Supporting Information for

Yet another perspective on hole interactions, Part II: LP-Hole vs LP-Hole Interactions

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Table S1: Sum of van der Waals radii and bond lengths (in Å), and binding energies (in kJ mol^{-1}) for different $F_3N\cdots LB$ complexes at MP2/6-311++G(d,p)[1], M06-2x/def2-TZVPD, MP2/def2-TZVPD, and M062X/6-311++G(d,p) level.

		MP2/ 6-311++G(d,p)		M062X/ def2-TZVPD		MP2/ def2-TZVPD		M062X/ 6-311++G(d,p)	
LB	**R_{vdW}(N+ LB)**	**R(N···LB)**	**BE**	**R(N···LB)**	**BE**	**R(N···LB)**	**BE**	**R(N···LB)**	**BE**
HF	3.02	3.4	-3	3.5[a]	-2	3.5	+1	3.2[a]	-4
ClF	3.02	3.3	-5	3.5[a]	-2	3.4	+2	3.1[a]	-5
HNC	3.25	4.1	-3	4.1	-1	4.1[a]	+1	3.8	-3
HCN	3.10	3.8	-3	3.9	-2	4.8[a]	+2	3.5	-3

[a] Multiple imaginary frequencies

F. Blanco, I. Alkorta, I. Rozas, M. Solimannejad, J. Elguero, *Phys. Chem. Chem. Phys.* **2011**, *13*, 674–683.

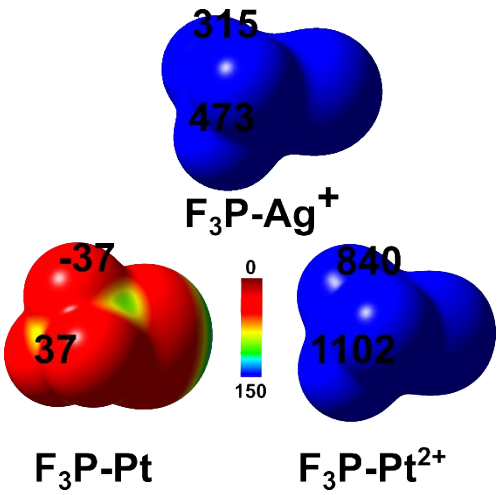

Figure S1. Electrostatic potential maps of F_3P-Ag^+, F_3P-Pt, and F_3P-Pt^{2+} . All values in kJ mol^{-1}.

Optimized Geometries

1. NF_3_FH
N 0.000000 0.000000 -1.193634
F 0.000000 1.215806 -0.599040
F 1.052919 -0.607903 -0.599040
F -1.052919 -0.607903 -0.599040
F 0.000000 0.000000 360844
H 0.000000 0.000000 3.281936

2. NF_3_ClF
N 0.000000 0.000000 - 267184
F 0.000000 1.215354 -1.670863
F 1.052527 -0.607677 -1.670863
F -1.052527 -0.607677 -1.670863
F 0.000000 0.000000 1.290688
Cl 0.000000 0.000000 903964

3. NF_3_CNH
N 0.000000 0.000000 -1.745406
F 0.000000 1.216010 -1.151533
F 1.053095 -0.608005 -1.151533
F -1.053095 -0.608005 -1.151533
H 0.000000 0.000000 4.518344
C 0.000000 0.000000 358658
N 0.000000 0.000000 3.519850

4. NF_3_NCH
N 0.000000 0.000000 -1.670826
F 0.000000 1.216015 -1.077070
F 1.053100 -0.608008 -1.077070
F -1.053100 -0.608008 -1.077070
H 0.000000 0.000000 4.474807
N 0.000000 0.000000 265335
C 0.000000 0.000000 3.407419

5. $NF_3\_F^-$
F 0.000000 0.000000 126594
N 0.000000 0.000000 -1.016732
F 0.000000 1.221474 -0.445267
F -1.057827 -0.610737 -0.445267
F 1.057827 -0.610737 -0.445267

6. $NCl_3\_F^-$
F 0.000000 0.000000 068725
N 0.000000 0.000000 -0.835636
Cl 0.000000 1.633022 -0.250374
Cl 1.414238 -0.816511 -0.250374
Cl -1.414238 -0.816511 -0.250374

7. $NBr_3\_F^-$
F 0.000000 0.000000 122779
N 0.000000 0.000000 -0.762386
Br 0.000000 1.790463 -0.131127
Br 1.550587 -0.895232 -0.131127
Br -1.550587 -0.895232 -0.131127

8. $NI_3\_F^-$
F 0.000000 0.000000 068214
N 0.000000 0.000000 -0.742776
I 0.000000 1.972448 -0.084368
I 1.708190 -0.986224 -0.084368
I -1.708190 -0.986224 -0.084368

9. $PF_3\_F^-$
P 0.000000 0.000000 0.866083
F 0.000000 1.405577 0.196529
F -1.217265 -0.702788 0.196529
F 1.217265 -0.702788 0.196529
F 0.000000 0.000000 - 033059

10. $PCl_3\_F^-$
P 0.000000 0.000000 0.957033
F 0.000000 0.000000 - 116185
Cl 0.000000 1.846004 0.091964
Cl 1.598686 -0.923002 0.091964
Cl -1.598686 -0.923002 0.091964

11. $PI_3\_F^-$
P 0.000000 0.000000 1.020505
F 0.000000 0.000000 -1.994628
I 0.000000 219709 0.016629
I 1.922325 -1.109855 0.016629
I -1.922325 -1.109855 0.016629

12. $Cl_2\_PH_3$
H -3.439139 0.038471 1.190695
H -3.428367 -1.052903 -0.571500
H -3.423174 1.019097 -0.635393
P - 684539 -0.000165 0.000170
Cl 0.485732 -0.000291 0.001953
Cl 488313 0.000162 -0.001151

13. FCl_PH_3
H - 365790 -0.978138 -0.751804
H - 362608 1.142844 -0.470526
H - 362793 -0.161318 1.225174
P -1.696793 0.000107 0.000148
F 391105 0.000689 0.000739
Cl 0.648420 -0.000658 -0.000689

14. FBr_PH_3
H - 657573 1.054565 0.642337
H - 656077 -1.083749 0.593608
H - 660472 0.027630 -1.232774
P -1.991562 -0.000049 0.000138
F 336379 -0.000299 0.000635
Br 0.480575 0.000142 -0.000313

15. FI_PH_3
H 945759 1.173345 0.381073
H 954907 -0.255379 -1.200530
H 949932 -0.911280 0.827168
P 276046 0.000432 0.000522
F - 385128 0.001889 0.002207
I -0.406135 -0.000569 -0.000668

16. $Cl_2\_PH_3\_NCH$
H 0.000000 1.195600 -1.866061
H -1.035420 -0.597800 -1.866061
H 1.035420 -0.597800 -1.866061
P 0.000000 0.000000 -1.120150
N 0.000000 0.000000 -5.065683
C 0.000000 0.000000 -6.207721
H 0.000000 0.000000 -7.275321
Cl 0.000000 0.000000 4.015120
Cl 0.000000 0.000000 007343

17. $FCl\_PH_3\_NCH$
H 0.907132 -0.861388 -0.895441
H 0.905406 -0.331330 1.201136
H 0.901210 1.219498 -0.306102
P 0.272765 0.007102 -0.000259
Cl -1.905646 -0.000133 -0.000092
F -3.740316 -0.007421 0.000347
N 3.585368 -0.001855 0.000298
C 4.726811 -0.006682 0.000121
H 5.795170 -0.011177 -0.000086

18. $FBr\_PH_3\_NCH$
H 1.508546 -0.773602 -0.957266
H 1.504796 -0.433647 1.159606
H 1.502549 1.230040 -0.193526
P 0.849691 0.006084 0.002078
F -3.453245 -0.005522 -0.001635
N 4.262341 -0.003287 0.000177
C 5.403932 -0.004690 -0.002319
H 6.472130 -0.006017 -0.004634
Br -1.568976 -0.000205 -0.000228

19. $FI\_PH_3\_NCH$
H 1.977375 -0.638699 -1.045203
H 1.974734 -0.568549 1.087275
H 1.969379 1.243262 -0.039751

P 1.305421 0.009472 0.000076
F -3.338016 -0.008057 0.000452
N 4.763977 -0.001476 0.000641
C 5.905604 -0.009715 -0.000379
H 6.973728 -0.017612 -0.001323
I -1.343695 -0.000365 -0.000159

20. $ClNa\_NF_3$
Na 0.000000 0.000000 1.093376
Cl 0.000000 0.000000 3.454610
F 0.000000 1.216138 - 200005
F -1.053207 -0.608069 - 200005
F 1.053207 -0.608069 - 200005
N 0.000000 0.000000 -1.622198

21. $ClNa\_PF_3$
Na 0.000000 0.000000 1.642413
Cl 0.000000 0.000000 4.002849
P 0.000000 0.000000 -1.569861
F 0.000000 1.362074 - 317298
F -1.179591 -0.681037 - 317298
F 1.179591 -0.681037 - 317298

22. $ClNa\_NF_3\_^-CN$
Na 0.000000 0.000000 1.912652
Cl 0.000000 0.000000 4.311223
F 0.000000 1.223363 -1.125415
F -1.059463 -0.611681 -1.125415
F 1.059463 -0.611681 -1.125415
N 0.000000 0.000000 -5.146757
C 0.000000 0.000000 -3.981287
N 0.000000 0.000000 -0.575533

23. $ClNa\_PF_3\_^-CN$
Na 0.000000 0.000000 273791
Cl 0.000000 0.000000 4.676164
P 0.000000 0.000000 -0.652989
F 0.000000 1.397833 -1.305041
F -1.210558 -0.698916 -1.305041
F 1.210558 -0.698916 -1.305041
N 0.000000 0.000000 -5.112655
C 0.000000 0.000000 -3.947826

24. $H_3B\_NF_3\_F^-$
B 0.000000 0.000000 - 136506
H 1.014582 0.585769 - 400262
H 0.000000 -1.171539 - 400262
H -1.014582 0.585769 - 400262
N 0.000000 0.000000 -0.502638
F 0.000000 1.224345 0.013438
F -1.060314 -0.612173 0.013438
F 1.060314 -0.612173 0.013438
F 0.000000 0.000000 337661

25. $H_3B\_NCl_3\_F^-$
B 0.000000 0.000000 - 226831
H -1.013816 0.585327 - 509202
H 1.013816 0.585327 - 509202
H 0.000000 -1.170654 - 509202
N 0.000000 0.000000 -0.550600
F 0.000000 0.000000 276727
Cl 0.000000 1.635741 0.039714
Cl -1.416593 -0.817871 0.039714
Cl 1.416593 -0.817871 0.039714

26. $H_3B\_NBr_3\_F^-$
B 0.000000 0.000000 - 275932
H 0.000000 -1.169254 - 571174
H -1.012604 0.584627 - 571174
H 1.012604 0.584627 - 571174
N 0.000000 0.000000 -0.608932
F 0.000000 0.000000 200818
Br 0.000000 1.795156 0.033794
Br 1.554650 -0.897578 0.033794
Br -1.554650 -0.897578 0.033794

27. $H_3B\_NI_3\_F^-$
B 0.000000 0.000000 - 311222
H -1.010653 0.583501 - 627616
H 1.010653 0.583501 - 627616
H 0.000000 -1.167002 - 627616
N 0.000000 0.000000 -0.658242
F 0.000000 0.000000 072599
I 0.000000 1.985616 0.033920
I -1.719593 -0.992808 0.033920
I 1.719593 -0.992808 0.033920

28. XeO_NCH
O 0.000000 0.000000 399524
Xe 0.000000 0.000000 0.490403
N 0.000000 0.000000 - 616012
C 0.000000 0.000000 -3.756802
H 0.000000 0.000000 -4.825050

29. XeO_3_NCH (σ_D interaction)
O 0.097657 -1.400951 -0.853205
O 190663 0.012246 0.328450
O 0.078349 1.392901 -0.857333
Xe 0.446561 -0.000100 0.141756
N - 481884 -0.010031 0.499793
C -3.527830 0.004177 0.047087
H -4.507490 0.017000 -0.379166

30. XeO_3_NCH (lp interaction)
O 0.000000 1.636906 0.132550
O -1.417602 -0.818453 0.132550
O 1.417602 -0.818453 0.132550
Xe 0.000000 0.000000 0.763888
N 0.000000 0.000000 - 526766
C 0.000000 0.000000 -3.668091
H 0.000000 0.000000 -4.735248

31. XeO_3_F- (σ_D interaction)
O -0.094470 1.400649 0.904200
O 1.860506 -0.000027 -0.347382
O -0.094481 -1.400622 0.904227
Xe 0.088001 0.000003 -0.149791
F - 013830 -0.000016 -0.399961

32. XeO_3_F- (lp interaction)
O 0.000000 1.766918 0.005731
O -1.530196 -0.883459 0.005731
O 1.530196 -0.883459 0.005731
Xe 0.000000 0.000000 0.284796
F 0.000000 0.000000 -1.724059