1. SUPPLEMENTARY INFORMATION

to accompany

Three-body Interactions Effect Heterolytic Hydrogen Splitting by Frustrated Lewis Pairs

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Table of Contents

Supplementary Tables

Table S1. Interaction energy terms from SAPT pseudo-dimer calculations in the model system P(*t*-Bu)$_3$…H$_2$…B(C$_6$F$_5$) for several values of the H-H bond distance; $E_{ind+ex+\delta}$ denotes the total induction effect in combination with exchange-induction and higher-order terms; $\Delta E_{3\text{-b(CAM)}}$ and ΔE_{str} (H_2) refer to supermolecular CAM-B3LYP-D3 values in kcal/mol.

H_2 = 0.741								
Term	E_{es}	E_{exch}	$E_{ind+ex+\delta}$	δ_{HF}	$E_{disp+ex}$	SAPT0	$\Delta E_{3\text{-b(CAM)}}$	$\Delta E_{str}(H_2)$
A-B + H_2(TCBS)	-17.4	64.8	-23.7	-11.4	-16.7	6.9		
A+H_2(DCBS)	-5.2	33.4	-10.0[a]	-4.4	-10.1	8.1		
B+H_2(DCBS)	-11.7	31.6	-7.7[b]	-4.8	-5.9	6.3		
3-body	-0.5	-0.2	-6.1	-2.1	-0.7	-7.5	-7.8	0.0
A + B	-3.4	3.7	-0.6	-0.3	-9.6	-10.0		
H_2 = 0.841								
A-B + H_2(TCBS)	-20.1	73.6	-31.1	-14.5	-19.3	3.2		
A+H_2(DCBS)	-5.8	38.8	-12.6	-5.3	-11.6	8.7		
B+H_2(DCBS)	-13.7	35.0	-9.9	-5.9	-6.8	4.6		
3-body	-0.5	-0.2	-8.5	-3.2	-0.8	-10.1	-10.2	3.1
H_2=0.941								
A-B + H_2(TCBS)	-23.0	83.5	-40.7	-18.6	-22.1	-2.2		
A+H_2(DCBS)	-6.4	44.8	-15.9	-6.3	-13.3	9.2		
B+H_2(DCBS)	-16.0	38.9	-13.0	-7.5	-7.8	2.1		
3-body	-0.5	-0.2	-11.9	-4.8	-1.0	-13.5	-13.3	10.8
H_2 = 1.041								
A-B + H_2(TCBS)	-26.2	94.6	-53.1	-24.0	-25.2	-9.9		
A+H_2(DCBS)	-7.1	51.5	-19.9	-7.4	-15.1	9.4		
B+H_2(DCBS)	-18.5	43.2	-16.9	-9.5	-8.9	-1.2		
3-body	-0.6	0.0	-16.3	-7.1	-1.2	-18.1	-17.1	20.9
H_2 = 1.041 sp^3 B(C$_6$F$_5$)$_3$								
A-B + H_2(TCBS)	-15.8	75.4	-74.5	-42.0	-20.9	-35.7		
A+H_2(DCBS)	3.9	33.0	-26.9	-11.2	-10.8	-0.8		

B+H_2(DCBS)	-18.5	43.2	-16.9	-9.5	-8.9	-1.2		
3-body	-1.2	-0.7	-30.7	-21.4	-1.1	-33.7	-31.3	20.9
A + B	-3.1	2.7	-0.6	-0.3	-6.8	-7.9		
H_2 = 1.141Å sp^3 $B(C_6F_5)_3$								
A-B + H_2(TCBS)	-17.4	84.8	-94.0	-52.8	-23.8	-50.4		
A+H_2(DCBS)	5.1	38.1	-32.9	-13.4	-12.3	-2.0		
B+H_2(DCBS)	-21.3	47.9	-21.8	-12.0	-10.1	-5.4		
3-body	-1.2	-1.2	-39.3	-27.3	-1.3	-43.1	-38.2	32.1

Table S2. Two- and 3-body interactions (in kcal/mol) in the transition state of $P(Ad)_3$…H_2… $B(C_6F_5)_3$ from pseudo-dimer calculations in the geometry optimized in CAM-B3LYP-D3.

	E_{es}	E_{exch}	E_{ind}	$E_{ex\text{-}ind}$	δ_{HF}	$E_{disp+ex}$	SAPT0	$\Delta E_{3\text{-}b(CAM)}$
A-B + H_2(TCBS)	-17.6	52.3	-24.5	14.1	-11.2	-15.3	-2.1	
A+H_2(DCBS)	-7.4	29.0	-16.4	11.1	-4.6	-9.2	2.5	
B+H_2(DCBS)	-9.6	24.1	-6.2	4.0	-4.1	-5.5	2.8	
3-body	-0.6	-0.9	-1.9	-1.0	-2.5	-0.6	-7.4	-7.4
A + B(DCBS)	-6.7	11.7	-6.9	6.4	-0.9	-16.1	-12.5	
3-body/ total, %							50.4[a]	

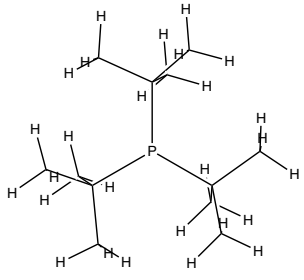
[a] This ratio in the supermolecular CAM-B3LYP-D3 calculation amounts to 65.6%

Table S3. Two-body and 3-body interactions (in kcal/mol) in $P(Ad)_3$ …H_2…$B(C_6F_5)_3$ model system from pseudo-dimer calculations; (P---B) = 4.745Å, (P…H) = 2.153Å, H-H = 1.041Å with sp^3 hybridized boron

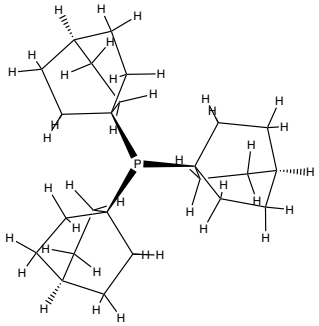
	E_{es}	E_{exch}	$E_{ind+ex+\delta}$	δ_{HF}	$E_{disp+ex}$	SAPT0	$\Delta E_{3\text{-}b(CAM)}$
A-B + H_2(TCBS)	-15.7	73.2	-79.1	-47.2	-21.3	-42.9	
A+H_2(DCBS)	3.7	32.8	-26.3	-11.0	-10.9	-0.7	
B+H_2(DCBS)	-18.0	38.9	-17.3	-10.6	-9.0	-5.5	
3-body	-1.4	1.5	-35.5	-25.6	-1.3	-36.8	-34.6
A + B(DCBS)	-4.3	3.7	-1.0	-0.5	-9.4	-10.9	
3-body/ total, %						68.2[a]	

[a] This ratio in the supermolecular CAM-B3LYP-D3 calculation amounts to 69.4%

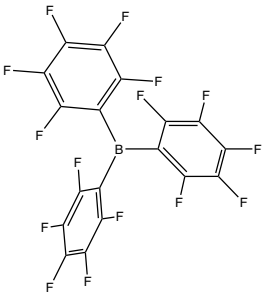
Supplementary 2-D structures of reactants considered



$P(t\text{-}Bu)_3$



$P(Ad)_3$



$B(C_6F_5)_3$

Supplementary Coordinate Files (in Å)

a. $P(t\text{-}Bu)_3+B(C_6F_5)_3$ FLP

```
74
P-tBut3+B(C6F5)3 CAM-B3LYP-D3(BJ)/DefTZVP optimized C3 group
P           0.00000        0.00000        2.58998
C           1.48687        0.97258        3.29385
C           0.09884       -1.77396        3.29385
C          -1.24370       -2.49339        3.11775
H          -1.60824       -2.43305        2.09556
H          -2.01672       -2.12681        3.78632
H          -1.09586       -3.55104        3.34794
C           1.08333       -2.54437        2.39965
H           2.09552       -2.15515        2.43207
H           0.74596       -2.53331        1.36388
H           1.12169       -3.58610        2.72760
C           0.51901       -1.92709        4.75679
H           1.52784       -1.57154        4.94512
H           0.49797       -2.98735        5.02320
H          -0.15266       -1.40744        5.43563
C          -1.58571        0.80138        3.29385
C          -1.92841        0.51407        4.75679
H          -1.14255        0.83593        5.43563
H          -2.12492       -0.53738        4.94512
H          -2.83611        1.06242        5.02320
C          -1.53749        2.32378        3.11775
H          -0.83351        2.80993        3.78632
H          -2.52735        2.72456        3.34794
H          -1.30297        2.60930        2.09556
C          -2.74515        0.33400        2.39965
H          -2.56689        0.62063        1.36388
H          -3.66650        0.82164        2.72760
H          -2.91417       -0.73720        2.43207
C           2.78119        0.16962        3.11775
H           3.62322        0.82647        3.34794
H           2.91121       -0.17625        2.09556
H           2.85023       -0.68312        3.78632
C           1.40941        1.41302        4.75679
H           2.33814        1.92493        5.02320
H           1.29521        0.57151        5.43563
H           0.59707        2.10892        4.94512
C           1.66183        2.21037        2.39965
H           2.54481        2.76446        2.72760
H           0.81865        2.89235        2.43207
H           1.82093        1.91268        1.36388
B           0.00000        0.00000       -1.55695
```

```
C          0.60879        1.43870       -1.56377
C          1.79046        1.74558       -2.22971
C          2.36568        2.99815       -2.20508
C          1.76034        4.00603       -1.47844
C          0.58136        3.75156       -0.80551
C          0.02392        2.49321       -0.87303
F         -1.11710        2.31476       -0.20883
F          0.00000        4.71382       -0.09934
F          2.30510        5.20895       -1.43159
F          3.49090        3.24349       -2.86454
F          2.41768        0.81488       -2.94984
C          0.94155       -1.24658       -1.56377
C          0.61649       -2.42338       -2.22971
C          1.41364       -3.54781       -2.20508
C          2.58915       -3.52751       -1.47844
C          2.95826       -2.37925       -0.80551
C          2.14723       -1.26732       -0.87303
F          2.56319       -0.18994       -0.20883
F          4.08229       -2.35691       -0.09934
F          3.35853       -4.60075       -1.43159
F          1.06349       -4.64495       -2.86454
F         -0.50313       -2.50121       -2.94984
C         -1.55034       -0.19212       -1.56377
C         -2.40695        0.67780       -2.22971
C         -3.77932        0.54966       -2.20508
C         -4.34949       -0.47852       -1.47844
C         -3.53963       -1.37231       -0.80551
C         -2.17114       -1.22589       -0.87303
F         -1.44609       -2.12482       -0.20883
F         -4.08229       -2.35691       -0.09934
F         -5.66363       -0.60820       -1.43159
F         -4.55439        1.40147       -2.86454
F         -1.91455        1.68633       -2.94984
```

b. $P(Ad)_3$+$B(C_6F_5)_3$ FLP

```
98
P(Ad)3 - B(C6F5)3 optimized CAM-C3LYP-D3(BJ)/Def2-TZVP C3
P          0.00000        0.00000        1.81015
C          1.13201       -1.36069        2.51102
C          2.39880       -1.38495        1.62068
H          2.80980       -0.39518        1.46551
H          2.09849       -1.75301        0.63885
C          3.47312       -2.30230        2.23068
H          4.22702       -1.71178        2.75652
H          3.99654       -2.84579        1.44186
C          2.80845       -3.27169        3.20307
C          2.34632       -2.49254        4.43034
C          1.56286       -1.23881        3.98457
```

H	2.18742	-0.35819	4.11150
H	0.69738	-1.09750	4.62556
H	1.71944	-3.13492	5.05299
H	3.20207	-2.20251	5.04219
C	1.57987	-3.86298	2.52211
C	0.51209	-2.76363	2.32623
H	0.08927	-2.85429	1.33076
H	-0.29904	-2.91353	3.03458
H	1.86418	-4.29342	1.55956
H	1.16964	-4.67837	3.11963
H	3.50289	-4.06156	3.49332
C	-1.74440	-0.30001	2.51102
C	-2.64942	0.93833	2.32623
H	-2.51652	1.34983	1.33076
H	-2.37367	1.71575	3.03458
C	-4.13537	0.56329	2.52211
H	-4.65030	0.53228	1.55956
H	-4.63640	1.32625	3.11963
C	-4.23759	-0.79634	3.20307
C	-3.73041	-1.85666	2.23068
C	-2.39880	-1.38495	1.62068
H	-2.56739	-0.94084	0.63885
H	-1.74713	-2.23577	1.46551
H	-3.59596	-2.80481	2.75652
H	-4.46280	-2.03821	1.44186
C	-3.33176	-0.78570	4.43034
C	-1.85427	-0.73407	3.98457
H	-1.29915	-0.05520	4.62556
H	-1.40391	-1.71527	4.11150
H	-3.57464	0.07838	5.05299
H	-3.50846	-1.67182	5.04219
H	-5.26886	-1.00281	3.49332
C	0.61238	1.66070	2.51102
C	2.13733	1.82530	2.32623
H	2.42725	1.50445	1.33076
H	2.67271	1.19779	3.03458
C	2.55551	3.29969	2.52211
H	2.78612	3.76114	1.55956
H	3.46677	3.35212	3.11963
C	1.42914	4.06803	3.20307
C	0.25729	4.15896	2.23068
C	-0.00000	2.76990	1.62068
H	0.46890	2.69385	0.63885
H	-1.06266	2.63095	1.46551
H	-0.63106	4.51660	2.75652
H	0.46626	4.88400	1.44186
C	0.98544	3.27824	4.43034
C	0.29141	1.97288	3.98457

```
H          0.60177        1.15270        4.62556
H         -0.78351        2.07346        4.11150
H          1.85520        3.05654        5.05299
H          0.30639        3.87433        5.04219
H          1.76597        5.06437        3.49332
B         -0.00000       -0.00000       -2.28378
C          1.45254       -0.57768       -2.28879
C          2.49503        0.03143       -1.60068
C          3.76032       -0.50798       -1.51622
C          4.03483       -1.69439       -2.16675
C          3.04125       -2.32184       -2.89442
C          1.78223       -1.76240       -2.93870
F          0.86704       -2.41109       -3.65971
F          3.30632       -3.45363       -3.53531
F          5.24283       -2.22617       -2.09700
F          4.70794        0.09423       -0.80755
F          2.29826        1.17749       -0.95110
C         -0.22599        1.54678       -2.28879
C         -1.27473        2.14505       -1.60068
C         -1.44024        3.51052       -1.51622
C         -0.55003        4.34146       -2.16675
C          0.49014        3.79472       -2.89442
C          0.63517        2.42466       -2.93870
F          1.65455        1.95643       -3.65971
F          1.33777        4.59017       -3.53531
F         -0.69349        5.65351       -2.09700
F         -2.43557        4.03008       -0.80755
F         -2.16886        1.40161       -0.95110
C         -1.22655       -0.96910       -2.28879
C         -1.22030       -2.17648       -1.60068
C         -2.32008       -3.00254       -1.51622
C         -3.48480       -2.64707       -2.16675
C         -3.53140       -1.47289       -2.89442
C         -2.41740       -0.66226       -2.93870
F         -2.52159        0.45466       -3.65971
F         -4.64409       -1.13654       -3.53531
F         -4.54934       -3.42733       -2.09700
F         -2.27237       -4.12431       -0.80755
F         -0.12940       -2.57909       -0.95110
```

c. $P(^tBu)_3...H_2...B(C_6F_5)_3$ transition state geometry

```
76
P(tBu)3--H2--B(C6F5)3 Transition State CAM-B3LYP-D3(BJ)/Def2-
TZVP
C     0.00000000  0.00000000  0.00000000
P    -0.45276700  1.66268500  0.80695700
C     0.86524600  2.08354400  2.11463300
C     0.77506000  3.56218600  2.50914900
```

```
H   -0.23361600  3.84788900  2.79834000
H    1.11934100  4.23459200  1.72902900
H    1.42011700  3.71957300  3.37617200
C    0.49393500  1.30690500  3.38708900
H    0.53770900  0.22964900  3.26841500
H   -0.50961700  1.57312200  3.71705700
H    1.19075800  1.57822000  4.18338400
C    2.31671100  1.78520700  1.73587600
H    2.49962700  0.72702400  1.57188500
H    2.96850200  2.10146500  2.55433100
H    2.62793800  2.32370700  0.84355700
C   -0.42646000  3.01174200 -0.53363800
C    0.94921800  3.48579900 -1.00479300
H    1.55077700  2.67458600 -1.40775900
H    1.51928400  3.96630400 -0.21431800
H    0.81772400  4.22395800 -1.80027800
C   -1.21415600  2.53574600 -1.75966900
H   -0.69642200  1.76798000 -2.32702700
H   -1.35665200  3.38901500 -2.42600700
H   -2.20306700  2.16539000 -1.49076000
C   -1.22095900  4.21129700  0.00798800
H   -2.24282400  3.92205700  0.25119400
H   -1.27163100  4.97618000 -0.77018900
H   -0.78186300  4.66784200  0.88724300
C    0.31806900 -1.02948800  1.09039100
H    0.40516700 -2.01002300  0.61811000
H   -0.47754300 -1.09960800  1.82970900
H    1.25541200 -0.83647400  1.60332100
C    1.15496800  0.01275200 -1.00211700
H    1.33025700 -1.00705700 -1.35447100
H    2.08294900  0.37137800 -0.56354900
H    0.93879500  0.62005400 -1.87720000
C   -1.26461800 -0.53074000 -0.69554100
H   -1.06552700 -1.54309200 -1.05435400
H   -1.56847400  0.06126500 -1.55123200
H   -2.10191000 -0.58455300 -0.00183000
B   -4.63636700  1.67576300  2.50356800
C   -5.60986100  0.76646200  1.65309700
C   -6.24798300 -0.34473900  2.18219300
C   -7.10252500 -1.14243600  1.44660600
C   -7.33785900 -0.84163500  0.12017600
C   -6.72333700  0.25699600 -0.45057600
C   -5.89022500  1.03703600  0.32128800
F   -5.32570100  2.09305500 -0.27476400
F   -6.94546300  0.55224500 -1.72638000
F   -8.14957400 -1.59875100 -0.60117800
F   -7.69704700 -2.19176500  2.00238700
F   -6.07078600 -0.68209900  3.46253100
```

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C   -3.76321000  1.00365200  3.63225000
C   -3.61357200  1.53799800  4.90318200
C   -2.83354400  0.95109400  5.88036500
C   -2.15976100 -0.22009200  5.59823600
C   -2.28547200 -0.79330500  4.34840200
C   -3.08121200 -0.18306200  3.40366300
F   -3.17049900 -0.78522400  2.21374900
F   -1.63094400 -1.91552700  4.06512300
F   -1.39433500 -0.78800100  6.51689400
F   -2.72470000  1.50315200  7.08323000
F   -4.24856100  2.66120200  5.24598600
C   -4.85124300  3.24026600  2.50102900
C   -6.07481300  3.84375700  2.25047800
C   -6.24575000  5.21499200  2.22207600
C   -5.16189300  6.04029600  2.44237100
C   -3.92339500  5.48382900  2.70192400
C   -3.79870700  4.11333900  2.73852200
F   -2.58340100  3.62660700  3.00576200
F   -2.87262000  6.26888000  2.91502300
F   -5.30655900  7.35531800  2.40901100
F   -7.44028800  5.74298200  1.98272500
F   -7.16750600  3.10729600  2.03841500
H   -3.48370700  1.72445200  1.18171100
H   -2.69936000  1.68004100  1.24650900
```

d. $P(Ad)_3...H_2...B(C_6F_5)_3$ Transition state geometry

```
100
FLP-adamanene-H2 TS CAM-B3LYP-D3 Def2TZVP
P   -1.19035900  0.26565400  1.45293300
C    0.00000000  0.00000000  0.00000000
C   -0.49056800  0.90101300 -1.15891100
H   -0.68314000  1.91562800 -0.83522900
H   -1.44499800  0.49996600 -1.50257500
C    0.53558300  0.91190500 -2.30624300
H    1.13379400  1.82543200 -2.27460200
H    0.02217400  0.90784600 -3.26911600
C    1.44665100 -0.30429100 -2.17616800
C    2.34493400 -0.11725500 -0.95743800
C    1.48972200  0.28821100  0.26273400
H    1.62673000  1.34751300  0.46683000
H    1.83094900 -0.24312400  1.14727400
H    2.88171500 -1.04696700 -0.75626300
H    3.10091200  0.64429200 -1.15489900
C    0.57329700 -1.53128400 -1.94454600
C   -0.10666100 -1.43531800 -0.56042800
H   -1.15063300 -1.71873600 -0.65691600
H    0.35747400 -2.14153400  0.12400100
H   -0.17845100 -1.60148300 -2.73314300
```

H	1.17265300	-2.44087300	-2.00206900
H	2.05014600	-0.42916300	-3.07630800
C	-1.00639000	-1.19042800	2.65215200
C	-1.69850400	-0.88397200	3.99873500
H	-2.67841500	-0.44500700	3.81793100
H	-1.12014500	-0.15614700	4.56298100
C	-1.86523200	-2.17395500	4.83234700
H	-2.90789800	-2.49731700	4.82945300
H	-1.60058900	-1.98069800	5.87279400
C	-0.98427300	-3.27616000	4.25605700
C	-1.53416600	-3.65912200	2.88587800
C	-1.81358300	-2.38078500	2.07512900
H	-2.87252600	-2.12256500	2.13255300
H	-1.60084700	-2.55863900	1.03011900
H	-0.81318400	-4.29204400	2.36341200
H	-2.44857100	-4.24570000	2.98720000
C	0.42566700	-2.72123200	4.07908100
C	0.42762200	-1.66370300	2.95496400
H	1.05732800	-0.82440400	3.23630900
H	0.86550600	-2.08979800	2.05504100
H	0.76415000	-2.28100000	5.01974600
H	1.12437500	-3.52434800	3.83989200
H	-0.97153300	-4.14103300	4.92076800
C	-0.69020500	1.85400300	2.35756200
C	-0.50761800	3.01546100	1.35631800
H	-1.33397400	3.02518400	0.64997400
H	0.40506900	2.88060200	0.78108600
C	-0.46095400	4.37113500	2.09449700
H	-1.39246500	4.91889100	1.94041800
H	0.33813400	4.99030200	1.68465400
C	-0.24096200	4.13704100	3.58419800
C	-1.48581100	3.46094400	4.14976300
C	-1.89270300	2.29308500	3.23172400
H	-2.69788000	2.59788600	2.56332300
H	-2.28515500	1.48194000	3.83062000
H	-1.28031200	3.10033700	5.16051000
H	-2.30663800	4.17483500	4.23243700
C	0.94685400	3.19468900	3.75257300
C	0.56684900	1.78776300	3.24472200
H	1.40089100	1.35228400	2.70165500
H	0.37593400	1.13395400	4.09338100
H	1.80199700	3.58444500	3.19574300
H	1.25060600	3.14621600	4.79943600
H	-0.05144500	5.08205100	4.09525100
B	-5.52975200	0.31088100	0.17026400
C	-4.73349100	1.05038800	-0.97169400
C	-4.05649100	2.23697000	-0.72541000
C	-3.32163100	2.90162100	-1.68273800

```
C   -3.25112200  2.38457100 -2.96062400
C   -3.92211000  1.21610100 -3.25981000
C   -4.64402200  0.57594600 -2.27183700
F   -5.28212100 -0.54030300 -2.63099300
F   -3.86294200  0.71613600 -4.48913800
F   -2.53540600  2.99968400 -3.88930200
F   -2.66685200  4.01971200 -1.38327600
F   -4.08723200  2.78392900  0.49326700
C   -6.44817700  1.16745800  1.12880800
C   -6.62513700  0.84174400  2.46612000
C   -7.40388300  1.58207100  3.32855800
C   -8.06904000  2.69499700  2.84974700
C   -7.93774800  3.04954200  1.52223300
C   -7.13439600  2.29087000  0.69373800
F   -7.05672300  2.67986600 -0.58186100
F   -8.58167200  4.11272400  1.05462600
F   -8.83022200  3.41416800  3.65963300
F   -7.52664100  1.23494000  4.60475700
F   -6.00975800 -0.23028100  2.97643600
C   -5.71059000 -1.25643000  0.12988600
C   -4.66434700 -2.09445000 -0.23245400
C   -4.74781100 -3.46848600 -0.21274500
C   -5.93862600 -4.06576500  0.15567000
C   -7.01798800 -3.27668800  0.49751700
C   -6.88763800 -1.90091800  0.48307800
F   -7.97388800 -1.20193800  0.81814700
F   -8.16869300 -3.84381400  0.84044100
F   -6.04307200 -5.38482500  0.17575300
F   -3.70210100 -4.21855500 -0.54455800
F   -3.49645500 -1.57008800 -0.60945100
H   -3.49532900  0.26731700  1.28772900
H   -4.26337400  0.22625100  1.44253600
```

e. $P(t\text{-}Bu)_3H^+$ -- $HB(C_6F_5)_3^-$ ion-pair geometry

```
76
Ion-pair P(tBu)H+ HB(C6F5)3- optimized CAM-B3LYP-D3(BJ)/Def2-
TZVP
P          0.00000        0.00000        3.26305
C          1.53116        0.96164        3.72907
C          0.06722       -1.80684        3.72907
C         -1.29066       -2.49758        3.55181
H         -1.66332       -2.42255        2.53486
H         -2.04981       -2.13932        4.24037
H         -1.13785       -3.55632        3.76461
C          1.02917       -2.49515        2.74683
H          2.05196       -2.14480        2.81581
H          0.69245       -2.37680        1.71772
H          1.02969       -3.56164        2.97504
```

C	0.52467	-2.00291	5.17675
H	1.52563	-1.62528	5.36317
H	0.53758	-3.07308	5.38656
H	-0.15522	-1.53904	5.88975
C	-1.59838	0.84521	3.72907
C	-1.99691	0.54708	5.17675
H	-1.25524	0.90395	5.88975
H	-2.17035	-0.50860	5.36317
H	-2.93015	1.07099	5.38656
C	-1.51764	2.36653	3.55181
H	-0.82779	2.84485	4.24037
H	-2.51094	2.76357	3.76461
H	-1.26633	2.65175	2.53486
C	-2.67545	0.35629	2.74683
H	-2.40459	0.58872	1.71772
H	-3.59932	0.88908	2.97504
H	-2.88343	-0.70465	2.81581
C	2.80830	0.13105	3.55181
H	3.64879	0.79275	3.76461
H	2.92965	-0.22920	2.53486
H	2.87761	-0.70553	4.24037
C	1.47224	1.45584	5.17675
H	2.39258	2.00209	5.38656
H	1.41046	0.63509	5.88975
H	0.64471	2.13388	5.36317
C	1.64628	2.13886	2.74683
H	2.56962	2.67256	2.97504
H	0.83147	2.84945	2.81581
H	1.71214	1.78808	1.71772
B	0.00000	0.00000	-1.00751
C	0.45293	1.50302	-1.42155
C	1.27520	1.84017	-2.48173
C	1.68041	3.13529	-2.74896
C	1.25331	4.16654	-1.93650
C	0.42159	3.88171	-0.87324
C	0.04276	2.57401	-0.65214
F	-0.78293	2.36690	0.40023
F	-0.00000	4.86275	-0.06986
F	1.63697	5.41803	-2.17498
F	2.47669	3.40095	-3.78246
F	1.71494	0.89708	-3.32317
C	1.07519	-1.14376	-1.42155
C	0.95603	-2.02445	-2.48173
C	1.87503	-3.02292	-2.74896
C	2.98168	-3.16866	-1.93650
C	3.15086	-2.30596	-0.87324
C	2.20778	-1.32404	-0.65214
F	2.44126	-0.50541	0.40023

```
F          4.21126       -2.43137       -0.06986
F          3.87367       -4.12667       -2.17498
F          1.70697       -3.84535       -3.78246
F         -0.08057       -1.93372       -3.32317
C         -1.52812       -0.35926       -1.42155
C         -2.23124        0.18427       -2.48173
C         -3.55544       -0.11237       -2.74896
C         -4.23498       -0.99788       -1.93650
C         -3.57245       -1.57575       -0.87324
C         -2.25054       -1.24997       -0.65214
F         -1.65833       -1.86149        0.40023
F         -4.21126       -2.43137       -0.06986
F         -5.51063       -1.29136       -2.17498
F         -4.18365        0.44440       -3.78246
F         -1.63436        1.03664       -3.32317
H          0.00000        0.00000        0.19884
H          0.00000        0.00000        1.86015
```

f. $P(Ad)_3H^+$ -- $HB(C_6F_5)_3^-$ ion-pair geometry

```
100
Ion-pair P(Ad)3H+ HB(C6F5)3- Optimized CAM-B3LYP-D3(BJ)/Def3-
TZVP
C     0.00000000  0.00000000  0.00000000
C     0.45666600  1.11864900 -0.97056700
H    -0.29755200  1.87802900 -1.12263400
H     0.63284200  0.66311500 -1.94547700
C     1.74371100  1.76714200 -0.42968300
H     1.51560500  2.71990200  0.05243700
H     2.41774200  1.98766500 -1.25714700
C     2.40695600  0.82648200  0.57182100
C     1.55451500  0.76580300  1.83579800
C     0.08380700  0.49184300  1.45878200
H    -0.50082400  1.40065300  1.57547900
H    -0.34548800 -0.24463200  2.13625900
H     1.93185300 -0.01907100  2.49370600
H     1.62548600  1.70216600  2.38968400
C     2.46042700 -0.56798400 -0.03947700
C     1.03063800 -1.13601800 -0.18699100
H     0.92987100 -1.57610600 -1.17261400
H     0.86753400 -1.92312000  0.54524400
H     2.94738400 -0.52645700 -1.01439800
H     3.05782200 -1.23434700  0.58304000
H     3.41149700  1.17413100  0.81324600
P    -1.72951700 -0.49119000 -0.46722800
C    -2.16889200 -2.23459000  0.00000000
C    -3.66803200 -2.55914000 -0.18699100
H    -3.99877600 -2.25183000 -1.17261400
H    -4.26813100 -2.02433700  0.54524400
```

```
C   -3.89099500 -4.08139100 -0.03947700
H   -4.09851000 -4.52387200 -1.01439800
H   -4.76677900 -4.26556900  0.58304000
C   -2.65661600 -4.73231700  0.57182100
C   -1.51035800 -4.62826000 -0.42968300
C   -1.42844700 -3.18939900 -0.97056700
H   -1.91103900 -3.11420500 -1.94547700
H   -0.39369600 -2.91591700 -1.12263400
H   -0.57119100 -4.90709400  0.05243700
H   -1.65639500 -5.32224900 -1.25714700
C   -2.28294500 -3.96374100  1.83579800
C   -1.78484800 -2.55309100  1.45878200
H   -2.20800600 -1.81307400  2.13625900
H   -0.70548000 -2.50119100  1.57547900
H   -3.15133400 -3.89808900  2.49370600
H   -1.50751600 -4.49338600  2.38968400
H   -2.85781400 -5.77609900  0.81324600
C   -3.01965800  0.76102000  0.00000000
C   -2.55115700  2.22158800 -0.18699100
H   -2.11964600  2.35436600 -1.17261400
H   -1.78795400  2.47388700  0.54524400
C   -3.75798400  3.17580500 -0.03947700
H   -4.03742500  3.57675900 -1.01439800
H   -3.47959400  4.02634600  0.58304000
C   -4.93889100  2.43226500  0.57182100
C   -5.42190400  1.38754700 -0.42968300
C   -4.21677000  0.59718100 -0.97056700
H   -3.91035400  0.97752000 -1.94547700
H   -4.49730300 -0.43568200 -1.12263400
H   -6.13296600  0.71362200  0.05243700
H   -5.94989800  1.86101400 -1.25714700
C   -4.46012100  1.72436800  1.83579800
C   -3.48751000  0.58767800  1.45878200
H   -2.63505800  0.58413500  2.13625900
H   -3.98224800 -0.37303200  1.57547900
H   -3.96906900  2.44358900  2.49370600
H   -5.30652100  1.31765000  2.38968400
H   -5.74223400  3.12839900  0.81324600
H   -1.72951700 -0.49119000 -1.87022400
B   -1.72951700 -0.49119000 -4.70434100
C   -0.77185900  0.75605400 -5.10357600
C   -0.82360300  1.91423000 -4.35202000
C    0.00559900  2.99983100 -4.53883500
C    0.94524800  2.95866000 -5.54875300
C    1.02607700  1.83338500 -6.34378800
C    0.17479600  0.76769200 -6.11135900
F    0.30488100 -0.28270400 -6.93134800
F    1.92423700  1.78677100 -7.32611800
```

```
F    1.76071800  3.99072800 -5.75238900
F   -0.08603600  4.07643000 -3.75215000
F   -1.72951700  2.02464500 -3.35364600
C   -3.28849200 -0.28545600 -5.10357600
C   -4.26562900 -0.90935500 -4.35202000
C   -5.62038800 -0.73404600 -4.53883500
C   -6.05455700  0.10029900 -5.54875300
C   -5.12045500  0.73293700 -6.34378800
C   -3.77189800  0.52855200 -6.11135900
F   -2.92727000  1.16640700 -6.93134800
F   -5.52916600  1.53407400 -7.32611800
F   -7.35608900  0.29048400 -5.75238900
F   -6.50693300 -1.35170400 -3.75215000
F   -3.90829400 -1.74910700 -3.35364600
C   -1.12820100 -1.94416900 -5.10357600
C   -0.09931900 -2.47844500 -4.35202000
C    0.42623800 -3.73935500 -4.53883500
C   -0.07924200 -4.53253000 -5.54875300
C   -1.09417300 -4.03989200 -6.34378800
C   -1.59144900 -2.76981500 -6.11135900
F   -2.56616200 -2.35727300 -6.93134800
F   -1.58362200 -4.79441400 -7.32611800
F    0.40682000 -5.75478100 -5.75238900
F    1.40441800 -4.19829600 -3.75215000
F    0.44926000 -1.74910700 -3.35364600
H   -1.72951700 -0.49119000 -3.49926000
```