0.826817	1.487691	-0.499408
C	-1.814875	1.727084	0.461347
C	-2.362366	2.983417	0.687955
C	-1.947811	4.056642	-0.097154
C	-0.982376	3.863053	-1.082859
C	-0.440208	2.596449	-1.260123
F	-2.260237	0.726465	1.245820
F	0.489989	2.458169	-2.219168
F	-0.587766	4.891373	-1.840420
F	-2.471788	5.266516	0.096139
F	-3.282932	3.168043	1.640262
C	-1.142615	-1.173622	-0.667752
C	-0.775601	-2.399853	-0.097203
C	-1.655686	-3.463193	0.052440
C	-2.958685	-3.344931	-0.421651
C	-3.363992	-2.160285	-1.032340
C	-2.464914	-1.105875	-1.134153
F	0.461012	-2.587270	0.386606
F	-1.263738	-4.584506	0.668394
F	-3.812518	-4.358933	-0.295386
F	-4.609436	-2.046760	-1.504233
F	-2.917170	0.009306	-1.730497
C	0.414035	-0.944287	3.038910
C	1.689508	-1.494054	2.865331
C	2.817675	-0.677651	2.782263
C	2.690036	0.708291	2.876909
C	1.422981	1.269242	3.045563
C	0.297183	0.450923	3.120726
H	1.797133	-2.572333	2.786900
H	3.797940	-1.125393	2.641302
H	3.564593	1.346100	2.792320
H	1.310254	2.348073	3.102533
H	-0.686807	0.894003	3.245486
C	-0.805109	-1.824903	3.169591
H	-0.621274	-2.826752	2.771143
H	-1.097717	-1.937591	4.221338
H	-1.660979	-1.393602	2.640697

[C_{10min}][NTf₂]

-2487.04611366

N	3.672586	2.176459	-1.186281
C	2.344725	2.264728	-1.046544
N	2.077408	2.932227	0.080122
C	3.276083	3.272937	0.685395
C	4.275449	2.797971	-0.106411
C	4.346698	1.334853	-2.178523
H	1.633336	1.793390	-1.707042
C	0.749087	3.058555	0.716331
H	3.304411	3.782998	1.634107
H	5.346059	2.813494	0.014749
H	4.681969	0.422331	-1.680820
H	3.629004	1.073633	-2.955475
H	5.187721	1.882857	-2.607544

C	-0.367212	2.453698	-0.126645
H	0.831821	2.519415	1.663332
H	0.577623	4.121350	0.916672
C	-1.696731	2.433765	0.633647
H	-0.480310	3.008982	-1.067543
H	-0.096313	1.423190	-0.371038
C	-2.784023	1.683951	-0.142466
H	-2.030873	3.458155	0.852526
H	-1.544001	1.939977	1.603126
C	-4.110977	1.591200	0.614933
H	-2.420879	0.672932	-0.371269
H	-2.948527	2.176659	-1.111692
C	-5.187190	0.812806	-0.147287
H	-4.479942	2.603714	0.835673
H	-3.938070	1.110772	1.588848
C	-6.511347	0.704260	0.614171
H	-4.812299	-0.196285	-0.371205
H	-5.364664	1.293637	-1.120365
C	-7.585574	-0.082491	-0.142092
H	-6.888104	1.713799	0.835396
H	-6.330877	0.227473	1.588698
C	-8.909054	-0.194315	0.621077
H	-7.208322	-1.091610	-0.363744
H	-7.767959	0.393726	-1.116768
C	-9.975235	-0.984555	-0.141417
H	-9.285673	0.814604	0.841087
H	-8.724995	-0.669294	1.594915
H	-10.910925	-1.048692	0.425282
H	-9.636746	-2.007784	-0.344974
H	-10.200107	-0.513610	-1.106195
N	1.462968	-0.341502	0.003290
S	2.616555	-0.366440	1.133067
S	1.581659	-1.064051	-1.440851
O	2.216254	0.602936	2.162442
O	1.225929	-0.079629	-2.486664
C	2.459788	-2.030794	1.965177
C	0.096976	-2.187635	-1.347705
F	3.324931	-2.096119	2.981768
F	1.218599	-2.183716	2.435509
F	2.722282	-3.011418	1.099995
F	0.228161	-3.028813	-0.319333
F	0.000666	-2.886750	-2.480749
F	-1.019767	-1.466713	-1.184158
O	3.989161	-0.313837	0.609018
O	2.745264	-1.923731	-1.669954

[C₁₀min]/B(C₆F₅)₃
-2868.28964827

N	-3.196160	-2.184073	2.567930
C	-1.906646	-1.941419	2.307868
N	-1.582573	-0.748879	2.820333
C	-2.707136	-0.210647	3.420125
C	-3.720367	-1.109569	3.262591
C	-3.945818	-3.336658	2.058443
H	-1.253314	-2.600984	1.763673
C	-0.306839	-0.033422	2.588997
H	-2.688168	0.756781	3.896094

H	-4.752519	-1.075351	3.572620
H	-4.694365	-2.973073	1.351130
H	-3.252922	-4.004553	1.546056
H	-4.426156	-3.864379	2.883720
C	0.940892	-0.900096	2.761357
H	-0.364020	0.380837	1.579638
H	-0.294062	0.809031	3.282808
C	2.114551	-0.250789	2.019758
H	1.158489	-1.030544	3.827307
H	0.778345	-1.896699	2.339828
C	3.480089	-0.891415	2.275325
H	2.168960	0.819638	2.263601
H	1.897175	-0.311177	0.947539
C	4.528331	-0.338673	1.304589
H	3.409041	-1.981906	2.159829
H	3.791225	-0.708392	3.312327
C	5.953625	-0.836425	1.543953
H	4.517243	0.760177	1.347622
H	4.229831	-0.607136	0.280457
C	6.946455	-0.278856	0.519298
H	5.969179	-1.935018	1.510128
H	6.275773	-0.557442	2.556941
C	8.382802	-0.760452	0.736880
H	6.920428	0.819960	0.551588
H	6.616943	-0.557937	-0.492514
C	9.375043	-0.188119	-0.279725
H	8.409681	-1.858866	0.692324
H	8.707935	-0.490558	1.752117
C	10.808271	-0.673344	-0.053120
H	9.346211	0.909396	-0.233309
H	9.049958	-0.458402	-1.294050
H	11.496862	-0.246518	-0.789931
H	10.873391	-1.765245	-0.128867
H	11.167984	-0.389344	0.943017
B	-1.108814	0.568508	-1.174340
C	-2.198367	1.525377	-0.596503
C	-2.174966	2.916450	-0.791154
C	-3.122428	3.775994	-0.245444
C	-4.146176	3.250725	0.544545
C	-4.212122	1.875728	0.765274
C	-3.266748	1.049664	0.178755
F	-1.214190	3.465664	-1.539584
F	-3.061330	5.086223	-0.463383
F	-5.048473	4.053449	1.090469
F	-5.176946	1.358724	1.537524
F	-3.392148	-0.270930	0.448183
C	0.396336	0.930656	-1.238671
C	1.273264	0.275767	-2.123822
C	2.640047	0.525301	-2.158955
C	3.185575	1.456846	-1.275779
C	2.361182	2.122306	-0.369483
C	1.001279	1.860560	-0.375544
F	0.799749	-0.625489	-2.991869
F	0.274955	2.464064	0.586949
F	2.895701	2.936561	0.542592
F	4.491787	1.673688	-1.264282
F	3.431433	-0.120257	-3.011170

C	-1.594683	-0.883020	-1.527908
C	-2.738837	-1.108715	-2.298305
C	-3.359235	-2.350308	-2.387558
C	-2.850716	-3.414930	-1.641649
C	-1.704396	-3.229358	-0.874066
C	-1.077641	-1.991066	-0.866820
F	-3.298659	-0.082301	-2.953301
F	-4.452473	-2.520139	-3.126377
F	-3.465346	-4.593975	-1.642538
F	-1.264078	-4.217526	-0.070403
F	0.014282	-1.861393	-0.072515

(*t*Bu)₃P/[NTf₂]

-2642.74189040

P	-2.541284	0.132310	-0.109326
C	-4.391861	0.605187	-0.460212
C	-2.424124	-0.314185	1.769297
C	-2.172376	-1.484475	-1.106513
C	-1.135433	-1.116513	2.031545
H	-0.983720	-1.177578	3.118144
H	-1.181997	-2.141427	1.659723
H	-0.253281	-0.634794	1.607571
C	-3.604479	-1.083409	2.385457
H	-3.383942	-1.293306	3.442143
H	-4.541654	-0.521536	2.358845
H	-3.772338	-2.043856	1.890333
C	-2.220957	1.027017	2.512826
H	-2.079036	0.820924	3.583054
H	-1.323954	1.538580	2.150775
H	-3.068502	1.708275	2.421380
C	-0.633025	-1.616803	-1.161583
H	-0.174242	-1.845391	-0.202535
H	-0.369870	-2.431221	-1.851506
H	-0.168612	-0.698530	-1.528927
C	-2.623758	-1.289904	-2.566999
H	-2.217584	-2.111552	-3.172562
H	-3.710045	-1.307640	-2.685788
H	-2.240947	-0.353110	-2.985260
C	-2.783524	-2.795577	-0.586101
H	-2.492396	-3.622884	-1.250164
H	-2.425897	-3.046134	0.413881
H	-3.876261	-2.763957	-0.558792
C	-5.433149	-0.524863	-0.495027
H	-6.435668	-0.101929	-0.662573
H	-5.243401	-1.232120	-1.305864
H	-5.464305	-1.087039	0.440737
C	-4.409683	1.349048	-1.815991
H	-4.187606	0.701968	-2.664283
H	-5.408754	1.777819	-1.982474
H	-3.682943	2.167850	-1.819719
C	-4.842736	1.655543	0.575095
H	-4.978810	1.240036	1.574832
H	-4.128528	2.482634	0.642066
H	-5.809310	2.074297	0.260349
N	1.714272	0.117166	0.767417
S	2.758176	-1.092084	0.956155
S	2.095686	1.685460	0.709190

O	1.967370	-2.309429	1.180664
O	1.168112	2.449411	1.553460
C	3.488744	-1.363573	-0.742894
C	1.542264	2.078970	-1.029962
F	4.243858	-2.476244	-0.736730
F	2.521334	-1.521825	-1.660462
F	4.259634	-0.334303	-1.113205
F	2.186051	1.311199	-1.923787
F	1.819043	3.365714	-1.305173
F	0.227455	1.889056	-1.181618
O	3.917197	-0.822488	1.812097
O	3.523494	2.025210	0.724308