Electronic Supplementary Material (ESI) for Chemical Science

Supplementry data for:

Frustrated Lewis Pair Olefin Addition Reactions: P-, N-, C- and H-Based Nucleophilic Additions to an Olefin Tethered to Boron

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DFT calculations

DFT calculations were performed using Gaussian 09.[1] Geometry optimization of the two conformers of **2** was carried out using the M06 method and 6-311++G(d,p) for C atoms on B, olefinic C, B and H atoms and 6-31G(d) basis sets for all other atoms implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis contained no imaginary frequency showing that these are energy minima. For the reaction profile leading to **11**, geometry optimization of $\mathbf{2}_{\mathbf{open}}$, $\mathbf{2}_{\mathbf{closed}}$, $B(C_6F_5)_3$, $\mathbf{2}$-hyride anion, **11** anion, $HB(C_6F_5)_3$ anion, and $\mathbf{2}_{\mathbf{closed}}\cdots HB(C_6F_5)_3$ anion‡ was conducted at the B3LYP/6-31G(d) level of theory. Frequency analysis of $\mathbf{2}_{\mathbf{open}}$, $\mathbf{2}_{\mathbf{closed}}$, $B(C_6F_5)_3$, $\mathbf{2}$-hyride anion, **11** anion and $HB(C_6F_5)_3$ anion contained no imaginary frequency showing that these are energy minima while that of $\mathbf{2}_{\mathbf{closed}}\cdots HB(C_6F_5)_3$ anion‡ gave one imaginary frequency confirming that it is a first-order saddle point.

Coordinates of optimized structure of $\mathbf{2}_{\mathbf{open}}$ (gas phase)

M06/6-311++G(d,p) (for B, C's on B, olefinic C and H) and 6-31G(d) (for all other atoms)

F	1.58171	-1.97882	-1.73482
F	4.22383	-2.47751	-1.73788
F	5.87349	-1.03586	-0.14198
F	4.87067	0.89484	1.46878
F	2.23353	1.37676	1.51009
F	-1.32985	-1.15396	-2.23846
F	-2.97533	-3.27551	-1.89534
F	-3.205	-4.41933	0.54958
F	-1.77973	-3.46164	2.6474
F	-0.11973	-1.34186	2.28489
F	-0.7146	3.29373	-1.96626
F	-1.89986	1.51429	-2.10337
F	-2.74747	3.30435	-1.23567
F	-2.96862	0.57012	0.16122
F	-3.15259	2.36967	1.3132
F	-1.7509	0.85173	1.9218
O	-0.0378	1.33044	-0.13158
C	1.81994	-0.26368	-0.14037
C	2.36808	-1.26147	-0.93327
C	3.72852	-1.53312	-0.95417

C	4.57708	-0.79101	-0.14054
C	4.06072	0.20516	0.6804
C	2.69558	0.44995	0.66843
C	-0.71678	-1.18617	0.02426
C	-1.44154	-1.70408	-1.03124
C	-2.28729	-2.79223	-0.87288
C	-2.4045	-3.3819	0.38152
C	-1.6721	-2.89138	1.45765
C	-0.83142	-1.80815	1.25306
C	-1.1484	2.15674	0.05953
C	-0.68181	3.37839	0.87517
C	0.58285	4.01664	0.40842
C	0.72078	5.31955	0.23463
C	-1.63867	2.57206	-1.34087
C	-2.28251	1.47099	0.8634
B	0.27817	0.01828	-0.10724
H	-1.49167	4.11825	0.90665
H	-0.53511	3.0144	1.90426
H	1.43013	3.3525	0.26555
H	-0.10929	6.00675	0.37855
H	1.6702	5.75663	-0.05308

Coordinates of optimized structure of 2_{closed} (gas phase)

M06/6-311++G(d,p) (for B, C's on B, olefinic C and H) and 6-31G(d) (for all other atoms)

F	-0.04879	0.88189	-2.29415
F	-1.21746	3.23229	-2.98391
F	-2.36558	4.76896	-1.0592
F	-2.32971	3.9612	1.52376
F	-1.17219	1.64313	2.20249
F	1.89825	-1.7562	-1.5721
F	4.57551	-1.58583	-1.68152
F	5.89115	0.17056	-0.10074
F	4.51574	1.77008	1.60416
F	1.8311	1.60621	1.7247
F	-3.02883	-0.28777	0.75599
F	-2.52561	-0.69438	-1.29875
F	-3.78916	-2.05374	-0.19923
F	-1.40589	-3.14261	-1.75713
F	-2.31476	-4.24111	-0.13339
F	-0.18624	-3.94767	-0.17567
O	-0.28899	-1.40907	0.13757
C	-0.58786	1.18963	-0.03818
C	-0.61276	1.64198	-1.34728
C	-1.20531	2.83713	-1.72099
C	-1.79242	3.62363	-0.73631
C	-1.77354	3.20581	0.5888
C	-1.1687	1.99978	0.91801
C	1.77794	-0.09465	0.09879
C	2.51291	-0.90188	-0.76039

C	3.89642	-0.81866	-0.84367
C	4.57499	0.08815	-0.03735
C	3.86835	0.91018	0.83303
C	2.48626	0.80857	0.87605
C	-1.49085	-2.06068	0.3642
C	-1.60566	-2.42589	1.86229
H	-2.61828	-2.80772	2.04732
H	-0.90478	-3.25291	2.03468
C	-1.26492	-1.29654	2.77438
H	-2.05924	-0.60567	3.03985
C	-0.04515	-1.09974	3.2512
H	0.77467	-1.7732	3.00942
H	0.17842	-0.26363	3.90473
C	-2.72435	-1.26041	-0.112
C	-1.35475	-3.37339	-0.44927
B	0.20995	-0.1575	0.14759

Coordinates of optimized structure of 2_{open} (gas phase)

B3LYP/6-31G(d)

F	1.58844900	-2.24976500	-1.35630000
F	4.21198900	-2.77616400	-1.35519700
F	5.94597800	-1.12496900	-0.04764300
F	5.01124300	1.07165900	1.26920800
F	2.39578900	1.62342400	1.29272000
F	-1.05207500	-1.18609200	-2.28492000
F	-2.79688700	-3.25907800	-2.12357700
F	-3.36496900	-4.37193900	0.30055100
F	-2.18023800	-3.40854900	2.56423200
F	-0.44372200	-1.32325400	2.39584800
F	-0.74754800	2.80163000	-2.17853800
F	-2.18431500	1.22367000	-1.83037200
F	-2.69270900	3.27548700	-1.31135500
F	-2.91080500	0.61986800	0.58140500
F	-3.07521200	2.62070700	1.38494900
F	-1.60703500	1.23562600	2.20759800
O	0.01198400	1.33925000	0.00301900
C	1.86077500	-0.28767600	-0.03344000
C	2.39259300	-1.40965700	-0.68532400
C	3.75302100	-1.70221200	-0.70542500
C	4.64059800	-0.85874200	-0.04226500
C	4.16060500	0.26620700	0.62489400
C	2.79552800	0.53439100	0.61460200
C	-0.72658400	-1.17605600	0.05505400
C	-1.33847900	-1.70456300	-1.07824600
C	-2.22635200	-2.77376400	-1.01572600
C	-2.51373500	-3.34665600	0.22234100
C	-1.90879300	-2.85469200	1.37730300
C	-1.02438500	-1.78586800	1.27098500
C	-1.11336600	2.19179500	0.09308000

C	-0.60680600	3.54406800	0.67105500
C	0.57836100	4.15275000	-0.02994100
C	0.59635800	5.40222700	-0.49221400
C	-1.69345500	2.37253200	-1.33329900
C	-2.19985400	1.64848800	1.07040400
B	0.31295400	0.01468800	-0.00590300
H	-1.44156000	4.24794900	0.68831500
H	-0.33603700	3.32975700	1.71280300
H	1.46689500	3.53128300	-0.09551900
H	-0.27403000	6.05249000	-0.43161800
H	1.48649400	5.82532400	-0.94912200

Coordinates of optimized structure of 2_{closed} (gas phase)

B3LYP/6-31G(d)

F	-0.39496400	0.58054700	-2.32499900
F	-1.51953000	3.00418300	-3.07201300
F	-2.12661400	4.85418700	-1.12893100
F	-1.64029300	4.29451500	1.51110800
F	-0.57923500	1.92146100	2.24671300
F	1.77350400	-1.98257000	-1.62676600
F	4.49704800	-1.94898000	-1.80254500
F	5.95050100	-0.19449500	-0.27947400
F	4.68882800	1.53512400	1.43612800
F	1.95166500	1.50632700	1.63245200
F	-2.93102400	0.05445500	0.81662900
F	-2.64157700	-0.61043400	-1.27786100
F	-3.96706400	-1.76077000	0.09327100
F	-2.05772200	-3.26428000	-1.49625700
F	-2.78133700	-4.00175600	0.47239100
F	-0.61699000	-4.02005000	0.02186700
O	-0.36566100	-1.45005700	-0.00019200
C	-0.48255800	1.18998200	-0.04477900
C	-0.73761400	1.51067500	-1.37344100
C	-1.28313700	2.72183600	-1.76169800
C	-1.58638600	3.65535900	-0.77916300
C	-1.33859300	3.37103300	0.55557800
C	-0.78339500	2.14674000	0.91075900
C	1.80426100	-0.23478800	0.00603400
C	2.47132600	-1.11077400	-0.84662500
C	3.85664800	-1.09761300	-0.95400200
C	4.59363300	-0.20621600	-0.18682900
C	3.95543100	0.67306700	0.67829000
C	2.57189200	0.65130500	0.75529400
C	-1.63337600	-1.92413300	0.45054600
C	-1.61016600	-2.08011500	1.99616300
H	-2.62953400	-2.29432100	2.32565400
H	-0.97980900	-2.95094400	2.19605100
C	-1.01982400	-0.85908400	2.64057800
H	-1.66002800	0.00430900	2.74708100

C	0.27542500	-0.76828500	2.95735400
H	0.94743100	-1.61555300	2.85220200
H	0.69973800	0.16277400	3.31033300
C	-2.79933800	-1.05030900	0.00542200
C	-1.77377100	-3.31922400	-0.16345100
B	0.24358800	-0.20594100	0.09972700

Coordinates of optimized structure of $B(C_6F_5)_3$ (gas phase)

B3LYP/6-31G(d)

B	-0.00022	-0.00042	0.00053
C	0.88043	-1.29889	0.00016
C	0.51714	-2.4526	0.71261
C	2.08653	-1.38799	-0.71248
C	1.28918	-3.60837	0.73222
C	2.87448	-2.53296	-0.73314
C	2.47353	-3.64838	-0.00071
C	0.68421	1.41148	0.00034
C	0.16019	2.49994	-0.71462
C	1.86343	1.67421	0.71507
C	0.75821	3.75461	-0.73517
C	2.47855	2.9206	0.73502
C	1.92311	3.96565	-0.00036
C	-1.56509	-0.11315	0.00041
C	-2.38196	0.77804	0.71383
C	-2.24595	-1.11202	-0.71323
C	-3.76896	0.68799	0.73394
C	-3.63155	-1.22121	-0.73342
C	-4.39649	-0.31674	0.00029
F	-0.95403	2.35206	-1.45016
F	0.22965	4.75432	-1.44777
F	2.50448	5.16368	-0.0009
F	3.59131	3.12448	1.44691
F	2.43735	0.70791	1.45076
F	2.51674	-0.34794	-1.44559
F	4.00588	-2.57397	-1.44368
F	3.22077	-4.75057	-0.00098
F	0.90874	-4.67506	1.44219
F	-0.60774	-2.4675	1.44656
F	-1.56097	-2.00447	-1.44712
F	-1.83158	1.75903	1.44805
F	-4.50174	1.55065	1.44486
F	-5.72466	-0.41256	0.00019
F	-4.23341	-2.17998	-1.44415

Coordinates of optimized structure of 2·hydride anion (gas phase)

B3LYP/6-31G(d)

F	-1.76728900	1.28091600	-2.37276500
F	-4.43151200	1.54251200	-2.27108900
F	-5.84042300	0.54725300	-0.14029200
F	-4.50493700	-0.71645200	1.88700100
F	-1.86220900	-0.98451000	1.82117800
F	1.61615900	1.78254900	-2.22354300
F	2.75456600	4.09173200	-1.49569200
F	2.48075000	5.03148400	1.05682900
F	1.02034200	3.60580500	2.88147800
F	-0.14737300	1.29130000	2.16872800
F	-0.31772700	-3.12613200	-1.19761100
F	1.37192100	-2.34715400	-2.31947600
F	1.60138800	-4.15031600	-1.14858100
F	2.90898500	-0.59877400	-1.06263300
F	3.72722700	-2.49419600	-0.37925000
F	3.25697100	-0.91879100	1.05049000
O	0.49076800	-1.11205700	0.42256300
C	-1.66017100	0.10660100	-0.30372300
C	-2.39764100	0.75513200	-1.29880000
C	-3.78150800	0.91161000	-1.27120400
C	-4.50072000	0.40933600	-0.19269400
C	-3.81727600	-0.23365900	0.83137500
C	-2.42883800	-0.36227300	0.76331900
C	0.67460000	1.41224300	-0.06119400
C	1.42773400	2.18078700	-0.94936800
C	2.03466100	3.38732300	-0.59770000
C	1.90029900	3.86932500	0.69866500
C	1.15896800	3.14037300	1.62248900
C	0.56880700	1.94228900	1.22565500
C	1.39681600	-2.09571100	0.11410500
C	1.45546400	-3.05285400	1.34512300
C	0.14363500	-3.71439000	1.66450800
C	-0.00369200	-5.02388200	1.86967100
C	1.00999000	-2.92450600	-1.15600500
C	2.82843000	-1.51401200	-0.08425600
B	-0.02400200	-0.02675000	-0.48185300
H	2.24511200	-3.79831100	1.21625100
H	1.73527900	-2.40205400	2.18136500
H	-0.70679900	-3.04330200	1.75004800
H	0.83100000	-5.71786900	1.78244300
H	-0.96795300	-5.45520000	2.12804300
H	0.19832200	-0.25048500	-1.64213000

Coordinates of optimized structure of the anion of 11 (gas phase)

B3LYP/6-31G(d)

F	2.32425000	1.42970600	1.66442000
F	4.93651100	1.10340200	1.18836200
F	5.81397800	-0.97955800	-0.36682500
F	3.99589400	-2.72354100	-1.42977100

F	1.40067200	-2.43803500	-0.97632300
F	-0.82745500	2.33882200	2.30375500
F	-1.40031400	4.69465200	1.22230900
F	-1.18855700	5.08867100	-1.48057900
F	-0.36035300	3.02834300	-3.08281300
F	0.24288200	0.64815100	-2.02531700
F	-0.90863700	-3.83839100	0.14150300
F	-1.94798500	-3.09785200	-1.61478000
F	-3.07984300	-3.81848300	0.09586600
F	-2.94109900	-0.61973900	-1.55325300
F	-4.31217100	-1.46549500	-0.09187500
F	-3.20455200	0.34647100	0.36874900
O	-0.74133900	-1.15149500	-0.04760500
C	1.70048700	-0.46997000	0.36386100
C	2.68129600	0.38186600	0.88044400
C	4.04781300	0.23961200	0.65477000
C	4.49712700	-0.81381900	-0.13251000
C	3.56775100	-1.69555000	-0.66822300
C	2.20513000	-1.51547400	-0.41582600
C	-0.26541100	1.34173900	0.19789000
C	-0.68246300	2.43269200	0.95884800
C	-0.99557900	3.68350200	0.42522700
C	-0.89091700	3.88935800	-0.94367900
C	-0.47444500	2.83830100	-1.75258700
C	-0.17390700	1.60759200	-1.17298100
C	-1.93903400	-1.69786300	0.36116000
C	-2.13780400	-1.85527600	1.89406700
H	-3.20107000	-2.02073600	2.10082500
H	-1.61009100	-2.76803800	2.19312000
C	-1.56977100	-0.68674400	2.71060500
H	-1.69391800	-0.93082800	3.77721700
H	-2.15183800	0.22246100	2.53323000
C	-0.09620300	-0.45838700	2.34875200
H	0.45999200	-1.37139000	2.61924900
H	0.32661500	0.34674100	2.95627100
C	-1.97134700	-3.11988900	-0.27028100
C	-3.10422100	-0.85742600	-0.24125500
B	0.10420000	-0.20118900	0.74808100

Coordinates of optimized structure of $HB(C_6F_5)_3$ anion (gas phase)

B3LYP/6-31G(d)

B	-0.02322	-0.06778	-0.86514
C	0.05728	1.49241	-0.34064
C	-1.44319	-0.79833	-0.47681
C	1.32987	-0.86096	-0.37666
C	0.85949	2.41175	-1.02278
C	0.98753	3.75142	-0.66107
C	0.29306	4.22892	0.44455
C	-0.51172	3.35493	1.165

C	-0.60611	2.02162	0.76753
C	-2.63538	-0.24342	-0.95572
C	-3.89653	-0.79378	-0.7503
C	-4.01402	-1.97488	-0.02514
C	-2.8646	-2.572	0.47355
C	-1.62102	-1.97982	0.24416
C	2.16935	-1.52308	-1.27406
C	3.35951	-2.1489	-0.89912
C	3.754	-2.13008	0.43239
C	2.94978	-1.48849	1.36891
C	1.77139	-0.87916	0.94812
F	1.57472	2.02208	-2.10063
F	1.77621	4.5895	-1.36527
F	0.40182	5.52021	0.81396
F	-1.18489	3.80579	2.24318
F	-1.40129	1.24082	1.53131
F	-2.60073	0.90402	-1.67028
F	-5.00333	-0.20114	-1.24333
F	-5.22342	-2.53009	0.18686
F	-2.96185	-3.71826	1.17773
F	-0.56682	-2.64539	0.77127
F	1.86192	-1.59808	-2.58629
F	4.13204	-2.77262	-1.81258
F	4.89934	-2.72847	0.81351
F	3.32107	-1.47096	2.66533
F	1.02931	-0.28917	1.91165
H	-0.0031	-0.02444	-2.07349

Coordinates of optimized structure of 2_{closed}···HB(C_6F_5)$_3$ anion‡ (gas phase)

B3LYP/6-31G(d)

F	3.18865	0.79269	-2.53282
F	4.7025	2.83168	-3.38046
F	5.9569	4.46564	-1.57531
F	5.65752	4.00285	1.09941
F	4.16517	1.99497	1.97753
F	1.48702	-1.7366	-2.08317
F	2.65636	-3.88595	-3.13133
F	5.06522	-4.76936	-2.18654
F	6.29716	-3.41719	-0.1507
F	5.15428	-1.23576	0.90842
F	1.69531	1.30144	3.67943
F	2.83977	-0.37695	4.45558
F	0.66673	-0.38429	4.58149
F	3.15081	-2.52318	2.7878
F	1.11795	-2.7647	3.52799
F	1.51813	-2.8742	1.39724
O	2.62781	-0.10677	1.66024
C	3.6028	1.26572	-0.23541

C	3.79163	1.55472	-1.59128
C	4.56594	2.60982	-2.06304
C	5.20255	3.44237	-1.14864
C	5.04516	3.20303	0.21091
C	4.25519	2.13702	0.64618
C	3.25345	-1.37997	-0.51248
C	2.67883	-2.10084	-1.55916
C	3.2627	-3.23182	-2.12834
C	4.48732	-3.68362	-1.65126
C	5.1086	-2.99596	-0.61442
C	4.4891	-1.87142	-0.07638
C	1.6349	-0.70031	2.40085
C	0.1896	-0.44155	1.82277
H	-0.50801	-1.17447	2.22603
H	-0.11394	0.55649	2.14397
C	0.25649	-0.48642	0.3361
H	0.08745	-1.43516	-0.15654
C	0.9913	0.49882	-0.32767
H	0.94951	1.4946	0.10884
H	1.0048	0.47661	-1.41221
C	1.71497	-0.03522	3.80453
C	1.86657	-2.23361	2.53757
B	2.70022	-0.01792	0.21768
B	-2.71409	0.19366	-0.29362
C	-3.50971	0.21814	1.13855
C	-2.44413	1.66179	-0.9547
C	-3.39567	-0.91425	-1.28398
C	-3.41134	-0.87184	2.00618
C	-4.34825	1.23873	1.59288
C	-1.75236	2.63317	-0.22446
C	-2.79841	2.06915	-2.24383
C	-2.6829	-1.91569	-1.94141
C	-4.77381	-0.93927	-1.51396
C	-4.05465	-0.95514	3.23809
F	-2.63635	-1.93414	1.66847
C	-5.01483	1.2011	2.81659
F	-4.56533	2.33776	0.84158
C	-1.43014	3.89885	-0.70092
F	-1.34845	2.36004	1.0428
C	-2.49982	3.32837	-2.76655
F	-3.47093	1.24692	-3.0771
C	-3.27533	-2.88619	-2.74938
F	-1.33575	-1.99309	-1.82976
C	-5.41053	-1.88446	-2.31207
F	-5.56446	0.0057	-0.95949
C	-4.86914	0.09518	3.64649
F	-3.9049	-2.03389	4.02657
F	-5.80792	2.21766	3.19895
C	-1.81155	4.25255	-1.99107
F	-0.75662	4.77552	0.06378
F	-2.87506	3.65644	-4.01525
C	-4.65219	-2.87127	-2.93441

F	-2.53141	-3.83049	-3.35088
F	-6.74312	-1.85345	-2.49403
F	-5.50672	0.0425	4.8273
F	-1.51498	5.46737	-2.47941
F	-5.2449	-3.79525	-3.70879
H	-1.55975	-0.21657	-0.01316

Geometry optimization and frequency analysis of **2**$_{\mathbf{closed}}$, $B(C_6F_5)_3$, **11** anion, $HB(C_6F_5)_3$ anion, and **2**$_{\mathbf{closed}}$$\cdots HB(C_6F_5)_3$ anion[‡] were also performed at the B3LYP/6-31G(d) level of theory with IEF-PCM model for bromobenzene.

Coordinates of optimized structure of 2$_{\mathbf{closed}}$ (with IEF-PCM model for bromobenzene)

B3LYP/6-31G(d)

F	0.43247100	-0.99112000	-2.43627400
F	2.08398500	-3.09666200	-2.90135000
F	3.28980800	-4.36425100	-0.80317700
F	2.83398600	-3.51891000	1.75130100
F	1.18656800	-1.41905600	2.20877600
F	-2.27457200	1.76795100	-1.12287300
F	-4.90357700	1.25283900	-1.20733600
F	-5.89664000	-1.02043800	-0.07825400
F	-4.21803200	-2.78649400	1.15072200
F	-1.58249100	-2.29240400	1.25656900
F	2.97084100	0.74693500	0.51560500
F	2.23246100	1.14889400	-1.48971000
F	3.34912000	2.67091800	-0.40988400
F	0.45831500	3.08597600	-1.83398400
F	1.46994400	4.48860700	-0.50955700
F	-0.57325700	3.88029300	-0.09717400
O	0.04639600	1.35712600	0.30490100
C	0.76887300	-1.13547200	-0.10303000
C	1.01948900	-1.60469000	-1.38981900
C	1.86124100	-2.68154100	-1.64815500
C	2.47743400	-3.32745700	-0.57932200
C	2.24540800	-2.89316300	0.72389100
C	1.39940100	-1.81027800	0.93816300
C	-1.80692900	-0.23904600	0.07479300
C	-2.71057100	0.64310100	-0.53502700
C	-4.07737400	0.39214500	-0.60035400
C	-4.58706700	-0.77121700	-0.02976000
C	-3.72810500	-1.67327200	0.59174700
C	-2.36547300	-1.39767800	0.62790300
C	1.12205900	2.26305700	0.32819500
C	1.34240100	2.78216700	1.77766700
H	2.24697200	3.40087900	1.76693300

H	0.50070700	3.44136900	2.00508300
C	1.43207500	1.71632400	2.83804000
H	2.28571800	1.04598200	2.80069200
C	0.53358300	1.58436600	3.81457700
H	-0.33415200	2.23638300	3.89086100
H	0.63801500	0.82022200	4.57975300
C	2.43332900	1.69491200	-0.27752600
C	0.61522100	3.45073100	-0.55096600
B	-0.25775200	0.05250700	0.11414900

Coordinates of optimized structure of $B(C_6F_5)_3$ (with IEF-PCM model for bromobenzene)

B3LYP/6-31G(d)

B	0.00058400	-0.00045200	0.00097800
C	-0.90968600	-1.27869500	0.00152000
C	-2.11786900	-1.34005800	0.71312800
C	-0.57411300	-2.44050400	-0.71081400
C	-2.93281900	-2.46546200	0.73148200
C	-1.37378600	-3.57682500	-0.73180700
C	-2.55899600	-3.58933700	-0.00086800
C	1.56278100	-0.14956300	0.00040200
C	2.40027100	0.72091300	-0.71420400
C	2.22101200	-1.16278100	0.71440800
C	3.78433800	0.59826900	-0.73433900
C	3.60331400	-1.30363200	0.73419300
C	4.38896500	-0.41880000	0.00000900
C	-0.65136600	1.42701400	0.00016600
C	-0.10301800	2.50365700	0.71425200
C	-1.82379800	1.71715700	-0.71452100
C	-0.67210200	3.77130400	0.73404500
C	-2.40970700	2.97703400	-0.73445600
C	-1.83107700	4.00928900	-0.00039500
F	1.87422100	1.71537500	-1.44912400
F	4.53717800	1.44430500	-1.44705000
F	5.71560000	-0.54499800	0.00021500
F	4.18301100	-2.27660000	1.44674800
F	1.51658400	-2.04041800	1.44879700
F	0.55150300	-2.48380100	-1.44351700
F	-1.01757700	-4.65291600	-1.44281600
F	-3.33366300	-4.67360800	-0.00242800
F	-4.06687200	-2.47927600	1.44152400
F	-2.52556900	-0.29076900	1.44694400
F	-2.42165400	0.76424800	-1.44951000
F	1.00880100	2.33224200	1.44928400
F	-0.11954400	4.75982400	1.44676100
F	-2.38513600	5.22130300	-0.00061800
F	-3.51877000	3.20602100	-1.44722200

Coordinates of optimized structure of 11 anion (with IEF-PCM model for bromobenzene)

B3LYP/6-31G(d)

F	2.30160300	1.48726800	1.62357600
F	4.91423600	1.20318900	1.14605500
F	5.83122000	-0.89567500	-0.36513900
F	4.04425100	-2.69873100	-1.38360900
F	1.44834700	-2.45687800	-0.93147200
F	-0.86681100	2.31528500	2.30741900
F	-1.47835200	4.66139000	1.23550100
F	-1.27262100	5.07129200	-1.46582400
F	-0.40999600	3.02927000	-3.07523400
F	0.23234600	0.65930600	-2.02998400
F	-0.86803900	-3.85604400	0.14322200
F	-1.89075800	-3.11583700	-1.62228200
F	-3.03839500	-3.85122300	0.07167600
F	-2.91899400	-0.64765700	-1.55534400
F	-4.28741000	-1.51092100	-0.10246800
F	-3.19800700	0.30886700	0.36885200
O	-0.72033500	-1.16799700	-0.05295400
C	1.71013800	-0.44874000	0.36079600
C	2.67671900	0.43034700	0.85810900
C	4.04486300	0.31020800	0.63301200
C	4.51435100	-0.75084500	-0.13179800
C	3.60100000	-1.66183100	-0.64502100
C	2.23655000	-1.50125100	-0.39357300
C	-0.28599200	1.33405000	0.19852500
C	-0.72267200	2.41571600	0.96182300
C	-1.05700900	3.66286000	0.43344200
C	-0.95564500	3.87720600	-0.93436600
C	-0.52110500	2.83603300	-1.74608300
C	-0.20030800	1.60942800	-1.16998500
C	-1.91570400	-1.72466500	0.35850300
C	-2.11320500	-1.88614500	1.89062300
H	-3.17470700	-2.05977900	2.09801600
H	-1.57975200	-2.79493400	2.19057500
C	-1.55622300	-0.71408500	2.70925800
H	-1.67456500	-0.96413300	3.77407600
H	-2.14937000	0.18871200	2.53641400
C	-0.08611500	-0.46765200	2.34393400
H	0.48053900	-1.37491600	2.61226300
H	0.32978100	0.34042800	2.95315000
C	-1.93356300	-3.14446300	-0.27588600
C	-3.08663200	-0.89290200	-0.24277800
B	0.11009400	-0.20342400	0.74468500

Coordinates of optimized structure of $HB(C_6F_5)_3$ anion (with IEF-PCM model for bromobenzene)

B3LYP/6-31G(d)

B	-0.01986800	-0.07025500	-0.86482200
C	0.04337500	1.48983900	-0.33874400
C	-1.43426200	-0.81264800	-0.47926400
C	1.34045400	-0.85140500	-0.37996400
C	0.82502100	2.42468000	-1.02263900
C	0.93797800	3.76414100	-0.65715400
C	0.24773900	4.22720000	0.45700900
C	-0.53689100	3.33785700	1.18083500
C	-0.61547300	2.00568900	0.77809600
C	-2.62769400	-0.27612800	-0.97424200
C	-3.88572100	-0.83266200	-0.76971900
C	-3.99917700	-2.00267300	-0.02637400
C	-2.84842600	-2.58146000	0.49039700
C	-1.60865100	-1.98300000	0.26000900
C	2.18727900	-1.50156900	-1.27841500
C	3.38421400	-2.11591000	-0.90827800
C	3.77997500	-2.09750800	0.42272700
C	2.96917000	-1.46738500	1.36143600
C	1.78466500	-0.86948200	0.94354700
F	1.53589900	2.04966300	-2.11150800
F	1.70697800	4.61355900	-1.36626000
F	0.34096500	5.51579000	0.83048300
F	-1.20625800	3.77093000	2.26711000
F	-1.39157300	1.20923300	1.54840700
F	-2.59655600	0.86256000	-1.70686600
F	-4.99093800	-0.25584200	-1.28037300
F	-5.20322700	-2.56280200	0.18629100
F	-2.93910100	-3.71506600	1.21295900
F	-0.55184000	-2.63001200	0.80834900
F	1.87897700	-1.57309900	-2.59346500
F	4.15992200	-2.72619100	-1.82556900
F	4.92960300	-2.68365500	0.80050900
F	3.33871400	-1.44893200	2.65695400
F	1.03685300	-0.28931500	1.91115600
H	0.00210500	-0.02557200	-2.07505900

Coordinates of optimized structure of 2_{closed}···$HB(C_6F_5)_3$ anion‡ (with IEF-PCM model for bromobenzene)

B3LYP/6-31G(d)

F	3.16728900	0.72383400	-2.60094200
F	4.63027100	2.76226500	-3.53032200
F	5.85106900	4.49381300	-1.79399400
F	5.56871100	4.12666300	0.89859500
F	4.12741900	2.12009400	1.85776000

F	1.54934400	-1.82806300	-2.05754500
F	2.77480700	-3.98639100	-3.01237200
F	5.20177000	-4.77144300	-2.02409000
F	6.38882500	-3.30589100	-0.03862500
F	5.18742300	-1.11779400	0.92860600
F	1.63122900	1.42753300	3.58815300
F	2.85092100	-0.17156600	4.41399600
F	0.68061100	-0.26487600	4.56060100
F	3.21407700	-2.38155600	2.84638600
F	1.18442300	-2.65861000	3.58185500
F	1.60215400	-2.83066900	1.45867500
O	2.62527000	-0.02457000	1.62554900
C	3.57526400	1.29453500	-0.32452900
C	3.75476000	1.53579100	-1.69080100
C	4.50316800	2.58912700	-2.20491200
C	5.12279400	3.47102600	-1.32618400
C	4.97401800	3.28025700	0.04169100
C	4.21029900	2.21396700	0.51852500
C	3.29586600	-1.36490500	-0.49287700
C	2.74742400	-2.14160600	-1.51259300
C	3.36214200	-3.27855200	-2.03393000
C	4.59508800	-3.68075800	-1.53556600
C	5.19266800	-2.93584300	-0.52501400
C	4.54141200	-1.80794700	-0.03474700
C	1.64663100	-0.62122600	2.38402600
C	0.19416100	-0.42651400	1.79816600
H	-0.47674500	-1.17477100	2.21947600
H	-0.14675700	0.56457300	2.10063100
C	0.26008500	-0.50900300	0.31221400
H	0.10152000	-1.47421100	-0.15215100
C	0.98761300	0.46291600	-0.38241700
H	0.92837500	1.47544900	0.01456000
H	0.99162600	0.40506900	-1.46598100
C	1.70590100	0.09727400	3.76214900
C	1.92254300	-2.14115400	2.57704600
B	2.70086100	0.00997300	0.17740600
B	-2.69303300	0.17778700	-0.27013900
C	-3.58039100	-0.31146800	1.01741000
C	-2.50378600	1.79321000	-0.41964000
C	-3.24020200	-0.59859200	-1.60274600
C	-3.35115200	-1.56392200	1.59035600
C	-4.63494200	0.39904500	1.59475800
C	-2.14497600	2.57198000	0.68626100
C	-2.59236100	2.51889000	-1.61149700
C	-2.47624000	-1.46603900	-2.38060100
C	-4.56621300	-0.46512700	-2.02155600
C	-4.08007500	-2.08192500	2.65730400
F	-2.35237500	-2.35238400	1.11636400
C	-5.39474600	-0.07761000	2.66098100
F	-4.97462100	1.62103100	1.13135500
C	-1.91142400	3.94183800	0.64591500
F	-2.00108300	1.98802700	1.90321400

C	-2.36935400	3.89326300	-1.70249700
F	-2.90762200	1.91305900	-2.77803300
C	-2.97451100	-2.16089200	-3.48267200
F	-1.16810900	-1.67667700	-2.10186800
C	-5.10877000	-1.13319500	-3.11378300
F	-5.39569300	0.36984000	-1.35475900
C	-5.11740400	-1.33008600	3.19683500
F	-3.79711300	-3.29479700	3.16407900
F	-6.39747800	0.65797500	3.17308400
C	-2.02798800	4.61403800	-0.56616500
F	-1.57590500	4.61787500	1.75800600
F	-2.47885100	4.52488200	-2.88419400
C	-4.30288900	-1.99439000	-3.85212000
F	-2.18281700	-2.98596900	-4.19003000
F	-6.39484600	-0.95587400	-3.46549400
F	-5.83967600	-1.80593200	4.22297500
F	-1.80756400	5.93546800	-0.63627700
F	-4.80309900	-2.65215400	-4.90994500
H	-1.52721900	-0.23219100	-0.04492300

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