Tuning the Reduction Potentials of Benzoquinone Through the Coordination to Lewis Acids

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Supporting Information

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1) Plots of Influence of Lewis Acid Strength on the Reduction Potentials of Benzoquinone-Lewis Acid Adducts

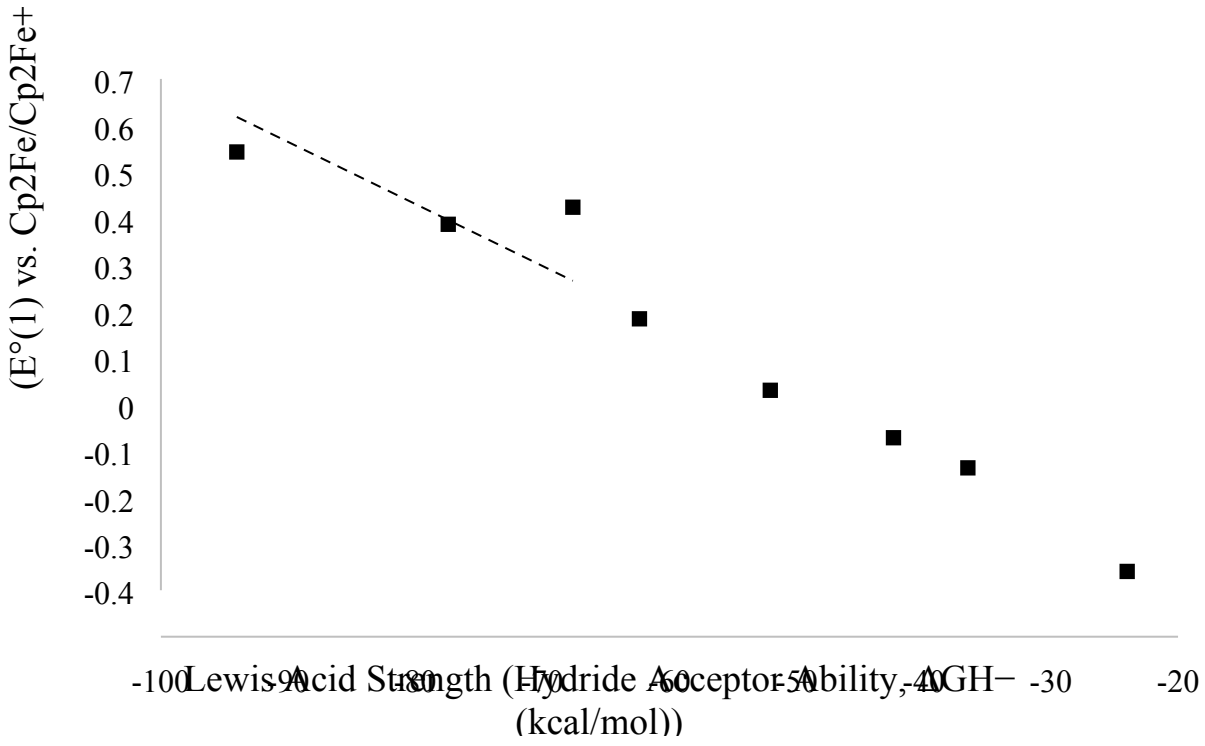

Figure S1. Plot showing the computed first reduction potential (E°(3)) of **LA_1-Q** as the Lewis acid strength is varied.

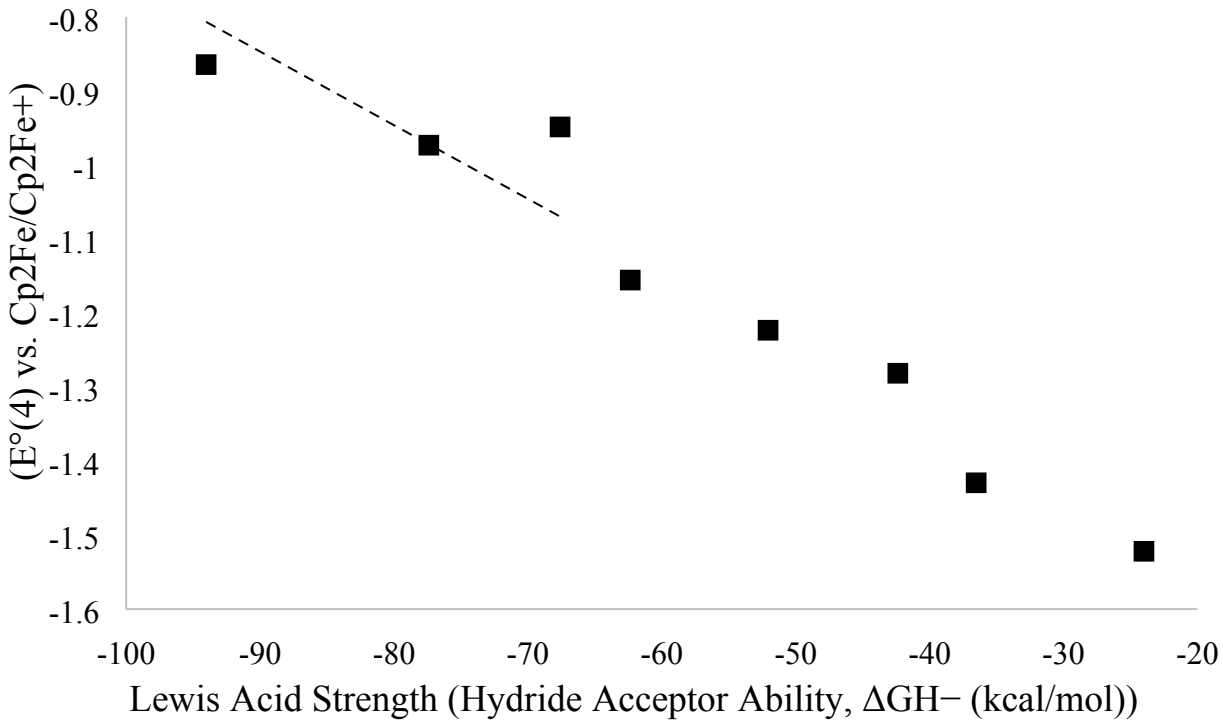

Figure S2. Plot showing the computed second reduction potential (E°(4)) of **LA_1-Q** as the Lewis acid strength is varied.

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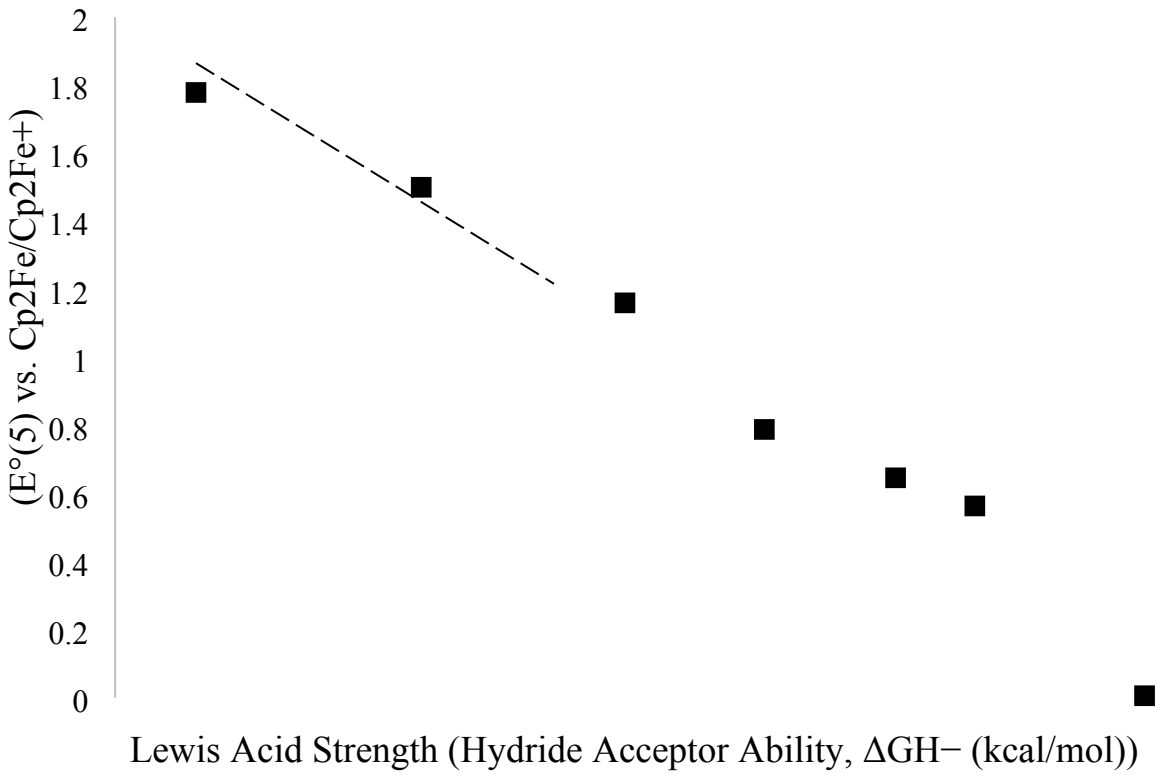


Figure S3. Plot showing the computed first reduction potential (E°(5)) of **LA_1-Q-LA_2**, where LA_1 = LA_2, as the Lewis acid strength is varied.

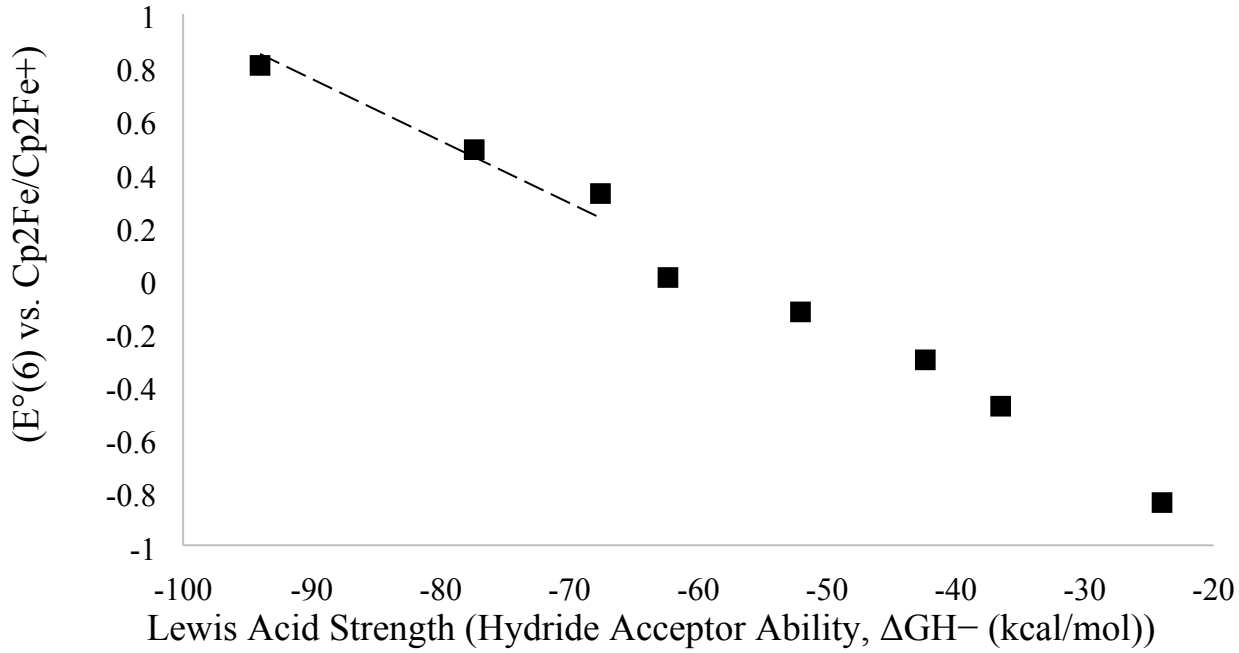


Figure S4. Plot showing the computed second reduction potential (E°(6)) of **LA_1-Q-LA_2**, where LA_1 = LA_2, as the Lewis acid strength is varied.

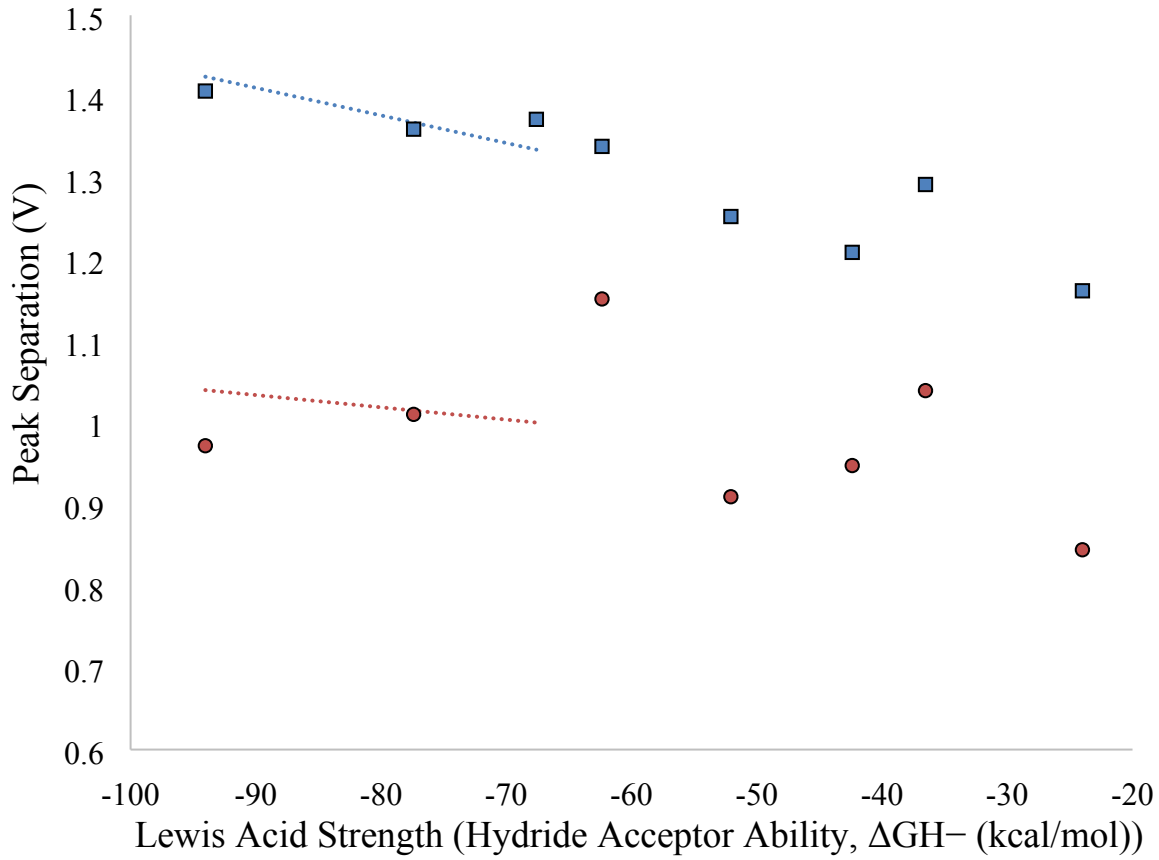


Figure S5. Plot showing the effect of Lewis acid strength on the difference between the first (E°(3) for **LA_1-Q** and E°(5) for **LA_1-Q-LA_2**) and second reduction potential (E°(4) for **LA_1-Q** and E°(6) for **LA_1-Q-LA_2**) of **Q**. The blue squares indicate the difference between E°(3) and E°(4) for **LA_1-Q** and the red circles indicate the difference between E°(5) and E°(6) for **LA_1-Q-LA_2**, where $LA_1 = LA_2$.

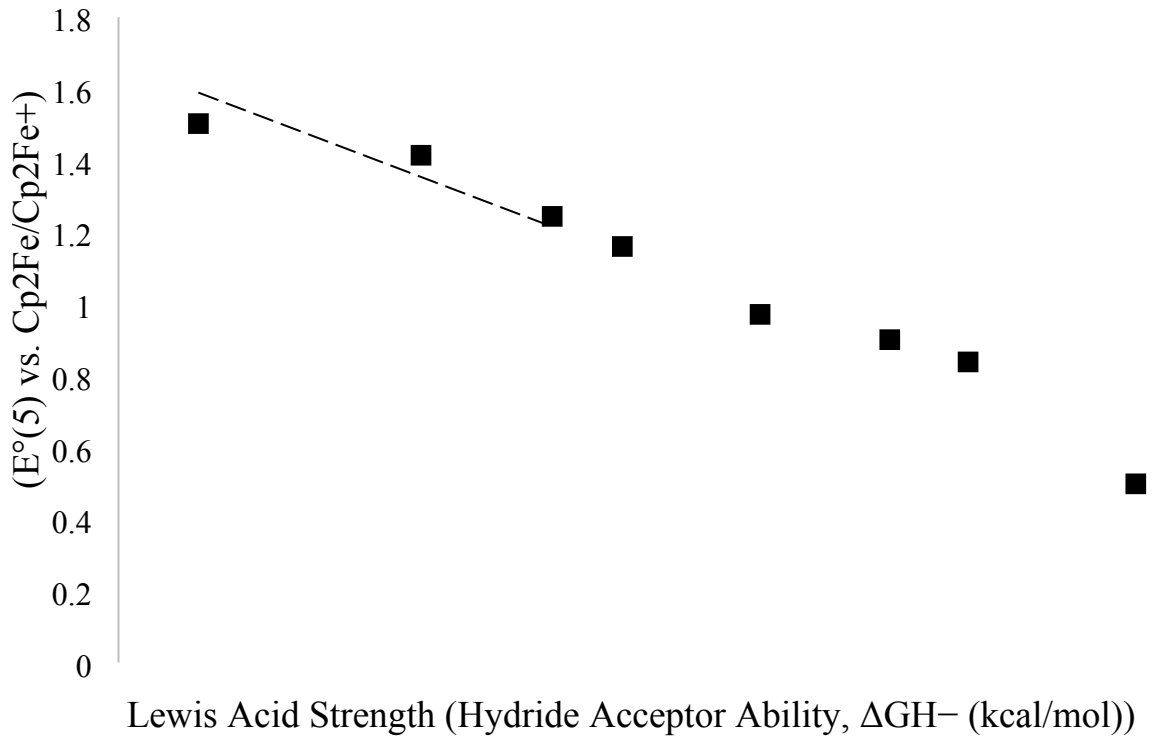


Figure S6. Plot showing the computed first reduction potential (E°(5)) of **LA_1-Q-LA_2**, where LA_1 = $B(C_6F_5)_3$, as the Lewis acid strength is varied.

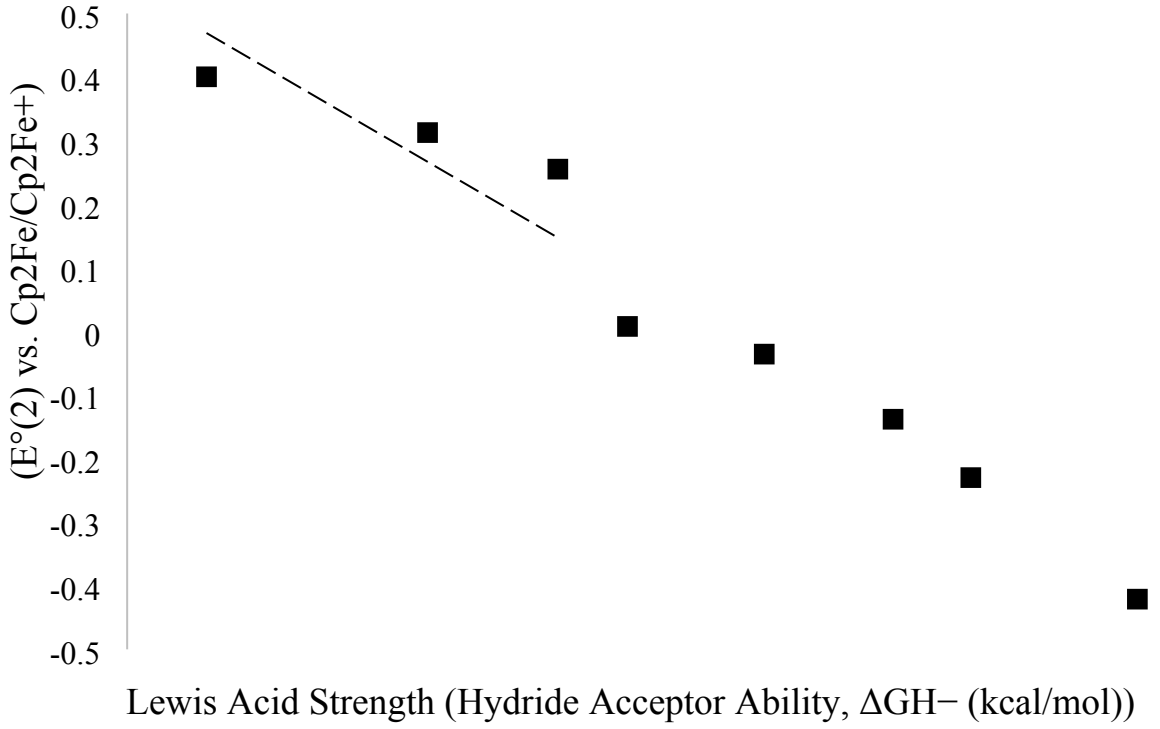


Figure S7. Plot showing the computed second reduction potential (E°(6)) of **LA_1-Q-LA_2**, where LA_1 = $B(C_6F_5)_3$**,** as the Lewis acid strength is varied.

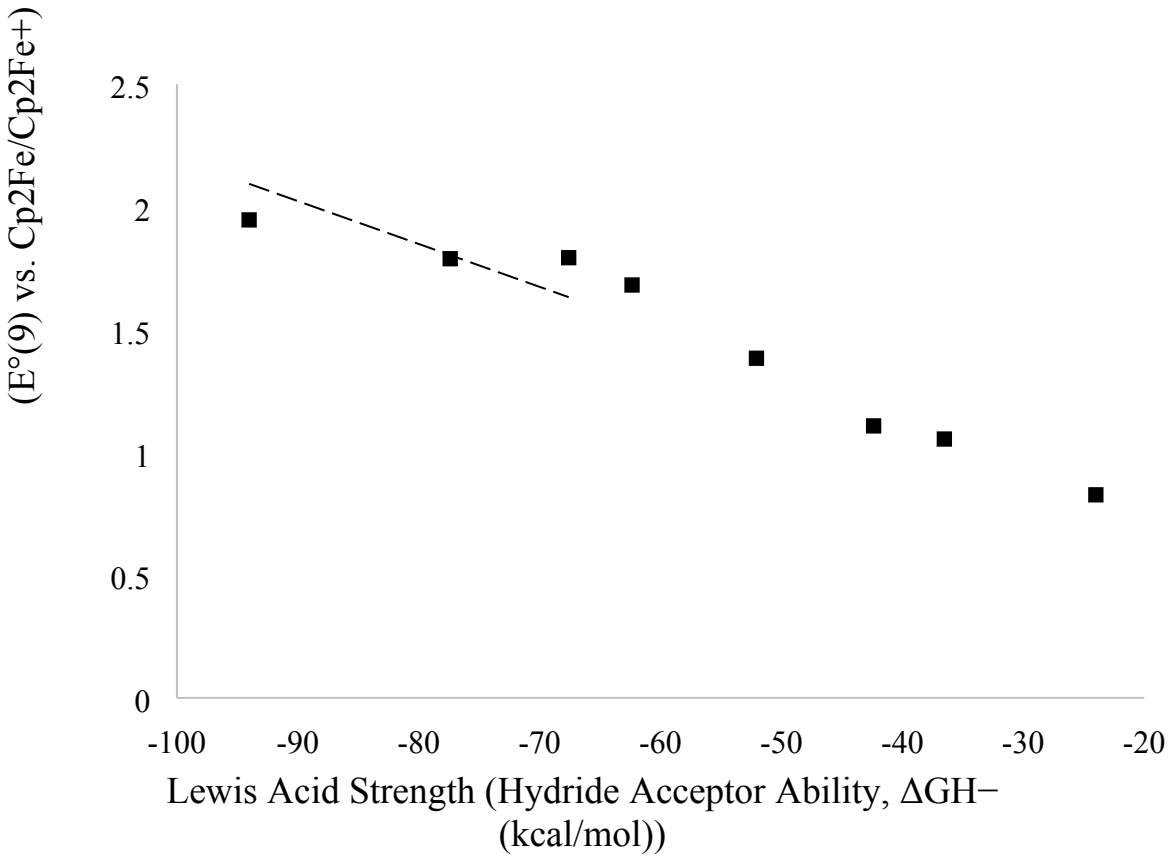


Figure S8. Plot showing the computed first reduction potential (E°(9)) of **[LA_1-HQ]$^+$** as the Lewis acid strength is varied.

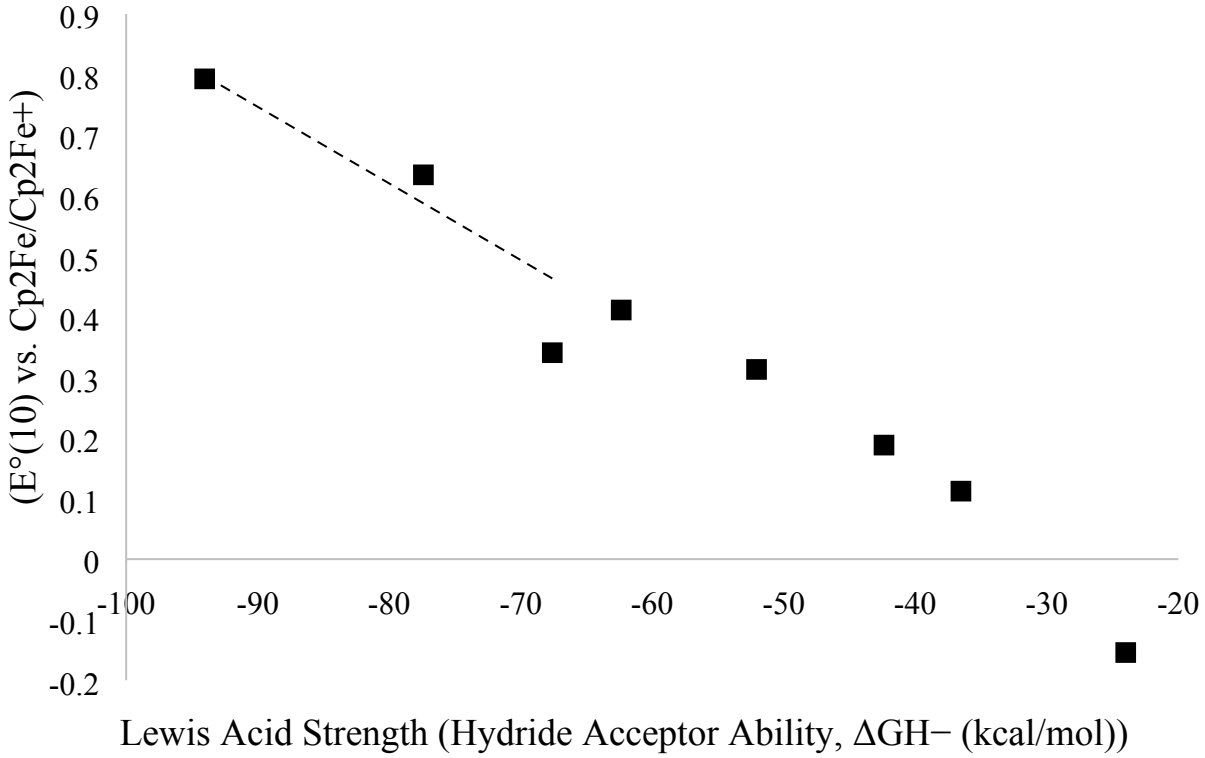


Figure S9. Plot showing the computed second reduction potential (E°(10)) of **[LA_1-HQ]$^+$** as the Lewis acid strength is varied.

2) Plot of Free Energies for the Binding of Q, $[Q]^{\bullet-}$, and $[Q]^{2-}$ to Lewis Acids of Varying Strengths

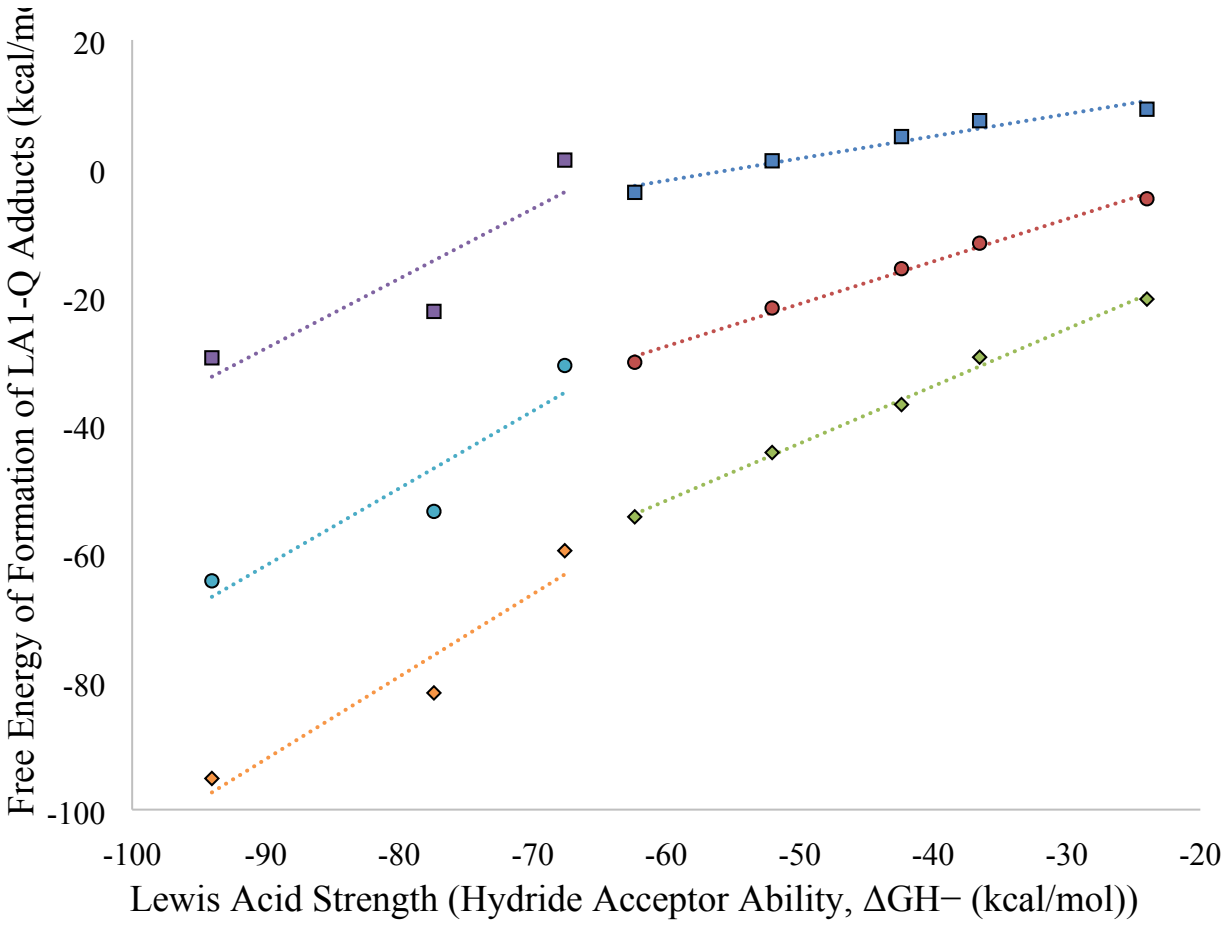


Figure S10. Plot showing the effect of Lewis acid strength on the binding of **Q** to a Lewis acid (ΔG_1), where the purple squares represent silicon-based Lewis acids and the blue squares represent boron-based Lewis acids. The light blue and red circles represent the effect of Lewis acid strength on the binding of $\mathbf{[Q]^{\bullet-}}$ to a Lewis acid (ΔG_2) for silicon-based and boron-based Lewis acids, respectively. The orange and light green diamonds represent the effect of Lewis acid strength on the binding of $\mathbf{[Q]^{2-}}$ to a Lewis acid (ΔG_3) for silicon-based and boron-based Lewis acids, respectively.

3) Plot of Free Energies for the Binding of Q, $[Q]^{\bullet-}$, and $[Q]^{2-}$ to Two Lewis Acids of Varying Strengths

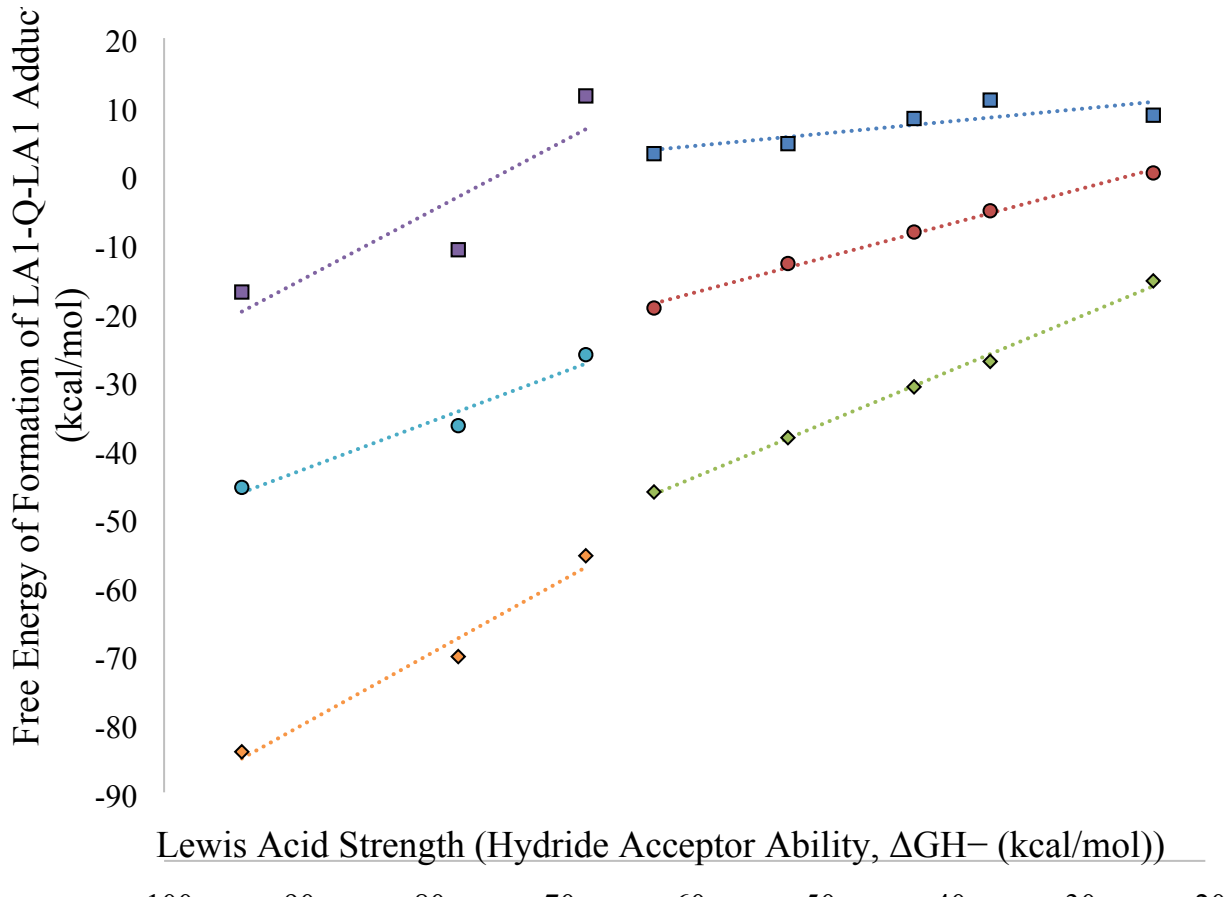


Figure S11. Plot showing the effect of Lewis acid strength on the binding of **LA_1-Q** to a Lewis acid (ΔG_4), where the purple squares represent silicon-based Lewis acids and the blue squares represent boron-based Lewis acids. The light blue and red circles represent the effect of Lewis acid strength on the binding of **$[LA_1\text{-}Q]^{\bullet-}$** to a Lewis acid ($\Delta G_5$) for silicon-based and boron-based Lewis acids, respectively. The orange and light green diamonds represent the effect of Lewis acid strength on the binding of **$[LA_1\text{-}Q]^{2-}$** to a Lewis acid (ΔG_6) for silicon-based and boron-based Lewis acids, respectively.

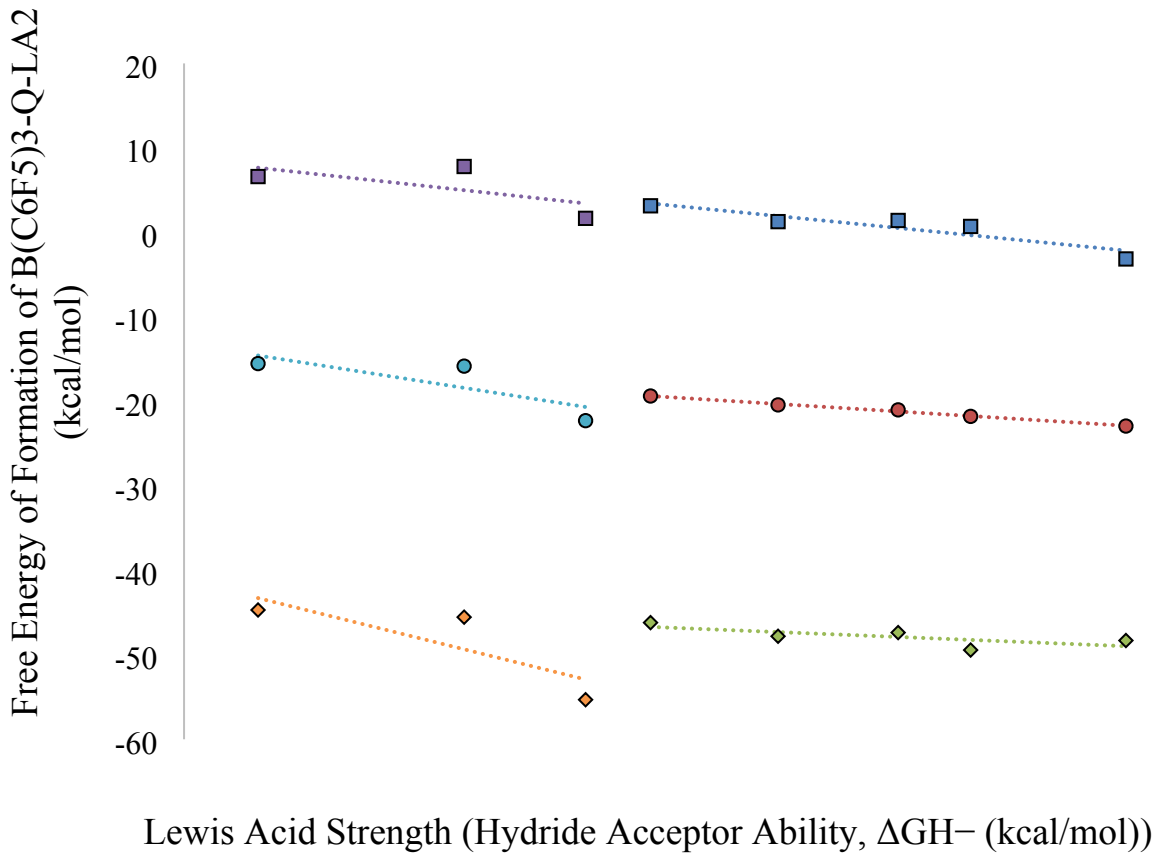
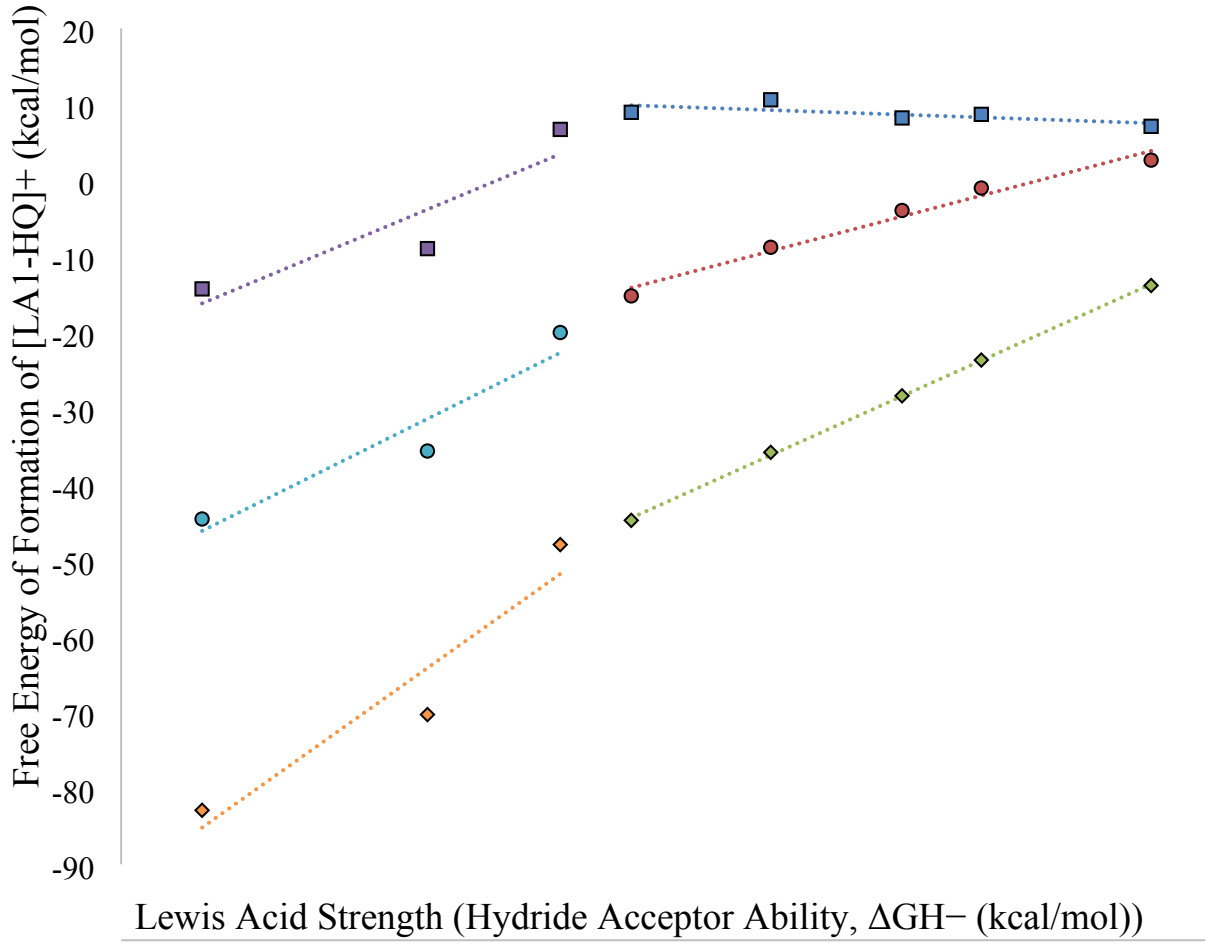


Figure S12. Plot showing the effect of Lewis acid strength on the binding of **$B(C_6F_5)_3$-Q** to a Lewis acid (ΔG_4), where the purple squares represent silicon-based Lewis acids and the blue squares represent boron-based Lewis acids. The light blue and red circles represent the effect of Lewis acid strength on the binding of **$[B(C_6F_5)_3\text{-}Q]^{\bullet-}$** to a Lewis acid ($\Delta G_5$) for silicon-based and boron-based Lewis acids, respectively. The orange and light green diamonds represent the effect of Lewis acid strength on the binding of **$[B(C_6F_5)_3\text{-}Q]^{2-}$** to a Lewis acid ($\Delta G_6$) for silicon-based and boron-based Lewis acids, respectively.

4) Plot of Free Energies for the Binding of $[HQ]^+$, $[HQ]^\bullet$, and $[HQ]^-$ to Lewis Acids of Varying Strengths



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5) Plot of Aromaticity of LA_1-Q, $[LA_1\text{-}Q]^{\bullet-}$, and $[LA_1\text{-}Q]^{2-}$

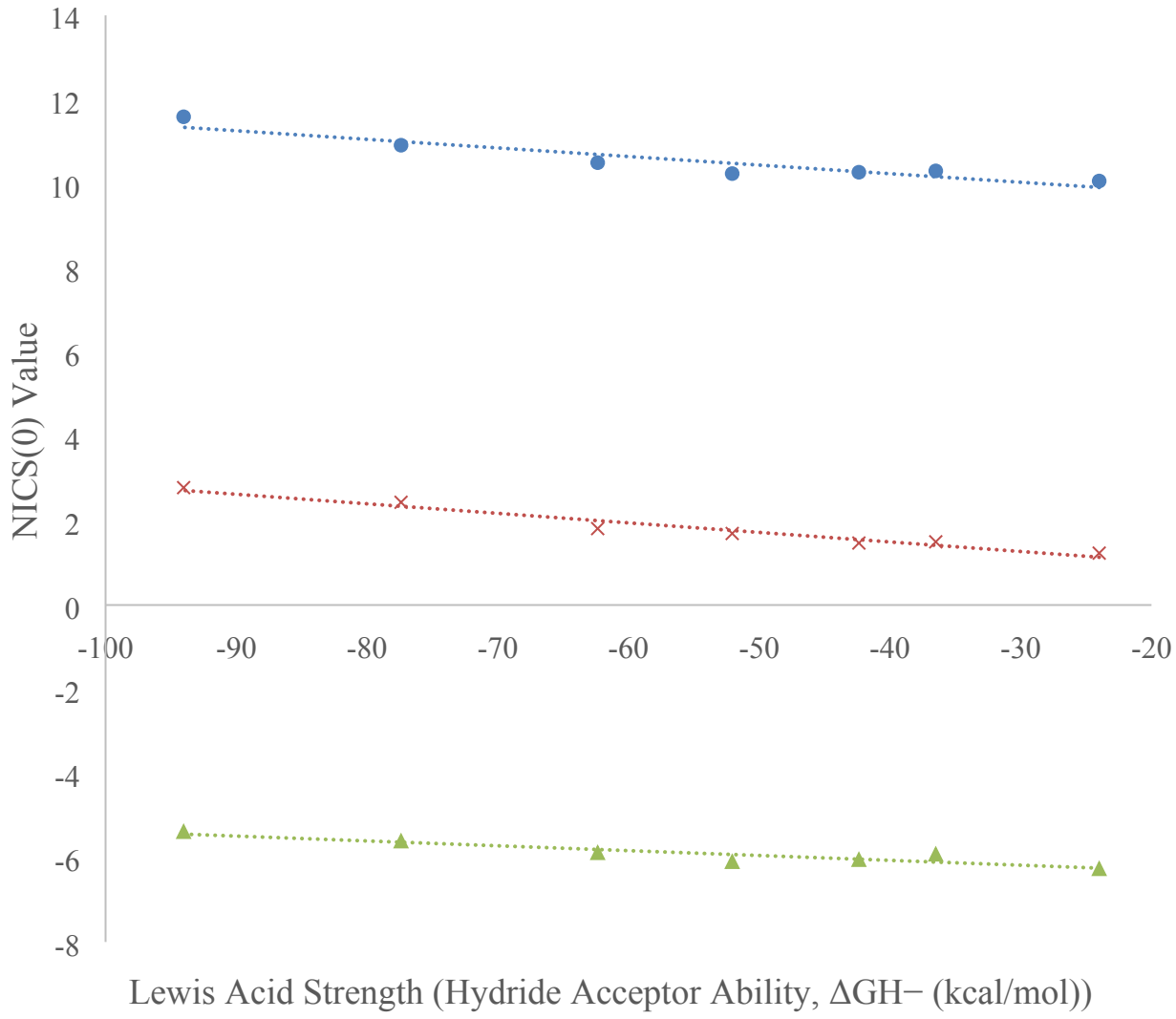

Figure S14. Plot showing the effect of Lewis acid strength on the aromaticity of **Q** (blue circles), **$[Q]^{\bullet-}$** (red squares), and **$[Q]^{2-}$** (light green triangles), through the computation of a NICS(0) value. A more negative value indicates a greater degree of aromaticity.

6) Plots of Frontier Molecular Energies of LA_1-Q, LA_1-Q-LA_1, $B(C_6F_5)_3$-Q-LA_2, and $[LA_1\text{-HQ}]^+$

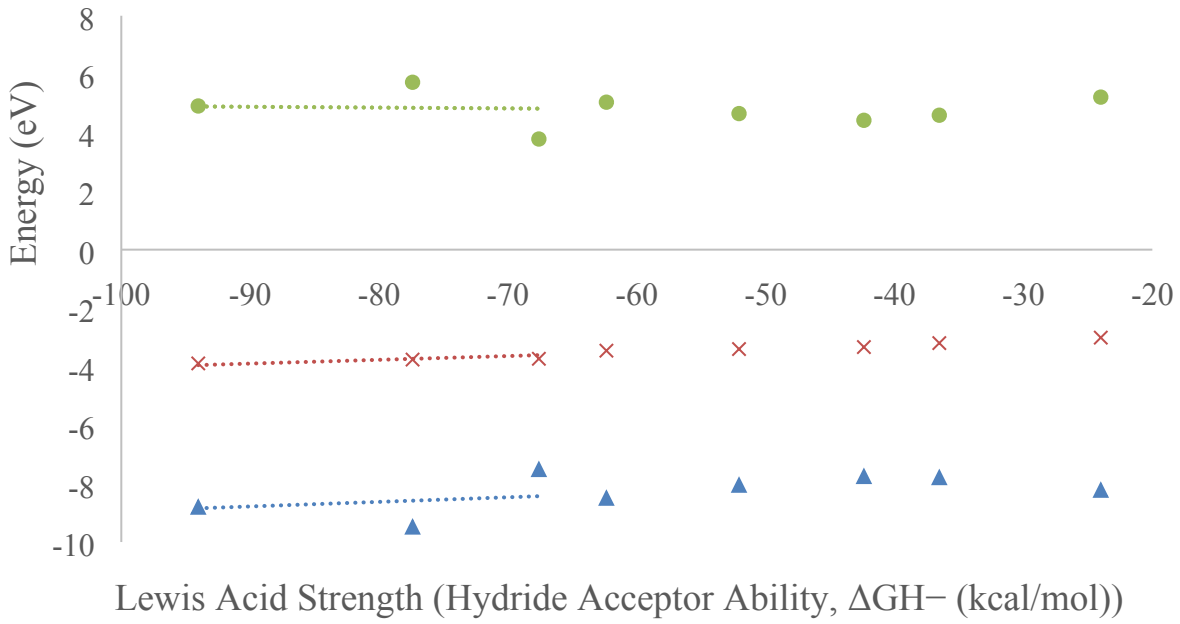

Figure S15. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **LA_1-Q**.

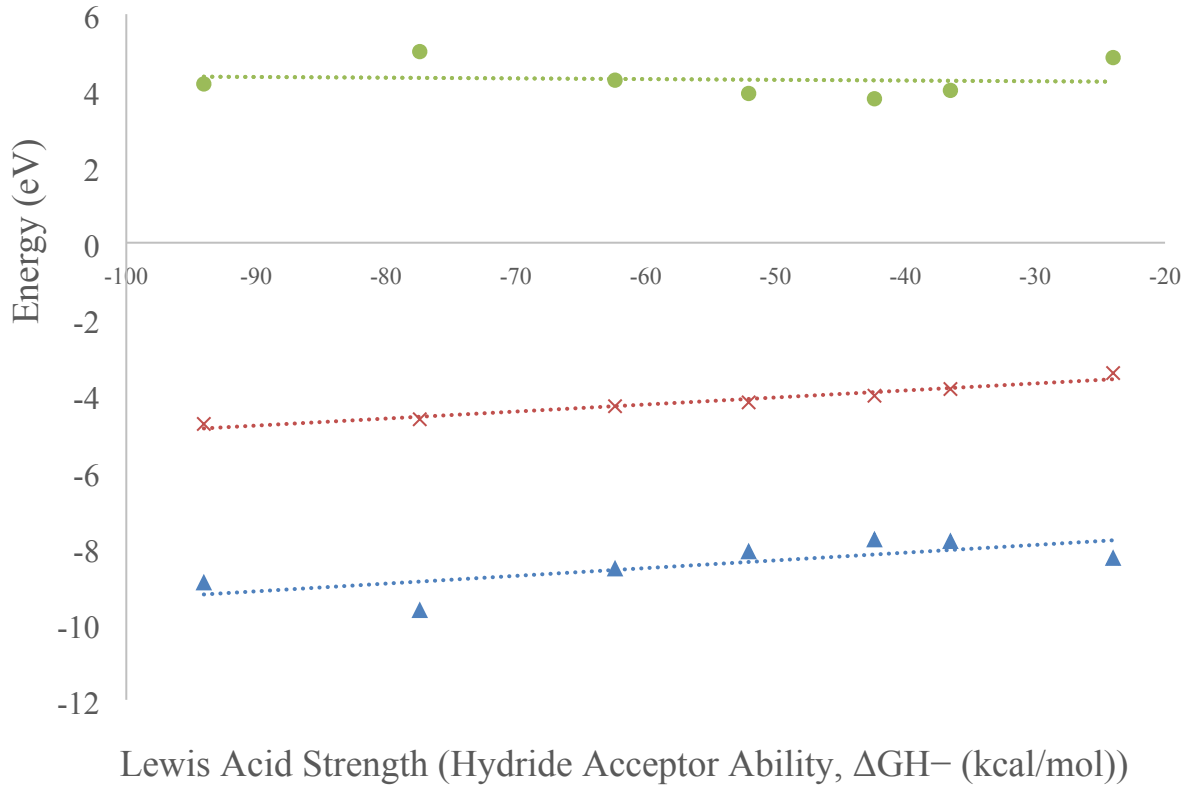

Figure S16. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **LA_1-Q-LA_1**.

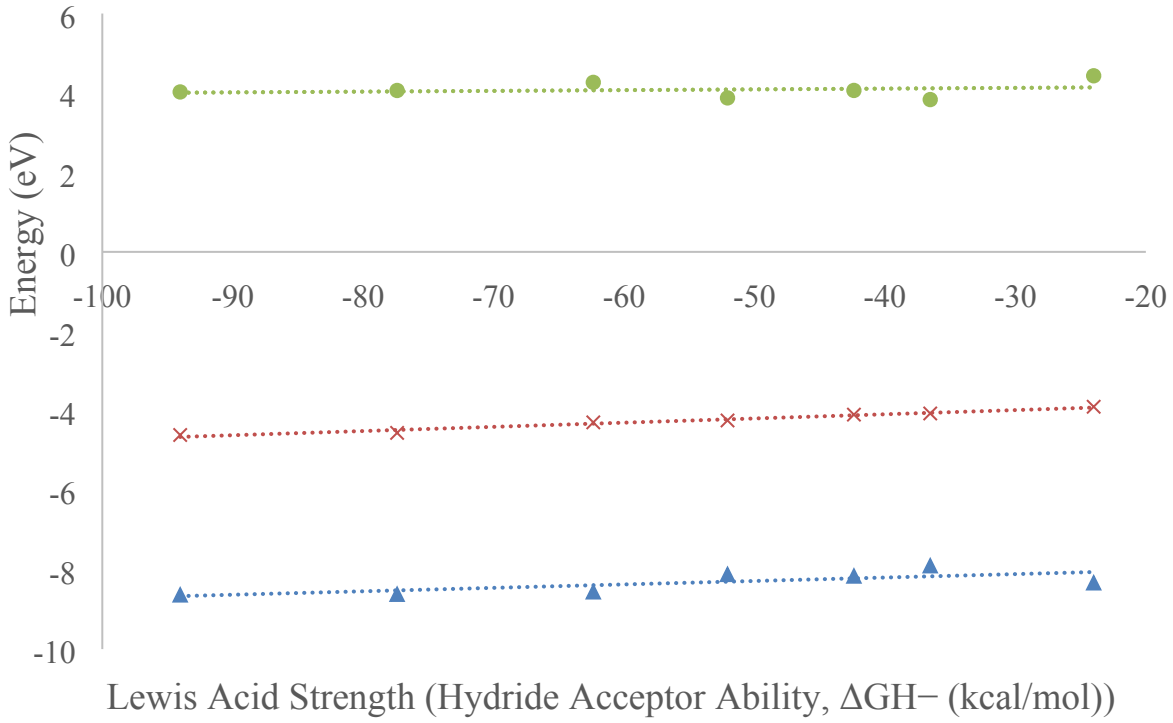

Figure S17. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **$B(C_6F_5)_3$-Q-LA_2**.

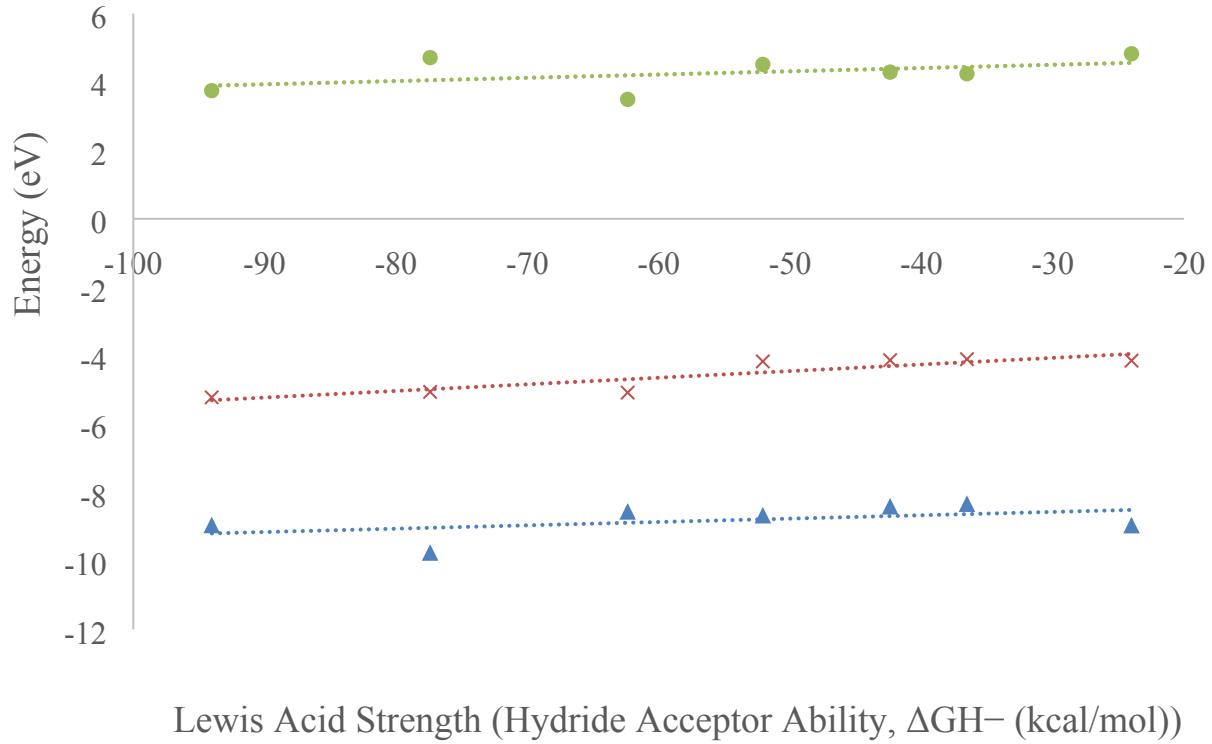

Figure S18. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **[LA_1-HQ]$^+$**.

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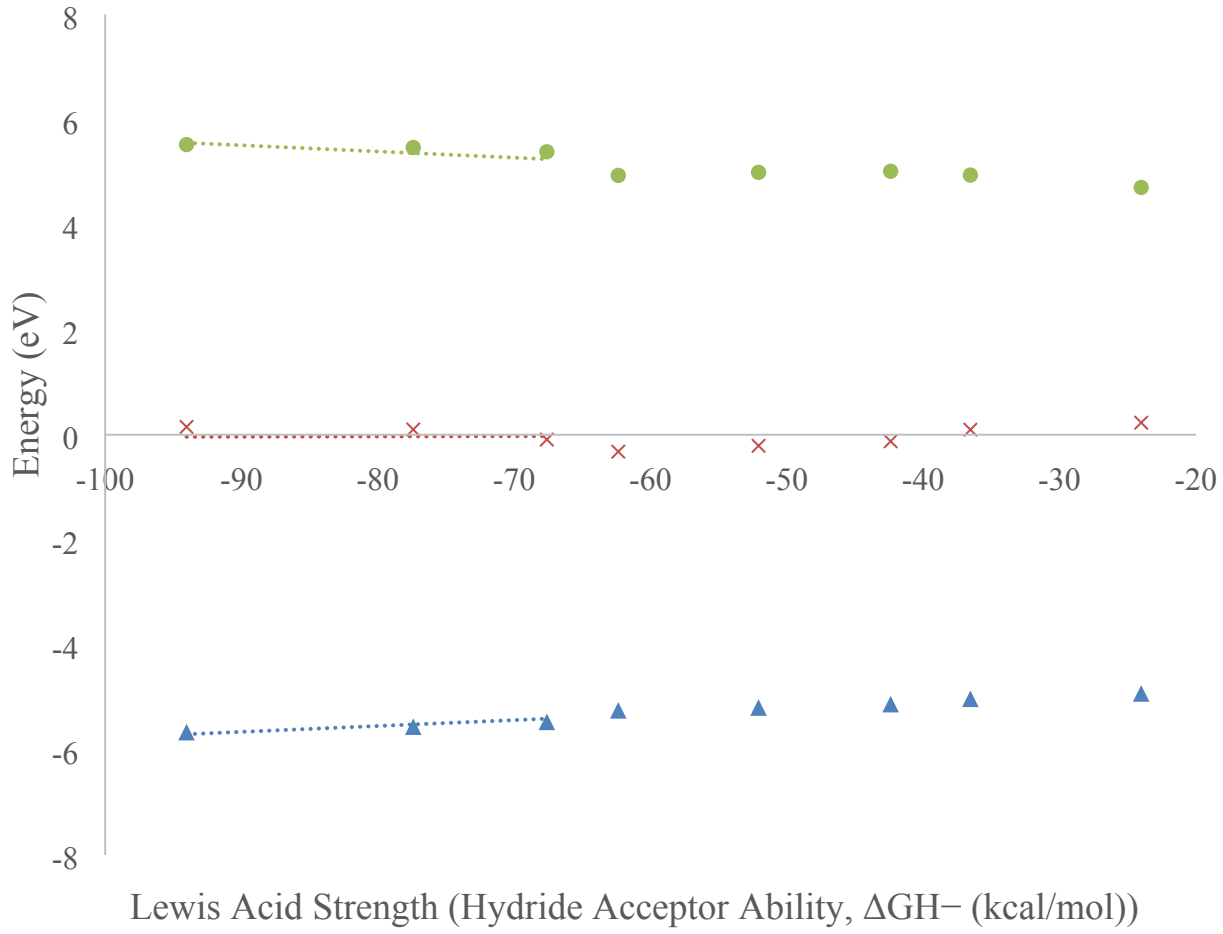


Figure S19. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **$[LA_1\text{-}Q]^{2-}$**.

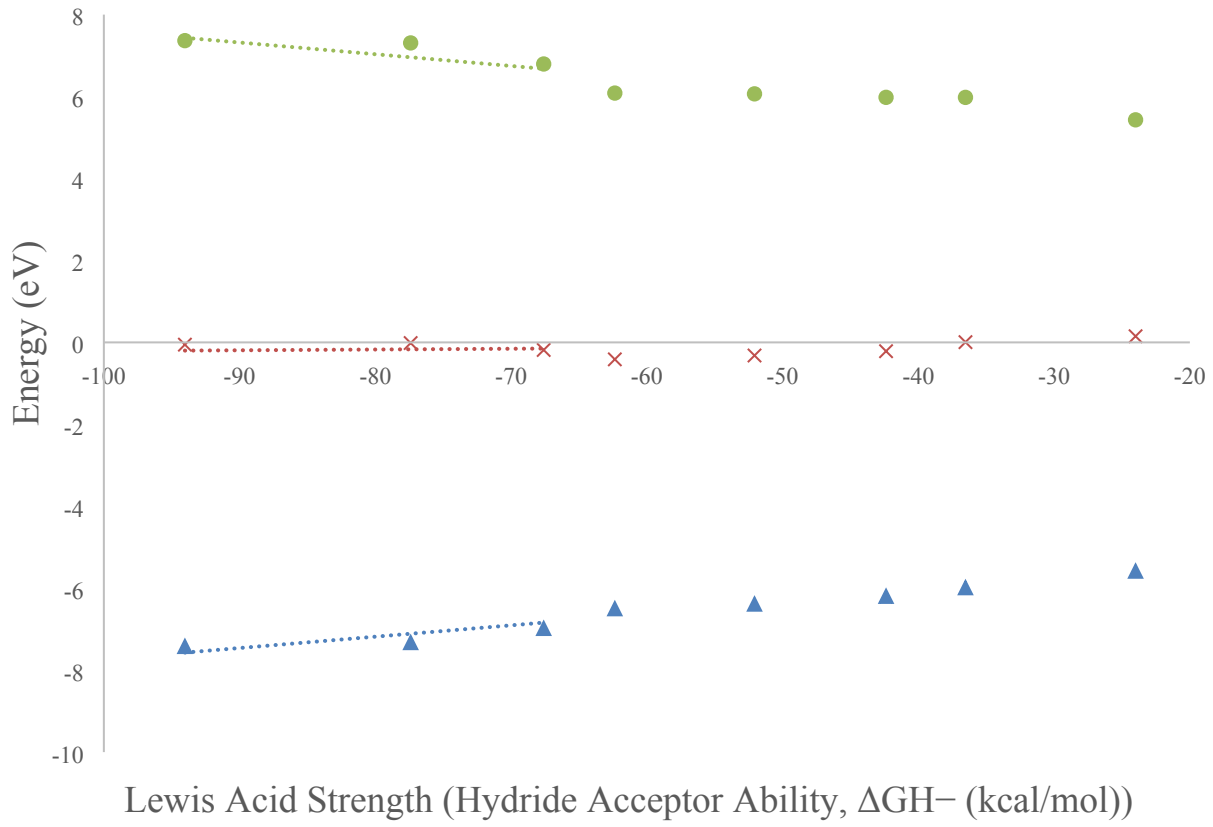


Figure S20. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **$[LA_1\text{-}Q\text{-}LA_1]^{2-}$**.

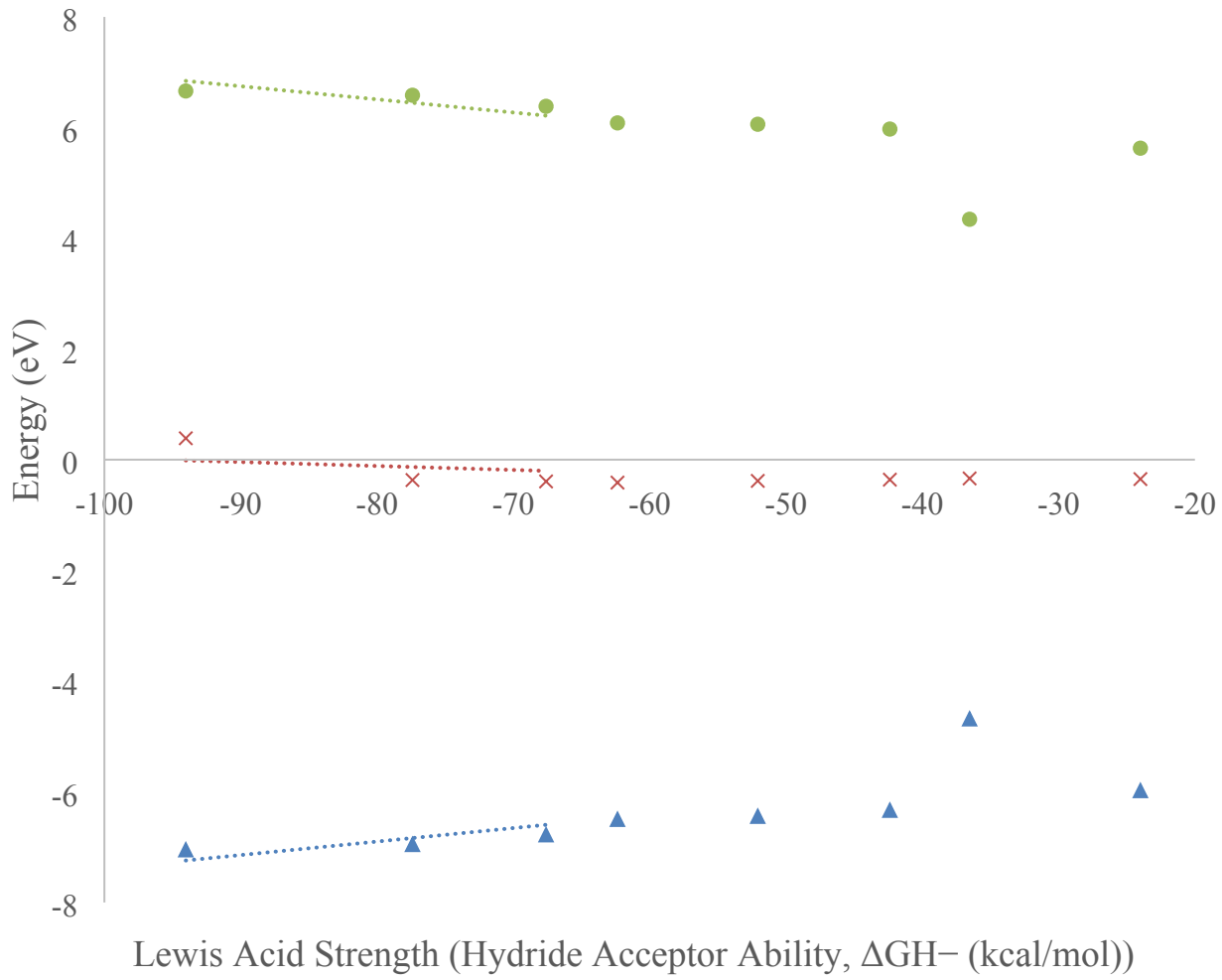


Figure S21. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **$[B(C_6F_5)_3\text{-}Q\text{-}LA_2]^{2-}$**.

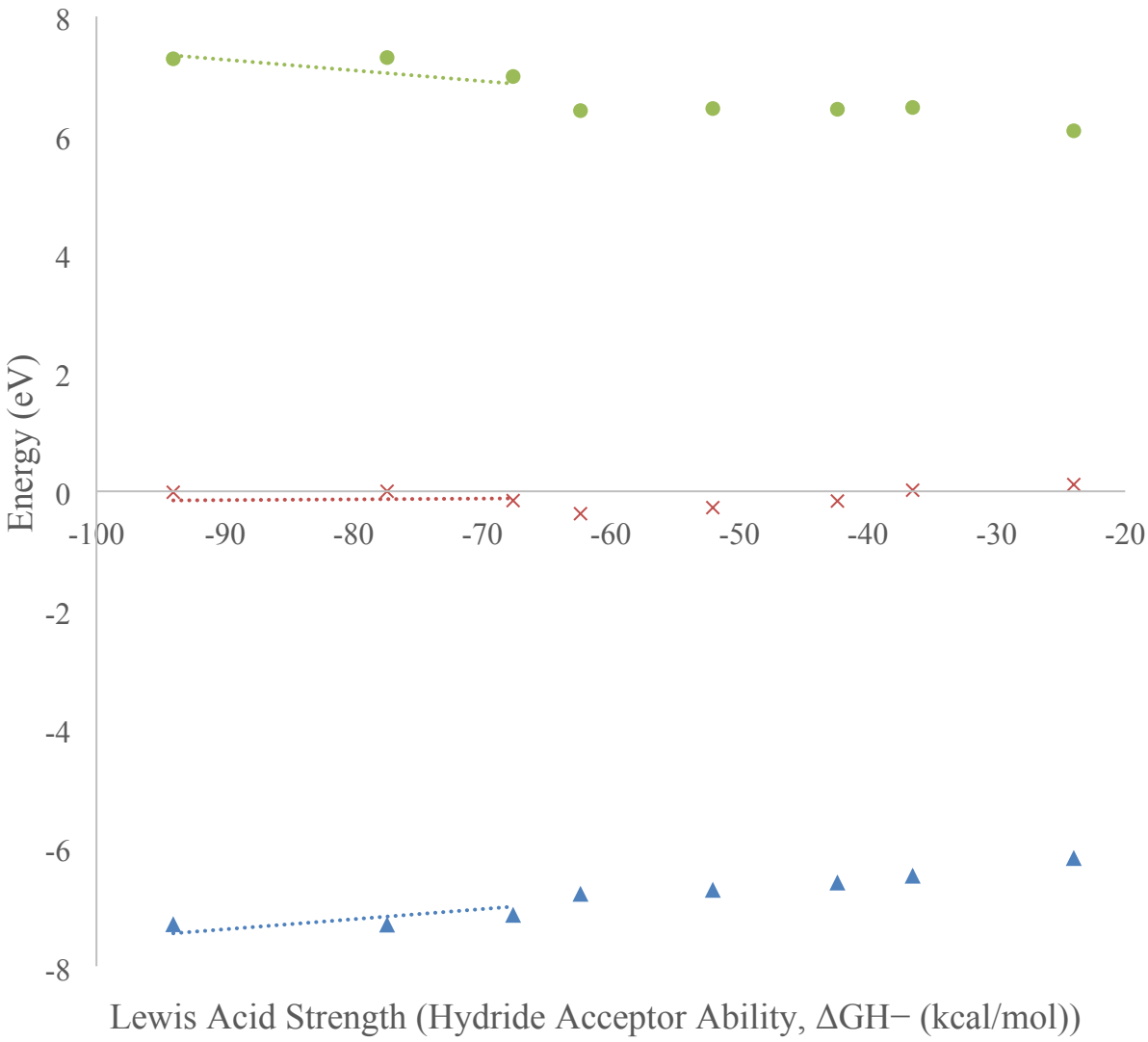


Figure S22. Plot showing the effect of Lewis acid strength on the energy of the HOMO (blue triangles), LUMO (red squares), and HOMO-LUMO gap (light green circles) of **[LA_1-HQ]$^-$**.

8) Plots of the Influence of Lewis Acid Strength on the Ability to Transfer H-atoms and Hydrides from $[LA_1\text{-}HQ]^{\bullet}$ and $[LA_1\text{-}HQ]^{-}$

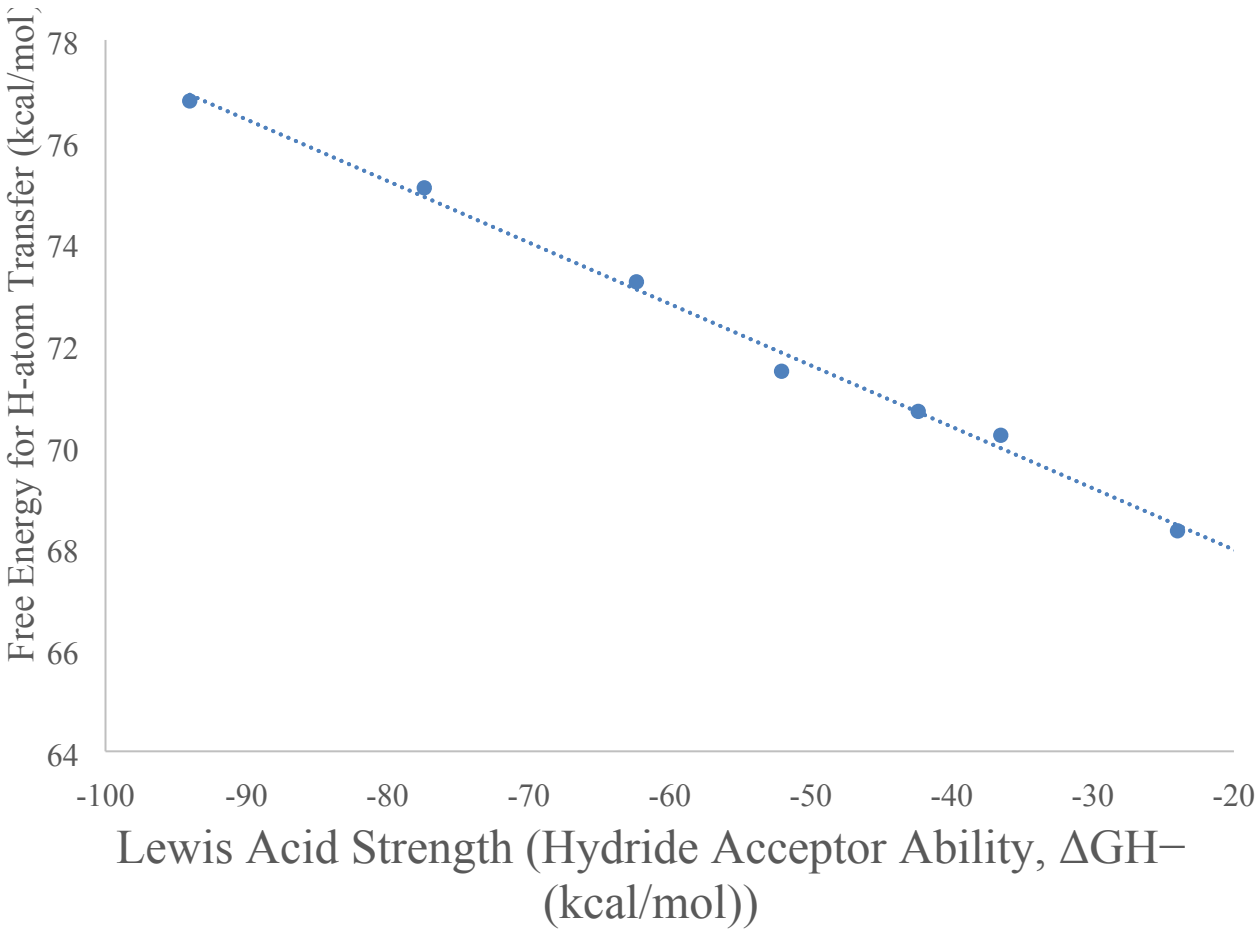


Figure S23. Plot showing the effect of Lewis acid strength on the ability to transfer a H-atom ($\Delta G_{H\bullet}$) from **$[LA_1\text{-}HQ]^{\bullet}$**.

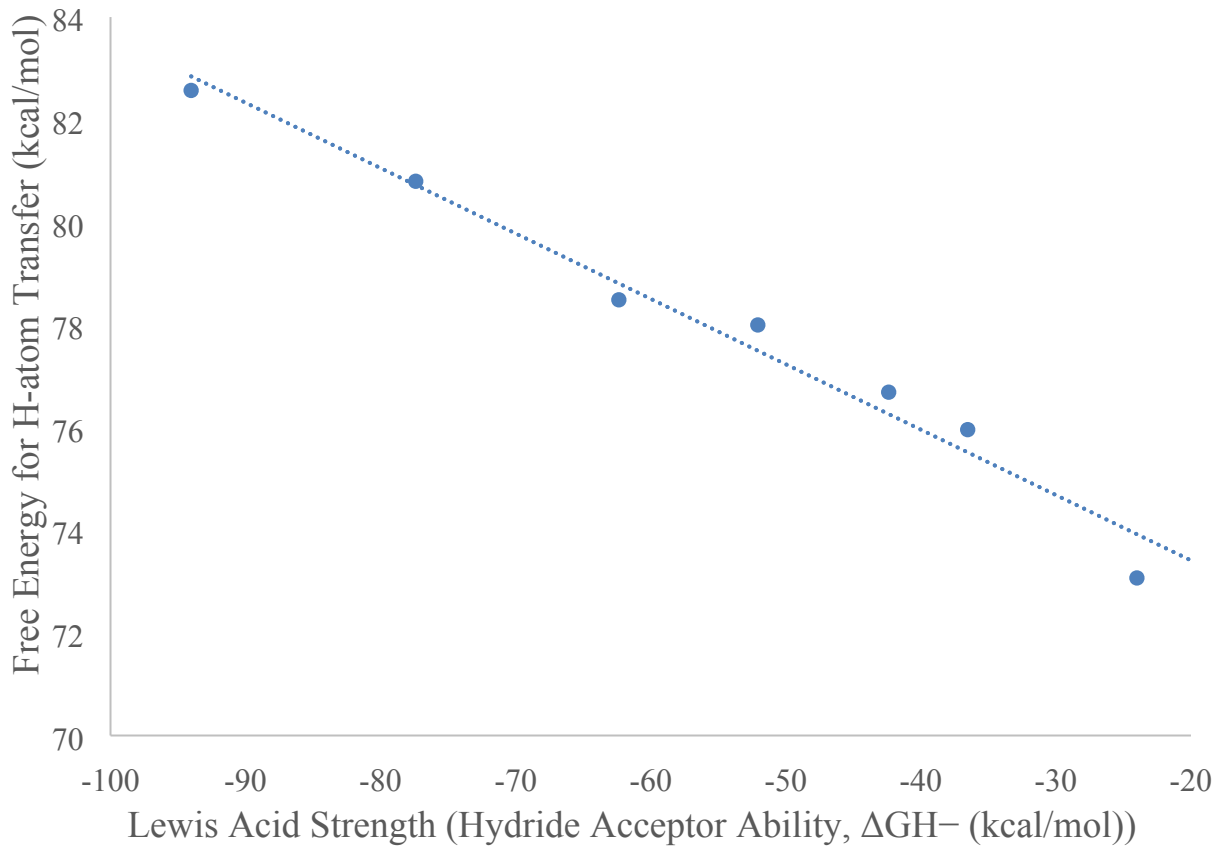


Figure S24. Plot showing the effect of Lewis acid strength on the ability to transfer a H-atom ($\Delta G_{H\bullet}$) from **[LA$_1$-HQ]**$^-$.

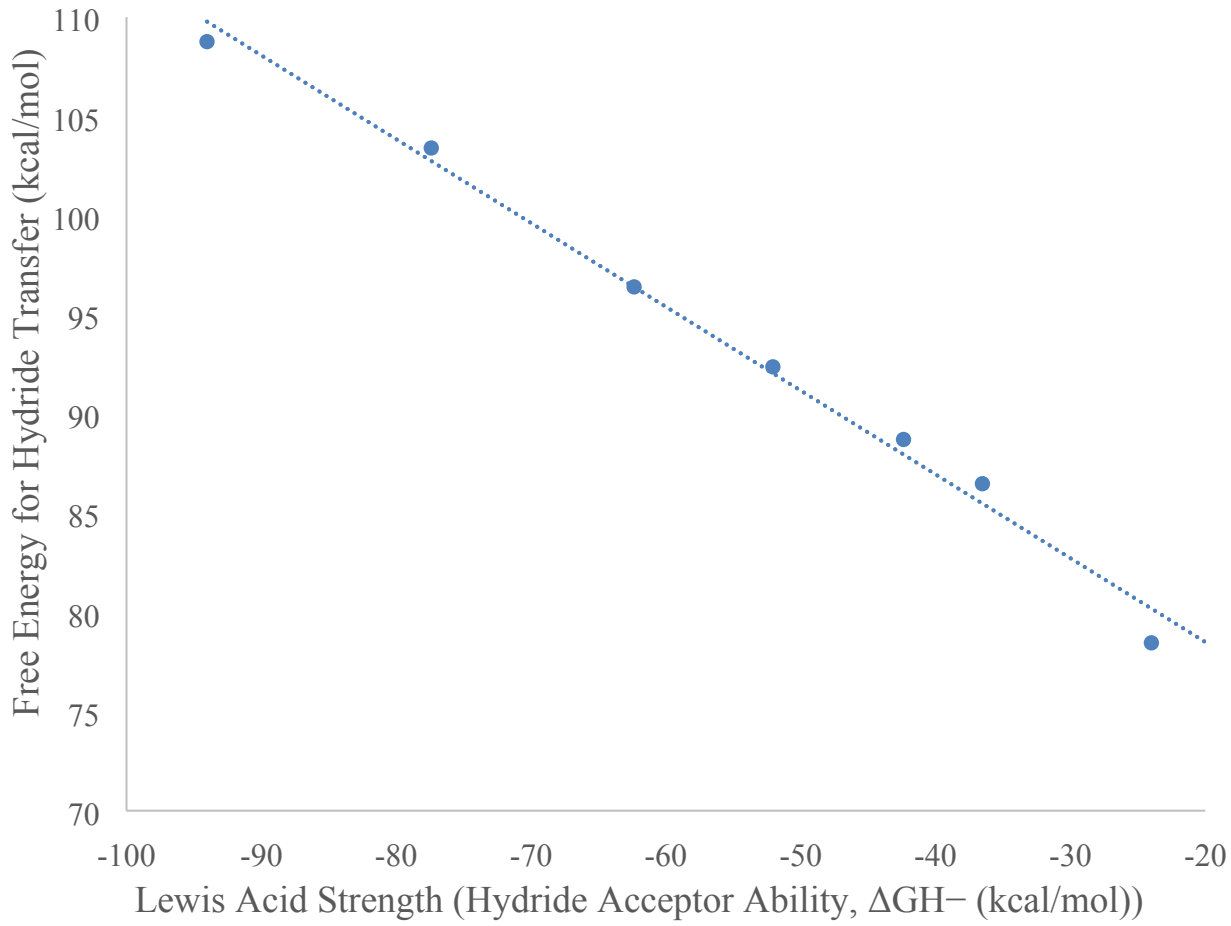


Figure S25. Plot showing the effect of Lewis acid strength on the ability to transfer a hydride (ΔG_{H-}) from **[LA$_1$-HQ]**$^-$.

9) Computed ΔG_{H^-} values of Lewis Acids

Table S1. Computed ΔG_{H^-} values (kcal/mol) of Lewis Acids. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K using either the polar continuum solvation model (PCM)[1] or the universal solvation model (SMD).[2]

Complex	ΔG_{H^-} in MeCN (PCM)	ΔG_{H^-} in MeCN (SMD)
$[SiPhH_2]^+$	-97.34	-94.03
$[SiEt_3]^+$	-83.85	-77.40
$[Si(C_6Me_5)_3]^+$	-74.48	-67.57
$B(C_6F_5)_3$	-66.72	-62.36
$BPh(C_6F_5)_2$	-55.48	-52.07
$BPh_2(C_6F_5)$	-44.98	-42.38
BPh_3	-37.76	-36.53
BEt_3	-23.70	-24.00

10) Computed Free Energy of Formation of Acetonitrile-Lewis Acid Adducts

Table S2. Computed free energy of formation of acetonitrile-Lewis acid adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K using either the polar continuum solvation model (PCM)[1] or the universal solvation model (SMD).[2]

Complex	ΔG_f (PCM)	ΔG_f (SMD)
$[MeCN\text{-}SiPhH_2]^+$	-31.89	-34.31
$[MeCN\text{-}SiEt_3]^+$	-28.19	-28.79
$[MeCN\text{-}Si(C_6Me_5)_3]^+$	-14.09	-13.91
$MeCN\text{-}B(C_6F_5)_3$	-10.55	-10.96
$MeCN\text{-}BPh(C_6F_5)_2$	-3.86	-4.58
$MeCN\text{-}BPh_2(C_6F_5)$	0.30	-0.74
$MeCN\text{-}BPh_3$	2.77	1.32
$MeCN\text{-}BEt_3$	4.38	3.30

11) Computed Free Energies of Formation for Lewis Acid-Q/$[Q]^{\bullet-}$/$[Q]^{2-}$ Adducts

Table S3. Computed free energy of formation (ΔG_1, ΔG_2, and ΔG_3 in kcal/mol) for **LA_1-Q/$[Q]^{\bullet-}$/$[Q]^{2-}$** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	ΔG_f
$[SiPhH_2\text{-}Q]^+$	-29.56
$[SiPhH_2\text{-}Q]^{\bullet}$	-64.33
$[SiPhH_2\text{-}Q]^-$	-95.14
$[SiEt_3\text{-}Q]^+$	-22.32
$[SiEt_3\text{-}Q]^{\bullet}$	-53.50
$[SiEt_3\text{-}Q]^-$	-81.80
$[Si(C_6Me_5)_3\text{-}Q]^+$	1.27
$[Si(C_6Me_5)_3\text{-}Q]^{\bullet}$	-30.75
$[Si(C_6Me_5)_3\text{-}Q]^-$	-59.63
$B(C_6F_5)_3\text{-}Q$	-3.76
$[B(C_6F_5)_3\text{-}Q]^{\bullet-}$	-30.25
$[B(C_6F_5)_3\text{-}Q]^{2-}$	-54.35
$B(C_6F_5)_2Ph\text{-}Q$	1.16
$[B(C_6F_5)_2Ph\text{-}Q]^{\bullet-}$	-21.79
$[B(C_6F_5)_2Ph\text{-}Q]^{2-}$	-44.32
$B(C_6F_5)Ph_2\text{-}Q$	4.94
$[B(C_6F_5)Ph_2\text{-}Q]^{\bullet-}$	-15.66
$[B(C_6F_5)Ph_2\text{-}Q]^{2-}$	-36.85
$BPh_3\text{-}Q$	7.42
$[BPh_3\text{-}Q]^{\bullet-}$	-11.68
$[BPh_3\text{-}Q]^{2-}$	-29.46
$BEt_3\text{-}Q$	9.20
$[BEt_3\text{-}Q]^{\bullet-}$	-4.76
$[BEt_3\text{-}Q]^{2-}$	-20.40

Table S4. Computed free energy of formation (ΔG_4, ΔG_5, and ΔG_6 in kcal/mol) for **LA_1-Q/$[Q]^{\bullet-}$/$[Q]^{2-}$-LA_1** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	**ΔG_f**
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{2+}$	-17.03
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{\bullet+}$	-45.53
$SiPhH_2\text{-}Q\text{-}SiPhH_2$	-84.09
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{2+}$	-10.87
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{\bullet+}$	-36.52
$SiEt_3\text{-}Q\text{-}SiEt_3$	-70.20
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{2+}$	11.56
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{\bullet+}$	-26.17
$Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3$	-55.50
$B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3$	3.15
$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{\bullet-}$	-19.37
$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{2-}$	-46.19
$B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph$	4.61
$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{\bullet-}$	-12.88
$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{2-}$	-38.28
$B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2$	8.27
$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{\bullet-}$	-8.28
$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{2-}$	-30.87
$BPh_3\text{-}Q\text{-}BPh_3$	10.96
$[BPh_3\text{-}Q\text{-}BPh_3]^{\bullet-}$	-5.18
$[BPh_3\text{-}Q\text{-}BPh_3]^{2-}$	-27.16
$BEt_3\text{-}Q\text{-}BEt_3$	8.76
$[BEt_3\text{-}Q\text{-}BEt_3]^{\bullet-}$	0.33
$[BEt_3\text{-}Q\text{-}BEt_3]^{2-}$	-15.41

Table S5. Computed free energy of formation (ΔG_4, ΔG_5, and ΔG_6 in kcal/mol) for **$B(C_6F_5)_3$-Q/$[Q]^{\bullet-}$/$[Q]^{2-}$-LA_2** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	ΔG_f
$[B(C_6F_5)_3\text{-Q-SiPhH}_2]^+$	6.61
$[B(C_6F_5)_3\text{-Q-SiPhH}_2]^\bullet$	-15.53
$[B(C_6F_5)_3\text{-Q-SiPhH}_2]^-$	-44.70
$[B(C_6F_5)_3\text{-Q-SiEt}_3]^+$	7.80
$[B(C_6F_5)_3\text{-Q-SiEt}_3]^\bullet$	-15.83
$[B(C_6F_5)_3\text{-Q-SiEt}_3]^-$	-45.55
$[B(C_6F_5)_3\text{-Q-Si}(C_6Me_5)_3]^+$	1.66
$[B(C_6F_5)_3\text{-Q-Si}(C_6Me_5)_3]^\bullet$	-22.29
$[B(C_6F_5)_3\text{-Q-Si}(C_6Me_5)_3]^-$	-55.32
$B(C_6F_5)_3\text{-Q-B}(C_6F_5)_2Ph$	1.27
$[B(C_6F_5)_3\text{-Q-B}(C_6F_5)_2Ph]^{\bullet-}$	-20.42
$[B(C_6F_5)_3\text{-BQ-B}(C_6F_5)_2Ph]^{2-}$	-47.81
$B(C_6F_5)_3\text{-Q-B}(C_6F_5)Ph_2$	1.41
$[B(C_6F_5)_3\text{-Q-B}(C_6F_5)Ph_2]^{\bullet-}$	-21.01
$[B(C_6F_5)_3\text{-Q-B}(C_6F_5)Ph_2]^{2-}$	-47.37
$B(C_6F_5)_3\text{-Q-BPh}_3$	0.70
$[B(C_6F_5)_3\text{-Q-BPh}_3]^{\bullet-}$	-21.78
$[B(C_6F_5)_3\text{-Q-BPh}_3]^{2-}$	-49.44
$B(C_6F_5)_3\text{-Q-BEt}_3$	-3.14
$[B(C_6F_5)_3\text{-Q-BEt}_3]^{\bullet-}$	-22.93
$[B(C_6F_5)_3\text{-Q-BEt}_3]^{2-}$	-48.31

Table S6. Computed free energy of formation (ΔG_7, ΔG_8, and ΔG_9 in kcal/mol) for **LA_1-[HQ]$^+$/[HQ]$^{\bullet}$/[HQ]$^-$** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	**ΔG_f**
$[SiPhH_2\text{-}HQ]^{2+}$	-14.28
$[SiPhH_2\text{-}HQ]^{\bullet+}$	-44.56
$SiPhH_2\text{-}HQ$	-82.90
$[SiEt_3\text{-}HQ]^{2+}$	-8.98
$[SiEt_3\text{-}HQ]^{\bullet+}$	-35.61
$SiEt_3\text{-}HQ$	-70.30
$[Si(C_6Me_5)_3\text{-}HQ]^{2+}$	6.71
$[Si(C_6Me_5)_3\text{-}HQ]^{\bullet+}$	-20.02
$HQ\text{-}Si(C_6Me_5)_3$	-47.93
$[B(C_6F_5)_3\text{-}HQ]^+$	8.96
$[B(C_6F_5)_3\text{-}HQ]^{\bullet}$	-15.20
$[B(C_6F_5)_3\text{-}HQ]^-$	-44.74
$[B(C_6F_5)_2Ph\text{-}HQ]^+$	10.61
$[B(C_6F_5)_2Ph\text{-}HQ]^{\bullet}$	-8.80
$[HQ\text{-}B(C_6F_5)_2Ph]^-$	-35.79
$[HQ\text{-}BPh_2(C_6F_5)]^+$	8.22
$HQ\text{-}BPh_2(C_6F_5)$	-3.96
$[HQ\text{-}BPh_2(C_6F_5)]^-$	-28.35
$[HQ\text{-}BPh_3]^+$	8.69
$HQ\text{-}BPh_3$	-1.00
$[HQ\text{-}BPh_3]^-$	-23.64
$[HQ\text{-}BEt_3]^+$	7.12
$HQ\text{-}BEt_3$	2.67
$[HQ\text{-}BEt_3]^-$	-13.83

12) Computed Reduction Potentials for Lewis Acid-Q/[Q]$^{\bullet-}$ Adducts

Table S7. Computed reduction potentials of benzoquinone (E°(1) and E°(2)) vs. Cp_2Fe/Cp_2Fe^+ using the 6-31G(d,p) basis set for all non metal atoms and the SDD basis set for iron in all geometry optimizations. The 6-311++G(d,p) basis set was used for all non metal atoms and the SDD basis set for iron in all single point solvation calculations. All solvation calculations were performed in MeCN at 298K using the universal solvation model (SMD).[2]

Functional	E°(1) (V)	E°(2) (V)	Average Difference from Experimental Values
Experiment	-0.94	-1.79	0
M06-2X	-0.96	-2.20	0.276
B3LYP	-1.05	-2.38	0.350
B3LYP-D3	-1.09	-2.50	0.351
X3LYP	-1.06	-2.43	0.375
TPPSh	-1.06	-2.46	0.397
M06	-0.51	-2.34	0.489
BP86	-0.41	-2.25	0.497
B97D	-0.46	-2.45	0.570
M06L	-0.46	-2.55	0.619

Table S8. Computed reduction potentials (E°(1), E°(2), E°(3), and E°(4)) vs. Cp_2Fe/Cp_2Fe^+ for **LA_1-Q/[Q]$^{\bullet-}$** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Redox Potential (V)
Q	-0.96
$[Q]^{\bullet-}$	-2.20
$[SiPhH_2\text{-}Q]^+$	0.54
$[SiPhH_2\text{-}Q]^{\bullet}$	-0.86
$[SiEt_3\text{-}Q]^+$	0.39
$[SiEt_3\text{-}Q]^{\bullet}$	-0.97
$[Si(C_6Me_5)_3\text{-}Q]^+$	0.42
$[Si(C_6Me_5)_3\text{-}Q]^{\bullet}$	-0.95
$[B(C_6F_5)_3\text{-}Q$	0.18
$[B(C_6F_5)_3\text{-}Q]^{\bullet-}$	-1.16
$B(C_6F_5)_2Ph\text{-}Q$	0.03
$[B(C_6F_5)_2Ph\text{-}Q]^{\bullet-}$	-1.22
$B(C_6F_5)Ph_2\text{-}Q$	-0.07
$[B(C_6F_5)Ph_2\text{-}Q]^{\bullet-}$	-1.28
$BPh_3\text{-}Q$	-0.14
$[BPh_3\text{-}Q]^{\bullet-}$	-1.43
$BEt_3\text{-}Q$	-0.36

Table S9. Computed reduction potentials (E°(3), and E°(4)) vs. Cp_2Fe/Cp_2Fe^+ for **LA_1-Q/[Q]$^{\bullet-}$-LA_1** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Redox Potential (V)
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{2+}$	1.78
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{\bullet+}$	0.81
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{2+}$	1.50
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{\bullet+}$	0.49
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{2+}$	2.06
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{\bullet+}$	0.32
$B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3$	1.16
$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{\bullet-}$	0.01
$B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph$	0.79
$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{\bullet-}$	-0.12
$B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2$	0.65
$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{\bullet-}$	-0.30
$BPh_3\text{-}Q\text{-}BPh_3$	0.56
$[BPh_3\text{-}Q\text{-}BPh_3]^{\bullet-}$	-0.48
$BEt_3\text{-}Q\text{-}BEt_3$	0.01
$[BEt_3\text{-}Q\text{-}BEt_3]^{\bullet-}$	-0.84

Table S10. Computed reduction potentials (E°(3), and E°(4)) vs. Cp_2Fe/Cp_2Fe^+ for **$B(C_6F_5)_3$-Q/$[Q]^{\bullet-}$-LA_1** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Redox Potential (V)
$[B(C_6F_5)_3\text{-BQ-SiPhH}_2]^+$	1.50
$[B(C_6F_5)_3\text{-BQ-SiPhH}_2]^\bullet$	0.40
$[B(C_6F_5)_3\text{-BQ-SiEt}_3]^+$	1.41
$[B(C_6F_5)_3\text{-BQ-SiEt}_3]^\bullet$	0.31
$[B(C_6F_5)_3\text{-BQ-Si}(C_6Me_5)_3]^+$	1.24
$[B(C_6F_5)_3\text{-BQ-Si}(C_6Me_5)_3]^\bullet$	0.26
$B(C_6F_5)_3\text{-BQ-B}(C_6F_5)_2Ph$	0.97
$[B(C_6F_5)_3\text{-BQ-B}(C_6F_5)_2Ph]^{\bullet-}$	-0.04
$B(C_6F_5)_3\text{-BQ-B}(C_6F_5)Ph_2$	0.90
$[B(C_6F_5)_3\text{-BQ-B}(C_6F_5)Ph_2]^{\bullet-}$	-0.14
$B(C_6F_5)_3\text{-BQ-BPh}_3$	0.84
$[B(C_6F_5)_3\text{-BQ-BPh}_3]^{\bullet-}$	-0.23
$B(C_6F_5)_3\text{-BQ-BEt}_3$	0.50
$[B(C_6F_5)_3\text{-BQ-BEt}_3]^{\bullet-}$	-0.42

Table S11. Computed reduction potentials (E°(7), E°(8), E°(9), and E°(10)) vs. Cp_2Fe/Cp_2Fe^+ for **LA_1-[HQ]$^+$/[HQ]$^\bullet$** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

Complex	Redox Potential
$[HQ]^+$	0.37
$[HQ]^{\bullet-}$	-1.14
$[H\text{-}HQ]^{2+}$	1.90
$[H\text{-}HQ]^{\bullet+}$	0.51
$[SiPhH_2\text{-}HQ]^{2+}$	1.95
$[SiPhH_2\text{-}HQ]^{\bullet+}$	0.79
$[SiEt_3\text{-}HQ]^{2+}$	1.79
$[SiEt_3\text{-}HQ]^{\bullet+}$	0.63
$[Si(C_6Me_5)_3\text{-}HQ]^{2+}$	1.79
$[Si(C_6Me_5)_3\text{-}HQ]^{\bullet+}$	0.34
$[B(C_6F_5)_3\text{-}HQ]^+$	1.68
$[B(C_6F_5)_3\text{-}HQ]^\bullet$	0.41
$[B(C_6F_5)_2Ph\text{-}HQ]^+$	1.38
$[B(C_6F_5)_2Ph\text{-}HQ]^\bullet$	0.31
$[B(C_6F_5)Ph_2\text{-}HQ]^+$	1.11
$[B(C_6F_5)Ph_2\text{-}HQ]^\bullet$	0.19
$[BPh_3\text{-}HQ]^+$	1.05
$[BPh_3\text{-}HQ]^\bullet$	0.11
$[BEt_3\text{-}HQ]^+$	0.83
$[BEt_3\text{-}HQ]^\bullet$	-0.15

13) Energies for Computed Structures

Table S12. Computed energies for the optimized structures of the **LA_1-Q** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

LA_1-Q	**Electronic Energies Gas Phase (Hartrees)**	**Free Energy Correction Gas Phase (Hartrees)**	**Enthalpy Correction Gas Phase (Hartrees)**
Q	-381.296290	0.055641	0.093408
$[Q]^{\bullet-}$	-381.355670	0.053848	0.091474
$[Q]^{2-}$	-381.201512	0.052440	0.089230
$[SiPhH_2\text{-}Q]^{+}$	-903.2852613	0.154655	0.212679
$[SiPhH_2\text{-}Q]^{\bullet}$	-903.5482001	0.152962	0.211156
$[SiPhH_2\text{-}Q]^{-}$	-903.6117445	0.152487	0.210111
$[SiEt_3\text{-}Q]^{+}$	-908.1319932	0.240792	0.307774
$[SiEt_3\text{-}Q]^{\bullet}$	-908.3893330	0.239408	0.306287
$[SiEt_3\text{-}Q]^{-}$	-908.4499292	0.234900	0.304999
$[Si(C_6Me_5)_3\text{-}Q]^{+}$	-1954.696430	0.710547	0.835130
$[Si(C_6Me_5)_3\text{-}Q]^{\bullet}$	-1954.104151	0.710086	0.833703
$[Si(C_6Me_5)_3\text{-}Q]^{-}$	-1954.996116	0.709442	0.832280
$B(C_6F_5)_3\text{-}Q$	-2588.832532	0.177776	0.283064
$[B(C_6F_5)_3\text{-}Q]^{\bullet-}$	-2588.975262	0.175760	0.281259
$[B(C_6F_5)_3\text{-}Q]^{2-}$	-2588.933186	0.173476	0.279217
$B(C_6F_5)_2Ph\text{-}Q$	-2092.833315	0.222392	0.318983
$[B(C_6F_5)_2Ph\text{-}Q]^{\bullet-}$	-2092.970377	0.221658	0.317300
$[B(C_6F_5)_2Ph\text{-}Q]^{2-}$	-2092.922892	0.219611	0.315303
$B(C_6F_5)Ph_2\text{-}Q$	-1596.834802	0.267048	0.354855
$[B(C_6F_5)Ph_2\text{-}Q]^{\bullet-}$	-1596.961582	0.266338	0.353097
$[B(C_6F_5)Ph_2\text{-}Q]^{2-}$	-1596.908295	0.264357	0.350905
$BPh_3\text{-}Q$	-1100.833671	0.312840	0.390995
$[BPh_3\text{-}Q]^{\bullet-}$	-1100.954617	0.311836	0.389146
$[BPh_3\text{-}Q]^{2-}$	-1100.893988	0.310876	0.386894
$BEt_3\text{-}Q$	-643.7095341	0.247352	0.309673
$[BEt_3\text{-}Q]^{\bullet-}$	-643.8180804	0.245967	0.307803
$[BEt_3\text{-}Q]^{2-}$	-643.7379794	0.243509	0.304935

Table S13. Computed energies for the optimized structures of the **LA_1-Q-LA_1** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

LA_1-Q-LA_1 Adduct	**Electronic Energies Gas Phase (Hartrees)**	**Free Energy Correction Gas Phase (Hartrees)**	**Enthalpy Correction Gas Phase (Hartrees)**
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{2+}$	-1425.162402	0.251926	0.331418
$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{\bullet+}$	-1425.583185	0.254196	0.331689
$SiPhH_2\text{-}Q\text{-}SiPhH_2$	-1425.845201	0.255021	0.331040
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{2+}$	-1434.858298	0.424141	0.521377
$[SiEt_3\text{-}Q\text{-}SiEt_3]^{\bullet+}$	-1435.267256	0.425583	0.521749
$SiEt_3\text{-}Q\text{-}SiEt_3$	-1435.523044	0.428732	0.520837
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{2+}$	-3526.448362	1.368152	1.575019
$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{\bullet+}$	-3526.828555	1.366112	1.574903
$Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3$	-3527.058856	1.366034	1.573958
$B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3$	-4796.356887	0.299854	0.472628
$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{\bullet-}$	-4796.556888	0.298581	0.471791
$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{2-}$	-4796.609130	0.297890	0.469771
$B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph$	-3804.362193	0.386337	0.544310
$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{\bullet-}$	-3804.550930	0.389467	0.543558
$[B(C_6F_5)_2Ph\text{-}BQ\text{-}B(C_6F_5)_2Ph]^{2-}$	-3804.593513	0.388100	0.541517
$B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2$	-2812.367177	0.476891	0.616226
$[B(C_6F_5)Ph_2\text{-}BQ\text{-}B(C_6F_5)Ph_2]^{\bullet-}$	-2812.540106	0.479319	0.615310
$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{2-}$	-2812.567501	0.477304	0.612951
$BPh_3\text{-}Q\text{-}BPh_3$	-1820.367395	0.570276	0.688473
$[BPh_3\text{-}Q\text{-}BPh_3]^{\bullet-}$	-1820.530343	0.570247	0.687364
$[BPh_3\text{-}Q\text{-}BPh_3]^{2-}$	-1820.546313	0.568818	0.684839
$BEt_3\text{-}Q\text{-}BEt_3$	-906.1156913	0.432239	0.525774
$[BEt_3\text{-}Q\text{-}BEt_3]^{\bullet-}$	-906.2631155	0.438745	0.524438
$[BEt_3\text{-}Q\text{-}BEt_3]^{2-}$	-906.2459751	0.436429	0.521362

Table S14. Computed energies for the optimized structures of the **$B(C_6F_5)_3$-Q-LA_2** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

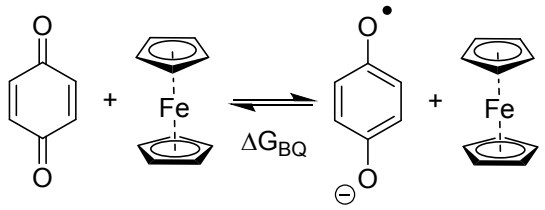
$B(C_6F_5)_3$-Q-LA_2 Adduct	**Electronic Energies Gas Phase (Hartrees)**	**Free Energy Correction Gas Phase (Hartrees)**	**Enthalpy Correction Gas Phase (Hartrees)**
$[B(C_6F_5)_3\text{-BQ-SiPhH}_2]^+$	-3110.795988	0.275339	0.401739
$[B(C_6F_5)_3\text{-BQ-SiPhH}_2]^\bullet$	-3111.103541	0.276055	0.401664
$[B(C_6F_5)_3\text{-BQ-SiPhH}_2]^-$	-3111.256659	0.275389	0.400487
$[B(C_6F_5)_3\text{-BQ-SiEt}_3]^+$	-3115.643494	0.362232	0.496768
$[B(C_6F_5)_3\text{-BQ-SiEt}_3]^\bullet$	-3115.946229	0.363120	0.496856
$[B(C_6F_5)_3\text{-BQ-SiEt}_3]^-$	-3116.098272	0.363663	0.495484
$[B(C_6F_5)_3\text{-BQ-Si}(C_6Me_5)_3]^+$	-4161.207390	0.834529	1.023795
$[B(C_6F_5)_3\text{-BQ-Si}(C_6Me_5)_3]^\bullet$	-4161.488592	0.835144	1.023682
$[B(C_6F_5)_3\text{-BQ-Si}(C_6Me_5)_3]^-$	-4161.633638	0.833398	1.022133
$B(C_6F_5)_3\text{-Q-B}(C_6F_5)_3$	-4796.356887	0.299854	0.472628
$[B(C_6F_5)_3\text{-Q-B}(C_6F_5)_3]^{\bullet-}$	-4796.556888	0.298581	0.471791
$[B(C_6F_5)_3\text{-Q-B}(C_6F_5)_3]^{2-}$	-4796.609130	0.297890	0.469771
$B(C_6F_5)_3\text{-BQ- B}(C_6F_5)_2Ph$	-4300.359748	0.342991	0.508522
$[B(C_6F_5)_3\text{-BQ- B}(C_6F_5)_2Ph]^{\bullet-}$	-4300.553976	0.343914	0.507669
$[B(C_6F_5)_3\text{-BQ-B}(C_6F_5)_2Ph]^{2-}$	-4300.601331	0.342092	0.505609
$B(C_6F_5)_3\text{-BQ- B}(C_6F_5)Ph_2$	-3804.362703	0.388823	0.544500
$[B(C_6F_5)_3\text{-BQ- B}(C_6F_5)Ph_2]^{\bullet-}$	-3804.549065	0.389561	0.543572
$[B(C_6F_5)_3\text{-BQ-B}(C_6F_5)Ph_2]^{2-}$	-3804.587830	0.387353	0.541295
$B(C_6F_5)_3\text{-BQ-BPh}_3$	-3308.363358	0.434741	0.580504
$[B(C_6F_5)_3\text{-BQ-BPh}_3]^{\bullet-}$	-3308.544598	0.434628	0.579495
$[B(C_6F_5)_3\text{-BQ-BPh}_3]^{2-}$	-3308.578356	0.433098	0.577310
$B(C_6F_5)_3\text{-BQ-BEt}_3$	-2851.236701	0.362334	0.499018
$[B(C_6F_5)_3\text{-BQ-BEt}_3]^{\bullet-}$	-2851.411056	0.368312	0.498021
$[B(C_6F_5)_3\text{-BQ-BEt}_3]^{2-}$	-2851.428078	0.366076	0.495543

Table S15. Computed energies for the optimized structures of the **LA_1-HQ** adducts. All calculations were implemented using the M06-2X/6-311++G(d,p)//M06-2X/6-31G(d,p) level of theory in MeCN at 298K.

LA_1-HQ	**Electronic Energies Gas Phase (Hartrees)**	**Free Energy Correction Gas Phase (Hartrees)**	**Enthalpy Correction Gas Phase (Hartrees)**
$[HQ]^+$	-381.6162449	0.068146	0.106186
$[HQ]^\bullet$	-381.8963541	0.066473	0.104643
$[HQ]^-$	-381.9486846	0.063862	0.103373
$[SiPhH_2\text{-}HQ]^{2+}$	-903.4715216	0.165995	0.224403
$[SiPhH_2\text{-}HQ]^{\bullet+}$	-903.9200251	0.166558	0.225159
$SiPhH_2\text{-}HQ$	-904.1891874	0.165959	0.224354
$[SiEt_3\text{-}HQ]^{2+}$	-908.3206774	0.251239	0.319486
$[SiEt_3\text{-}HQ]^{\bullet+}$	-908.7649338	0.252785	0.320180
$SiEt_3\text{-}HQ$	-909.0296311	0.252895	0.319304
$[Si(C_6Me_5)_3\text{-}HQ]^{2+}$	-1954.94447	0.718256	0.843651
$[Si(C_6Me_5)_3\text{-}HQ]^{\bullet+}$	-1954.487985	0.720181	0.846657
$Si(C_6Me_5)_3\text{-}HQ$	-1954.730343	0.723617	0.846695
$[B(C_6F_5)_3\text{-}HQ]^+$	-2589.124644	0.188224	0.294148
$[B(C_6F_5)_3\text{-}HQ]^\bullet$	-2589.450099	0.189259	0.295104
$[B(C_6F_5)_3\text{-}HQ]^-$	-2589.601155	0.188144	0.293776
$[B(C_6F_5)_2Ph\text{-}HQ]^+$	-2093.159331	0.234419	0.331444
$[B(C_6F_5)_2Ph\text{-}HQ]^\bullet$	-2093.448785	0.233959	0.330915
$[B(C_6F_5)_2Ph\text{-}HQ]^-$	-2093.595049	0.233651	0.329762
$[B(C_6F_5)Ph_2\text{-}HQ]^+$	-1597.156453	0.276741	0.367749
$[B(C_6F_5)Ph_2\text{-}HQ]^\bullet$	-1597.449060	0.279216	0.366861
$[B(C_6F_5)Ph_2\text{-}HQ]^-$	-1597.583928	0.278319	0.365453
$[BPh_3\text{-}HQ]^+$	-1101.173362	0.326034	0.404116
$[BPh_3\text{-}HQ]^\bullet$	-1101.447173	0.324550	0.402797
$[BPh_3\text{-}HQ]^-$	-1101.575245	0.323654	0.401371
$[BEt_3\text{-}HQ]^+$	-644.0283202	0.253846	0.321997
$[BEt_3\text{-}HQ]^\bullet$	-644.3215081	0.257782	0.320425
$[BEt_3\text{-}HQ]^-$	-644.4330483	0.257759	0.319785

14) Sample Calculation of Redox Potential for Benzoquinone

G_Q = -239305.9292 kcal/mol
$G_{Q^{\bullet-}}$ = -239397.7387 kcal/mol
G_{Fc} = -320499.3504 kcal/mol
G_{Fc+} = -320385.2878 kcal/mol



Q **Fc** **[Q]•–** **Fc+** (S1)

$$\Delta G_{BQ} = [Products] - [Reactants] = \left[G_{Q^{\bullet-}} + G_{Fc+}\right] - \left[G_Q + G_{Fc}\right] = 22.2531\ kcal/mol$$

This free energy value can now be converted to volts using Equation S2:

$$\Delta G = -nFE° \quad \text{(S2)}$$

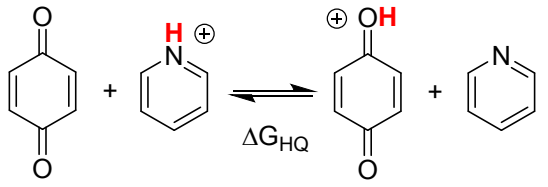
Where ΔG = ΔG_{BQ}, *n* = the number of electrons transferred (1 electron for this reaction), *F* is Faraday's constant (23.061 kcal/volt), and *E*° is the reduction potential in volts, solving for *E*° and inserting the values yields the following:

$$E° = -\frac{\left(22.2531\frac{kcal}{mol}\right)}{(1)\left(23.061\frac{kcal}{mol \cdot volt}\right)} = -0.964\ V$$

Since the reduction potential of ferrocenium (**Fc+**) is defined as 0.0 V, no further correction of the reduction potential is needed.

15) Sample Calculation of pK_a for Protonated Benzoquinone

G_Q = -239305.9292 kcal/mol
G_{HQ+} = -239550.529 kcal/mol
G_{Py} = -155737.9626 kcal/mol
G_{PyH+} = -156012.9224 kcal/mol



Q **[PyH]$^+$** **[HQ]$^+$** **Py** (S3)

$$\Delta G_{HQ} = [Products] - [Reactants] = \left[G_{HQ+} + G_{Py}\right] - \left[G_Q + G_{PyH+}\right] = 30.36\ kcal/mol$$

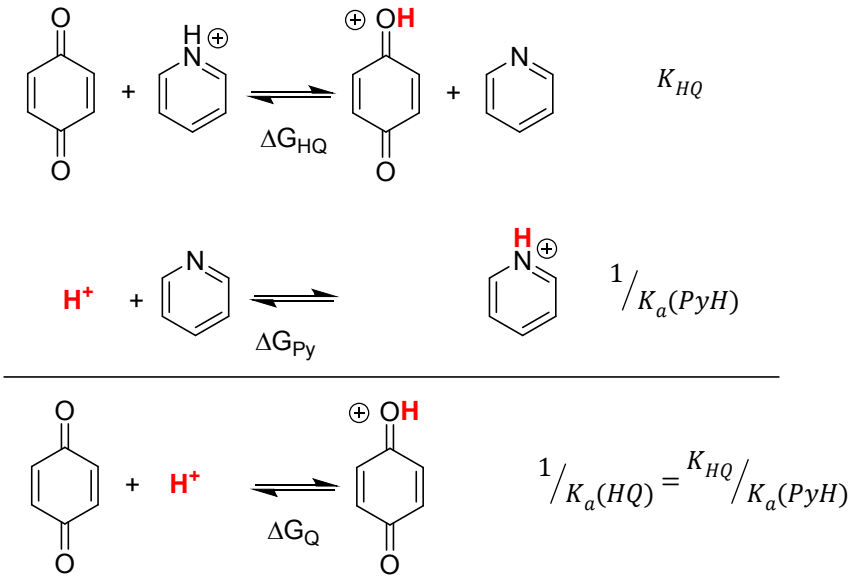
This free energy value can now be converted to an equilibrium constant using Equation S4:

$$\Delta G_{HQ} = -RT\ ln(K_{HQ}) \quad \text{(S4)}$$

Where ΔG_{HQ} is the change in free energy for the reaction of benzoquinone with pyridinium, R = 1.9871 kcal K^{-1} mol^{-1}, T is ambient temperature (298.15 K), and K_{HQ} is the equilibrium constant for the reaction of benzoquinone with pyridinium, solving for K_{HQ} and inserting the values yields the following:

$$K_{HQ} = e^{-\left(\frac{\Delta G_{HQ}}{RT}\right)} = e^{-\left(\frac{\left(30.36\frac{kcal}{mol}\right)\left(1000\frac{cal}{kcal}\right)}{\left(1.9871\frac{cal}{mol\cdot K}\right)(298.15\ K)}\right)} = 5.556 \times 10^{-23}$$

To determine the K_a value for **[HQ]$^+$**, the K_a expression for pyridinium needs to be substracted out, as follows:



Solving for Ka(HQ) results in Equation S5:

$$K_a(HQ) = \frac{K_a(PyH)}{K_{HQ}} \qquad \text{(S5)}$$

$K_a(PyH)$ is determined by converting the pK_a of pyridinium (12.33 in acetonitrile)[3] using Equation S6:

$$K_a = 10^{(-pK_a)} \qquad \text{(S6)}$$

Which results in a K_a(Py) of 4.677×10^{-13} for pyridinium. Using the values for K_a(PyH) and K_{HQ} the value for K_a(HQ) can be determined as follows:

$$K_a(HQ) = \frac{K_a(PyH)}{K_{HQ}} = \frac{4.677 \times 10^{-13}}{5.556 \times 10^{-23}} = 5.691 \times 10^{9}$$

To determine the pK_a value for protonated benzoquinone, the Equation S7 can be used:

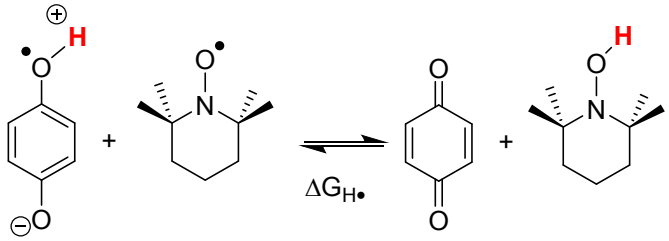
$$pK_a = -\log(K_a) \qquad \text{(S7)}$$

Using the values for the protonated benzoquinone the pK_a can be determind for **[HQ]**$^+$ from the following:

$$pK_a(HQ) = -\log(K_a(HQ)) = -\log(5.691 \times 10^{9}) = 9.93$$

16) Sample Calculation of the Ability to transfer a Hydrogen Atom from Protonated Semiquinone

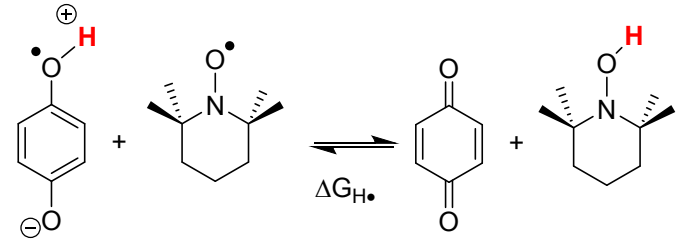
G_Q = -239305.9292 kcal/mol
$G_{HQ\cdot}$ = -239679.2155 kcal/mol
G_{TEMPO} = -303343.7728 kcal/mol
G_{TEMPOH} = -303721.7586 kcal/mol



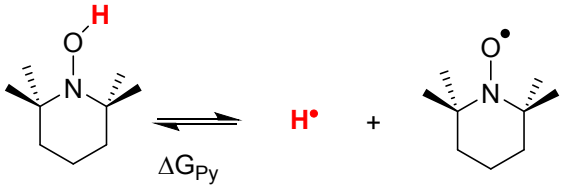
[HQ]• **TEMPO** **Q** **TEMPOH** (S8)

$$\Delta G_{HQ} = [Products] - [Reactants] = [G_Q + G_{TEMPOH}] - [G_{HQ\cdot} + G_{TEMPO}] = -4.70\ kcal/mol$$

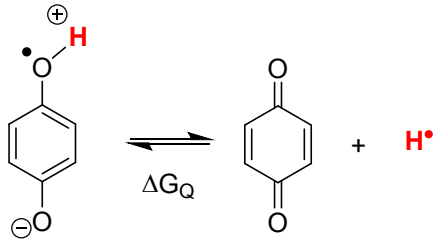
This free energy for hydrogen atom transfer from [HQ]• can then be determined from the following equilibrium expressions:



$\Delta G_{H\cdot}$



$\Delta G_{H\cdot}(TEMPOH)$



$\Delta G_{H\cdot}(Q) = \Delta G_{H\cdot} + \Delta G_{H\cdot}(TEMPOH)$

Given that $\Delta G_{H\cdot}(TEMPOH)$ is 66.5 kcal/mol,[4] $\Delta G_{H\cdot}(Q)$ can be determined to be **61.80 kcal/mol**

17) Plots Showing the Locations of the Frontier Molecular Orbitals

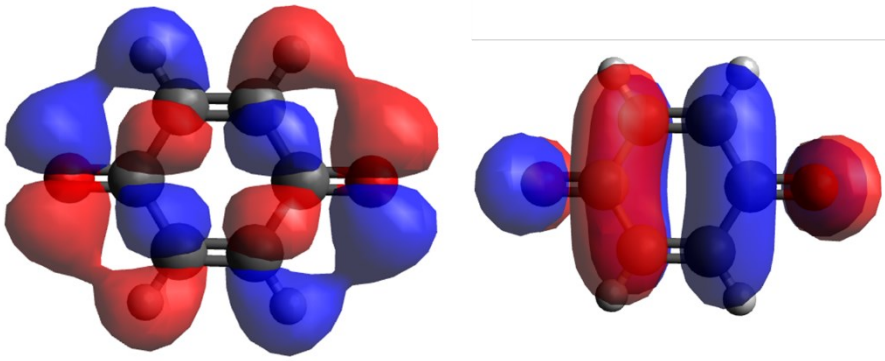


Figure 26. HOMO (left) and LUMO (right) images of benzoquinone (**Q**). Isovalue = 0.02 e^-/a.u.

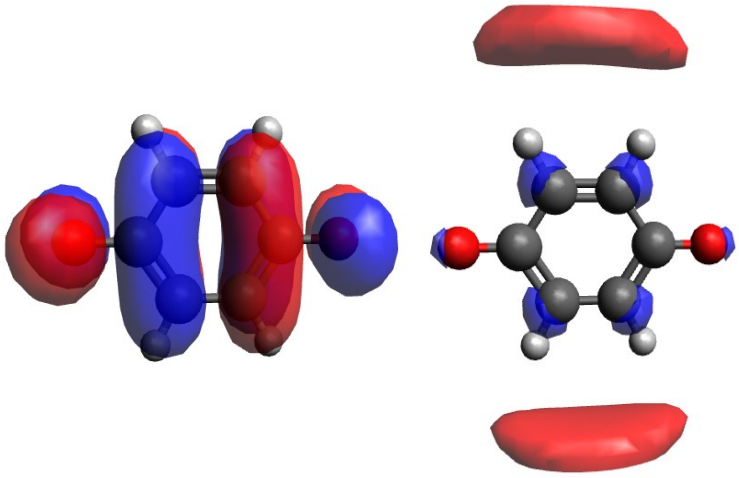


Figure S27. HOMO (left) and LUMO (right) images of hydroquinone dianion (**[Q]**$^{2-}$). Isovalue = 0.02 e^-/a.u.

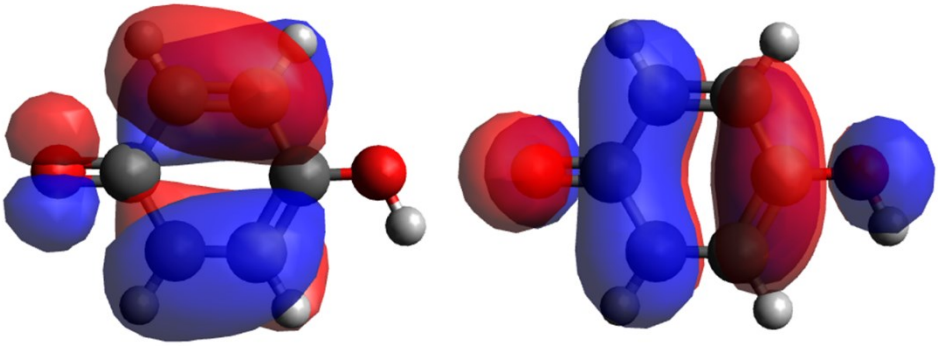


Figure S28. HOMO (left) and LUMO (right) images of **[HQ]$^+$**. Isovalue = 0.02 e$^-$/a.u.

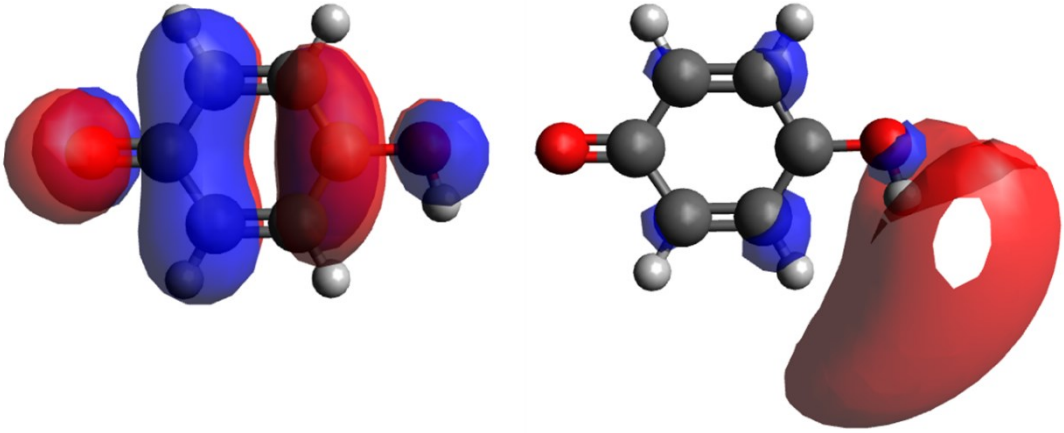


Figure S29. HOMO (left) and LUMO (right) images of **[HQ]$^-$**. Isovalue = 0.02 e$^-$/a.u.

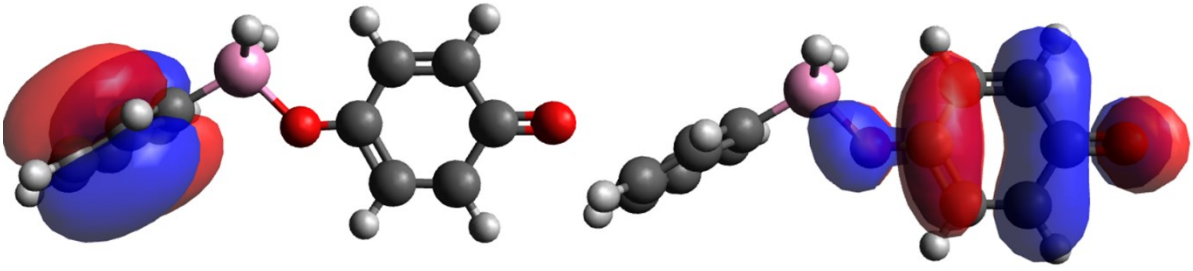


Figure S30. HOMO (left) and LUMO (right) images of **[SiH$_2$Ph-Q]$^+$**. Isovalue = 0.02 e$^-$/a.u.

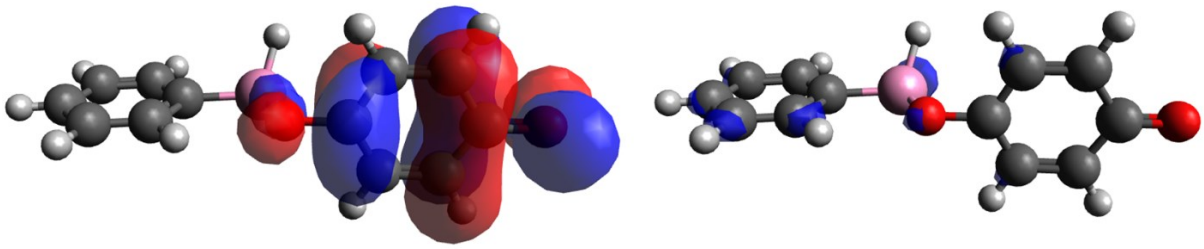


Figure S31. HOMO (left) and LUMO (right) images of **[SiH_2Ph-Q]**$^-$. Isovalue = 0.02 e^-/a.u.

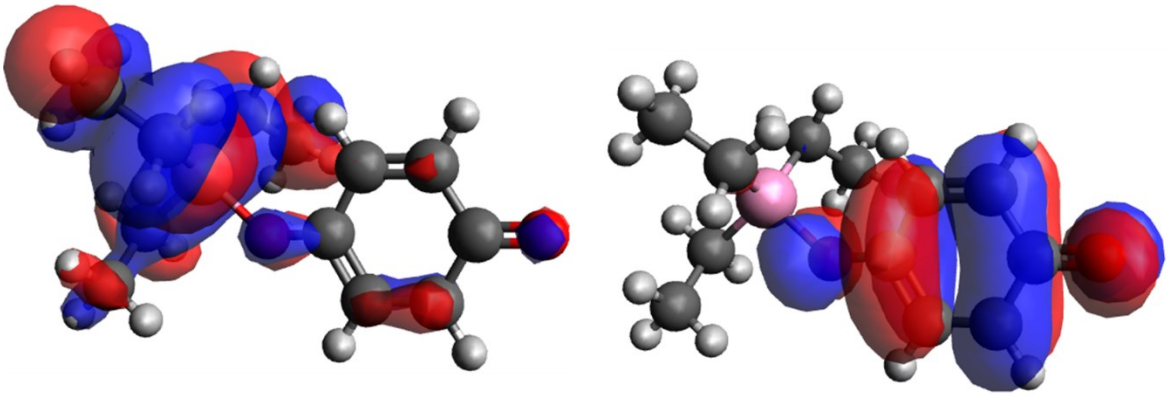


Figure S32. HOMO (left) and LUMO (right) images of **[$SiEt_3$-Q]**$^+$. Isovalue = 0.02 e^-/a.u.

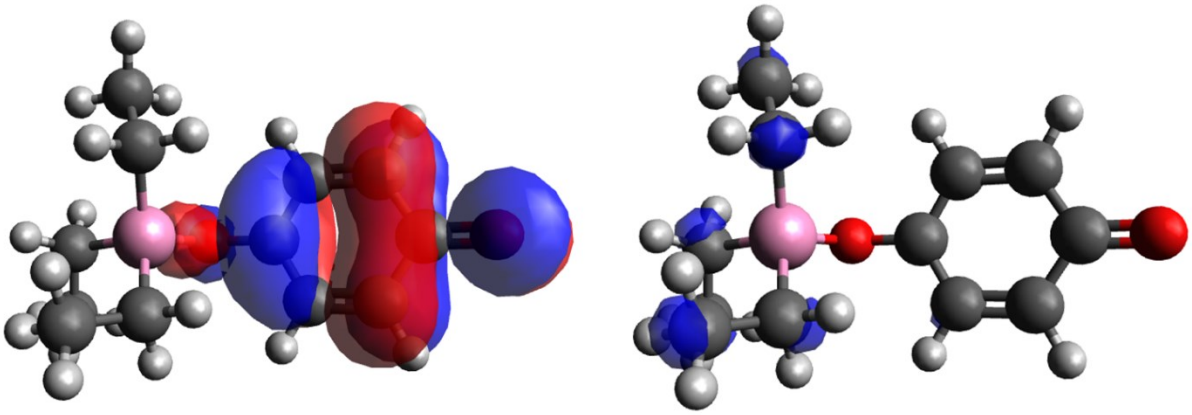


Figure S33. HOMO (left) and LUMO (right) images of **[$SiEt_3$-Q]**$^-$. Isovalue = 0.02 e^-/a.u.

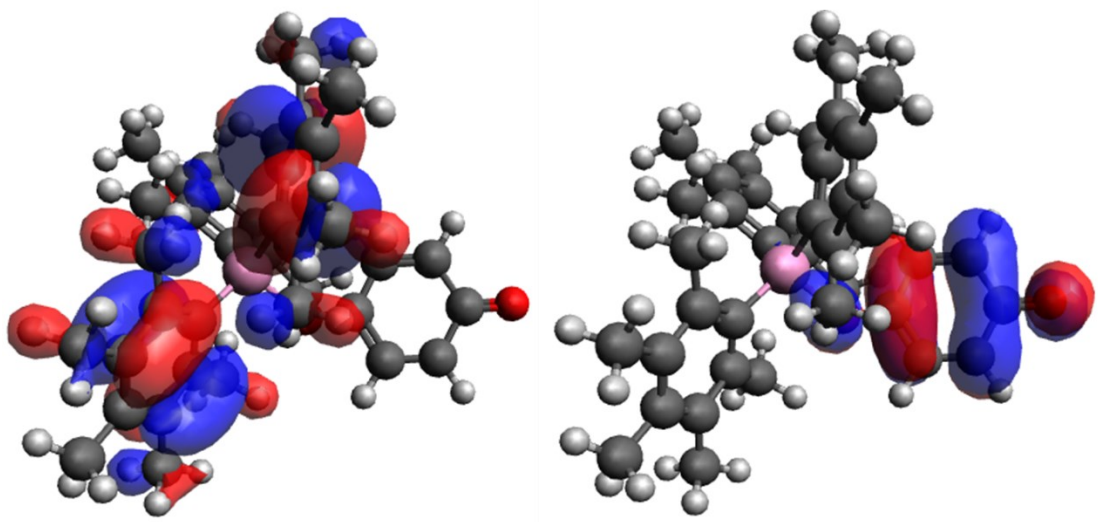


Figure S34. HOMO (left) and LUMO (right) images of **[Si(C_6Me_5)$_3$-Q]$^+$**. Isovalue = 0.02 e^-/a.u.

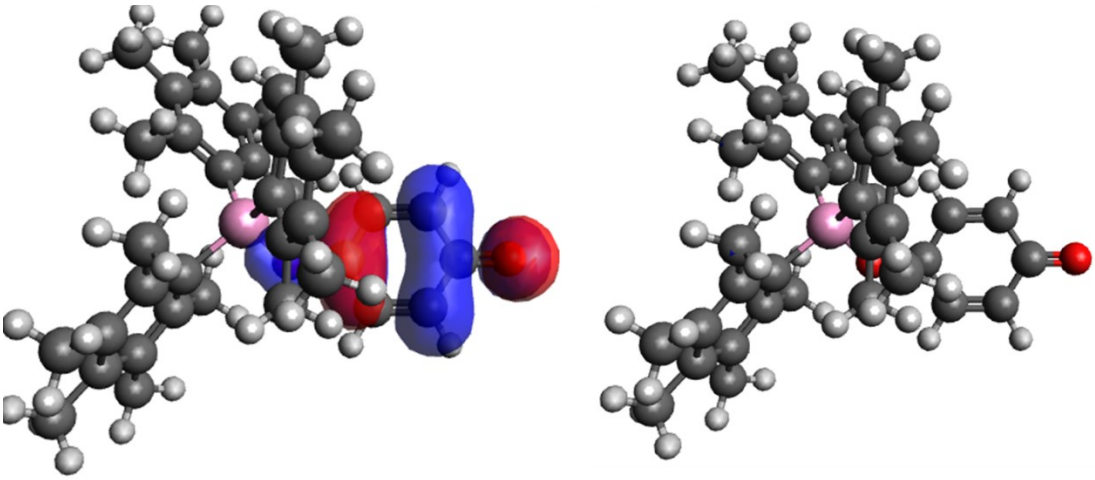


Figure S35. HOMO (left) and LUMO (right) images of **[Si(C_6Me_5)$_3$-Q]$^-$**. Isovalue = 0.02 e^-/a.u.

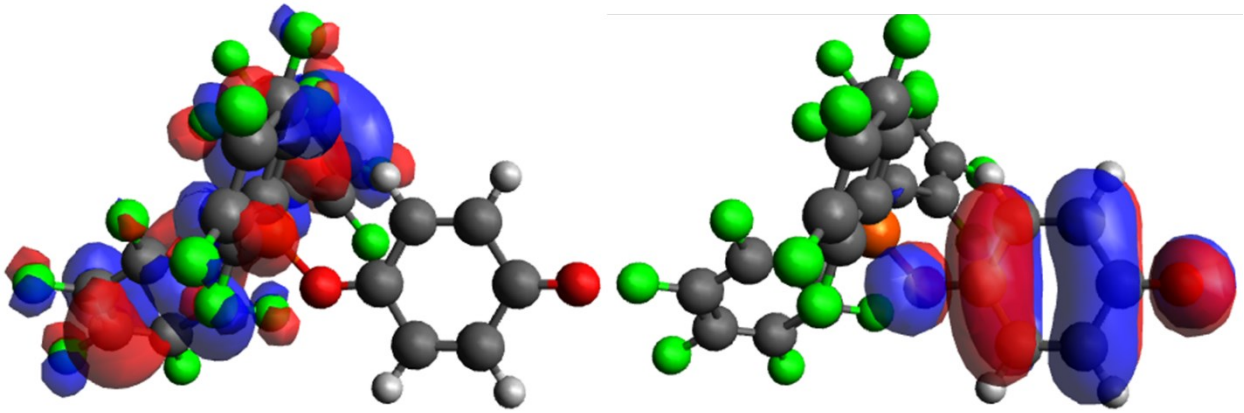


Figure S36. HOMO (left) and LUMO (right) images of **$B(C_6F_5)_3$-Q**. Isovalue = 0.02 e^-/a.u.

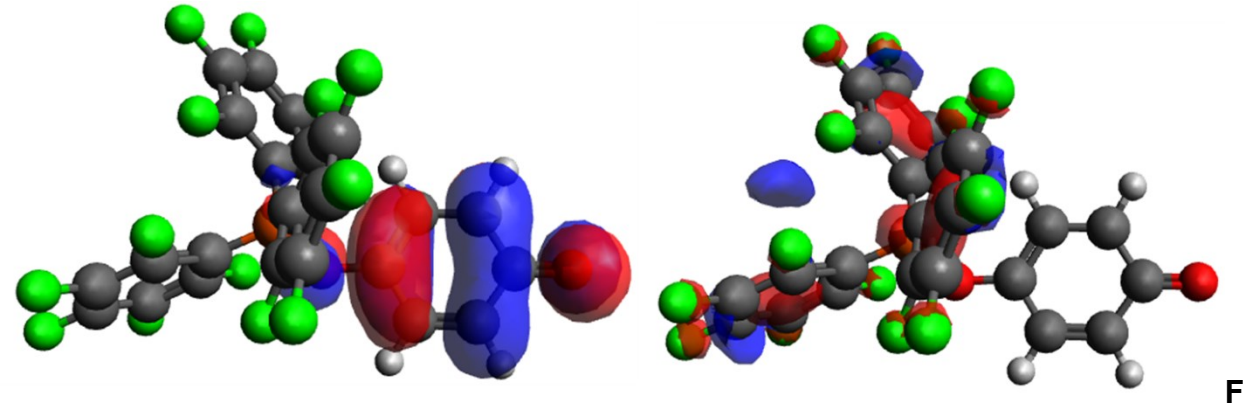


Figure S37. HOMO (left) and LUMO (right) images of **$[B(C_6F_5)_3\text{-}Q]^{2-}$**. Isovalue = 0.02 e^-/a.u.

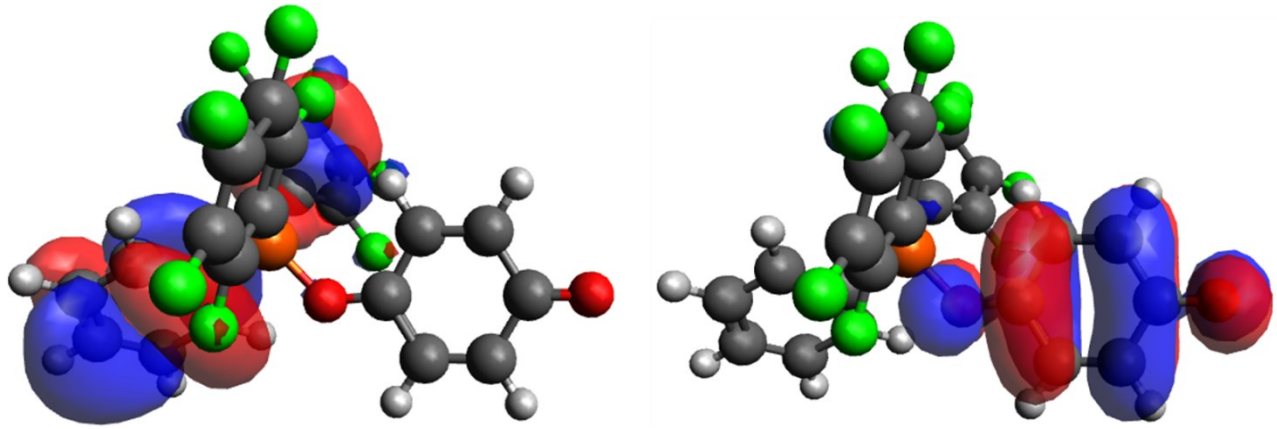


Figure S38. HOMO (left) and LUMO (right) images of **$B(C_6F_5)_2$Ph-Q**. Isovalue = 0.02 e^-/a.u.

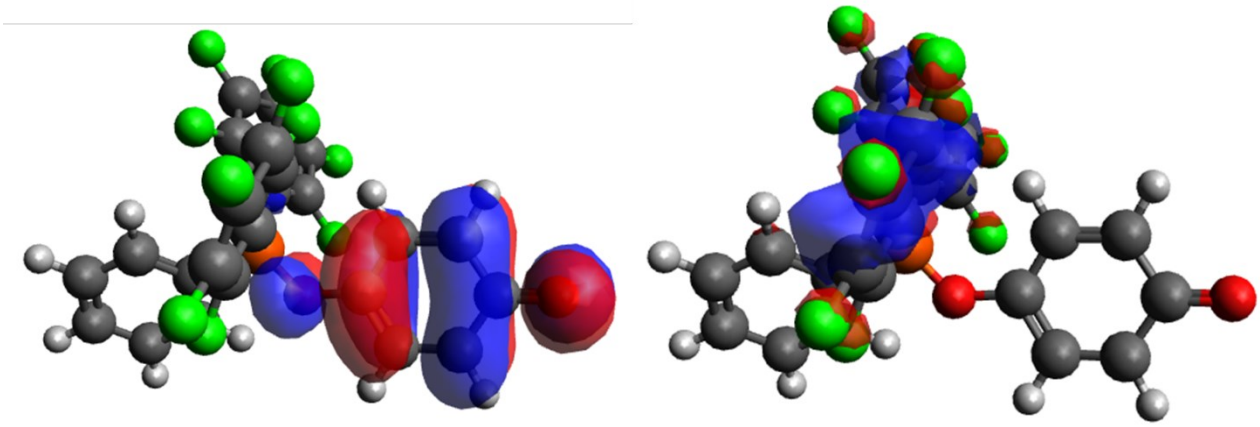


Figure S39. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_2$Ph-Q]$^{2-}$**. Isovalue = 0.02 e$^-$/a.u.

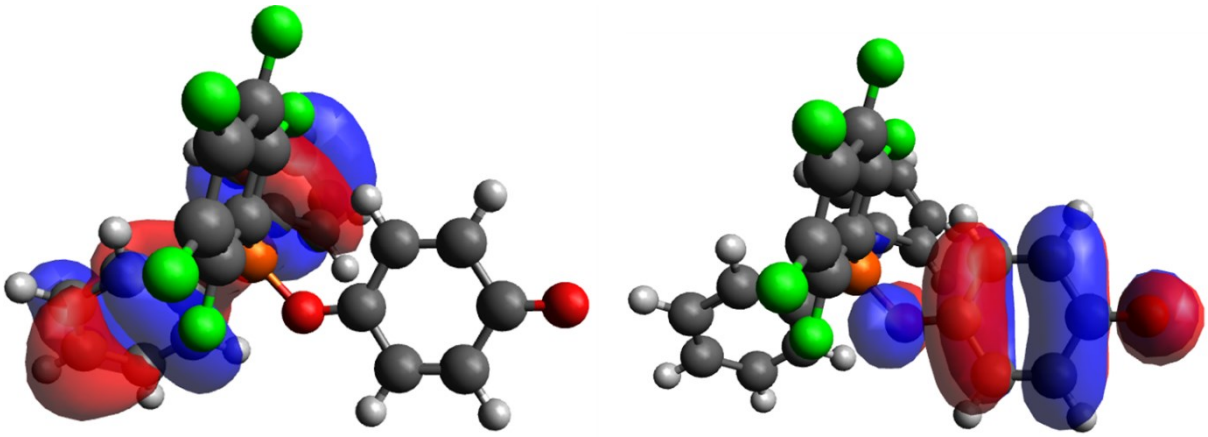


Figure S40. HOMO (left) and LUMO (right) images of **B(C_6F_5)Ph$_2$-Q**. Isovalue = 0.02 e$^-$/a.u.

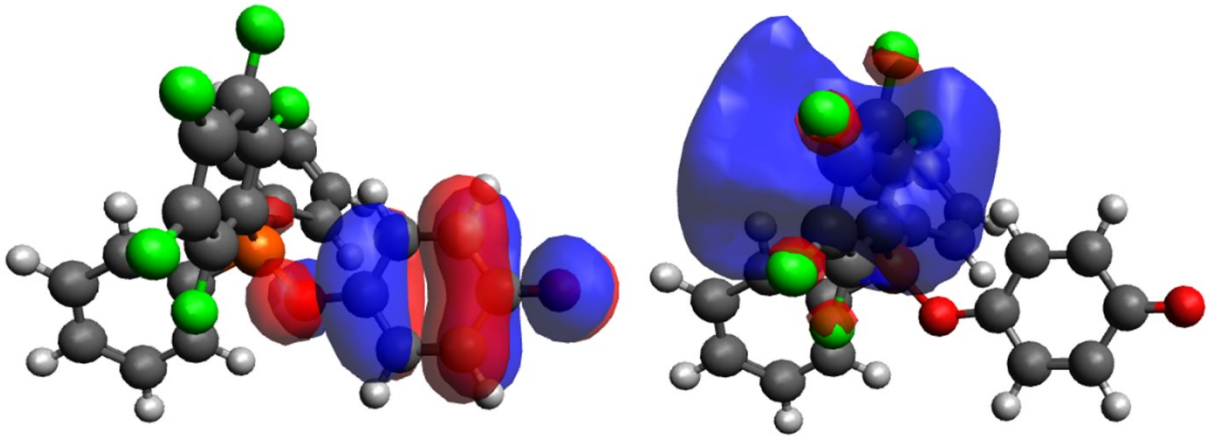


Figure S41. HOMO (left) and LUMO (right) images of **[B(C_6F_5)Ph$_2$-Q]$^{2-}$**. Isovalue = 0.02 e$^-$/a.u.

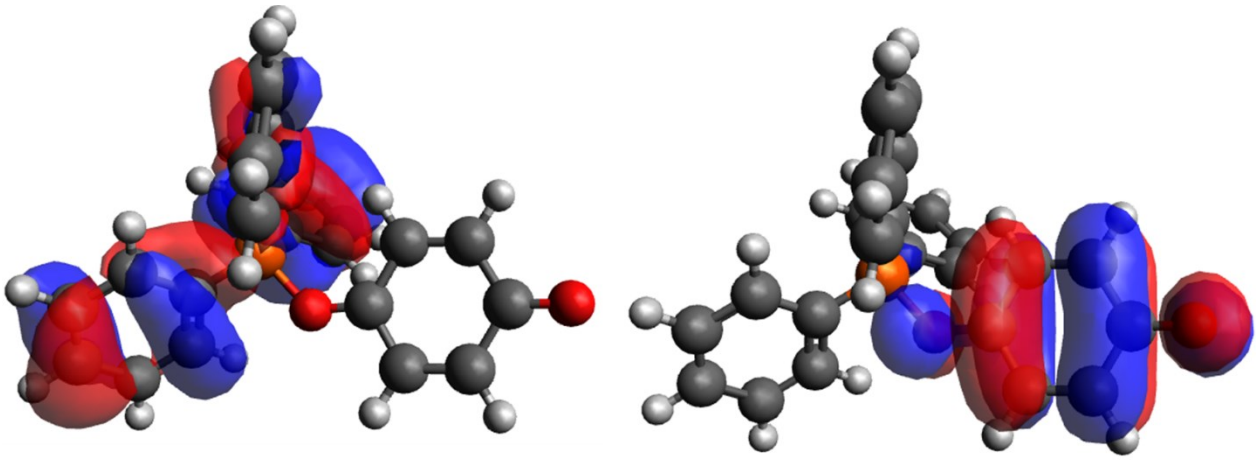


Figure S42. HOMO (left) and LUMO (right) images of **BPh_3-Q**. Isovalue = 0.02 e^-/a.u.

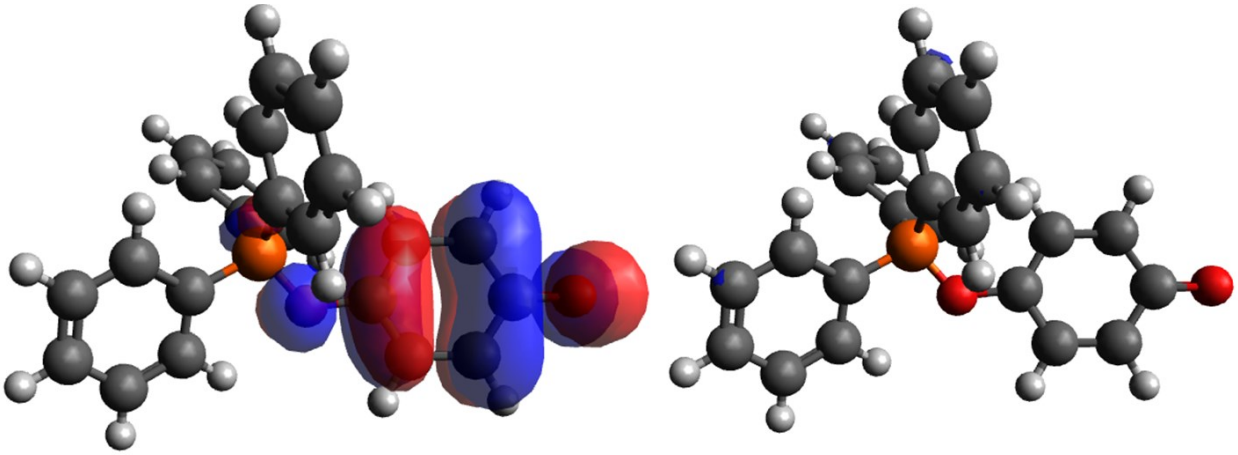


Figure S43. HOMO (left) and LUMO (right) images of **$[BPh_3\text{-}Q]^{2-}$**. Isovalue = 0.02 e^-/a.u.

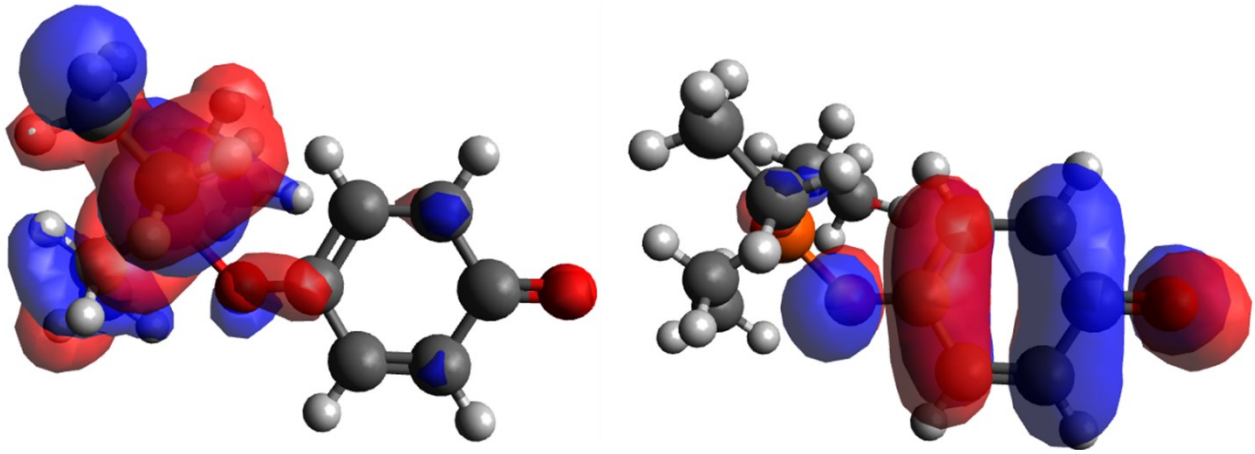


Figure S44. HOMO (left) and LUMO (right) images of **BEt_3-Q**. Isovalue = 0.02 e^-/a.u.

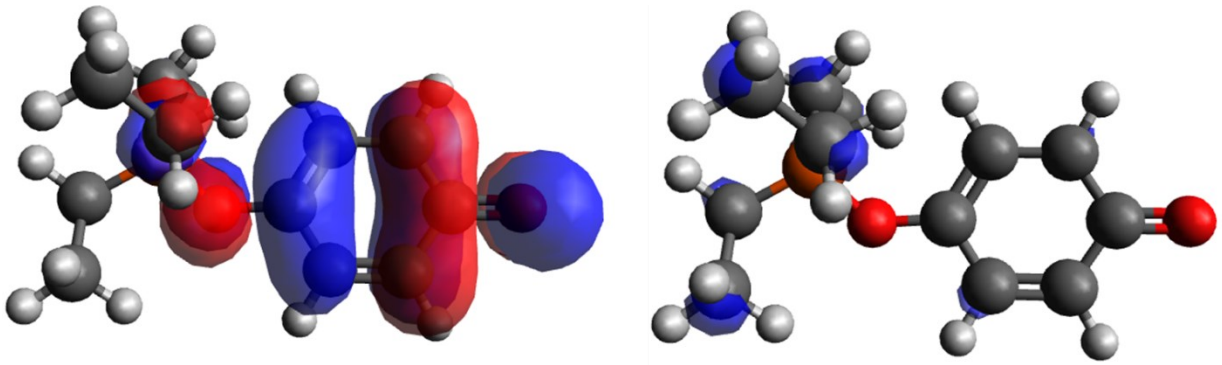


Figure S45. HOMO (left) and LUMO (right) images of **[BEt_3-Q]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

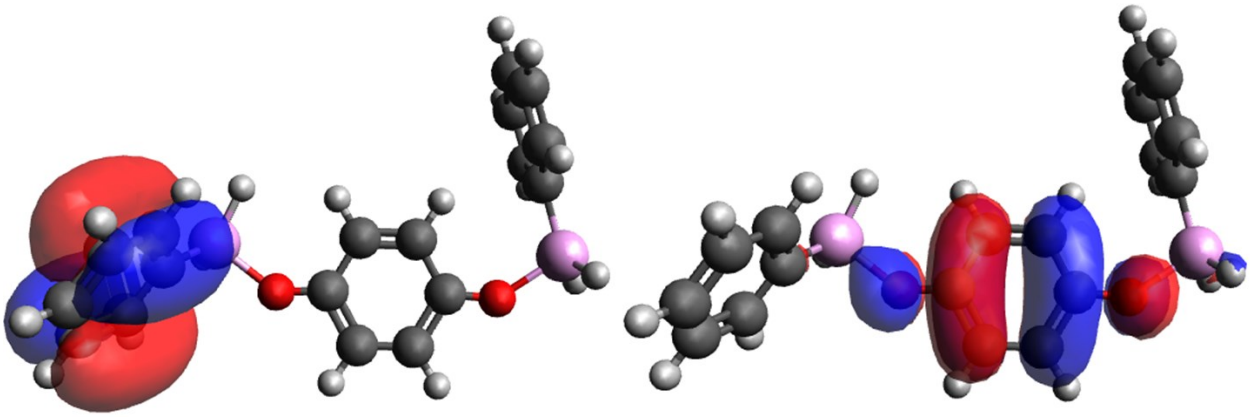


Figure S46. HOMO (left) and LUMO (right) images of **[SiH_2Ph-Q-SiH_2Ph]$^{2+}$**. Isovalue = 0.02 e^-/a.u.

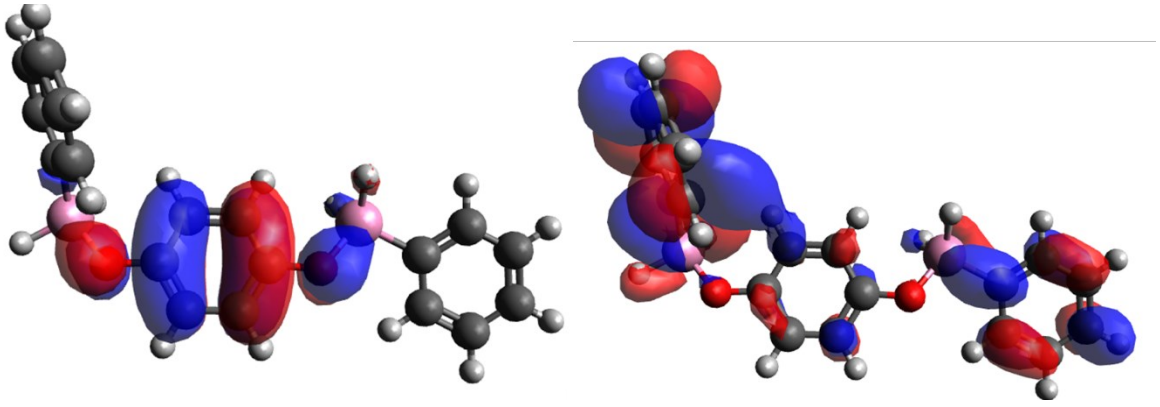


Figure S47. HOMO (left) and LUMO (right) images of **SiH_2Ph-Q-SiH_2Ph**. Isovalue = 0.02 e^-/a.u.

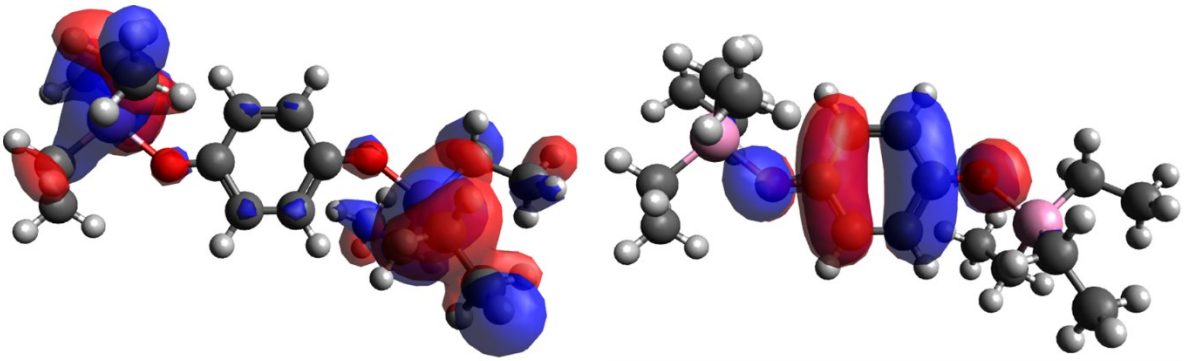


Figure S48. HOMO (left) and LUMO (right) images of **[$SiEt_3$-Q-$SiEt_3$]$^{2+}$**. Isovalue = 0.02 e^-/a.u.

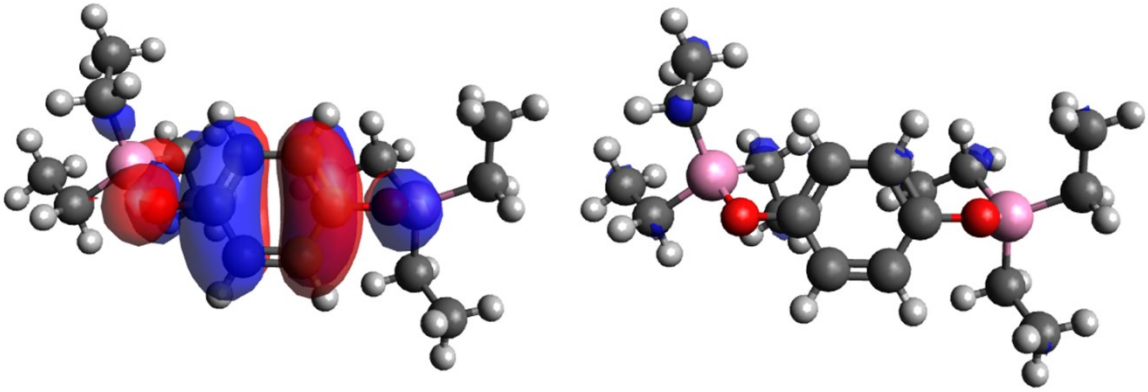


Figure S49. HOMO (left) and LUMO (right) images of **$SiEt_3$-Q-$SiEt_3$**. Isovalue = 0.02 e^-/a.u.

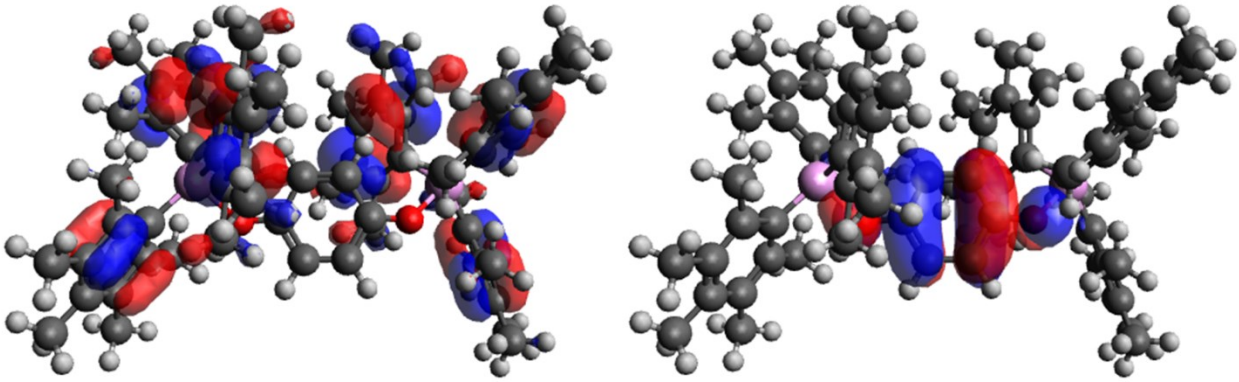


Figure S50. HOMO (left) and LUMO (right) images of **[$Si(C_6Me_5)_3$-Q-$Si(C_6Me_5)_3$]$^{2+}$**. Isovalue = 0.02 e^-/a.u.

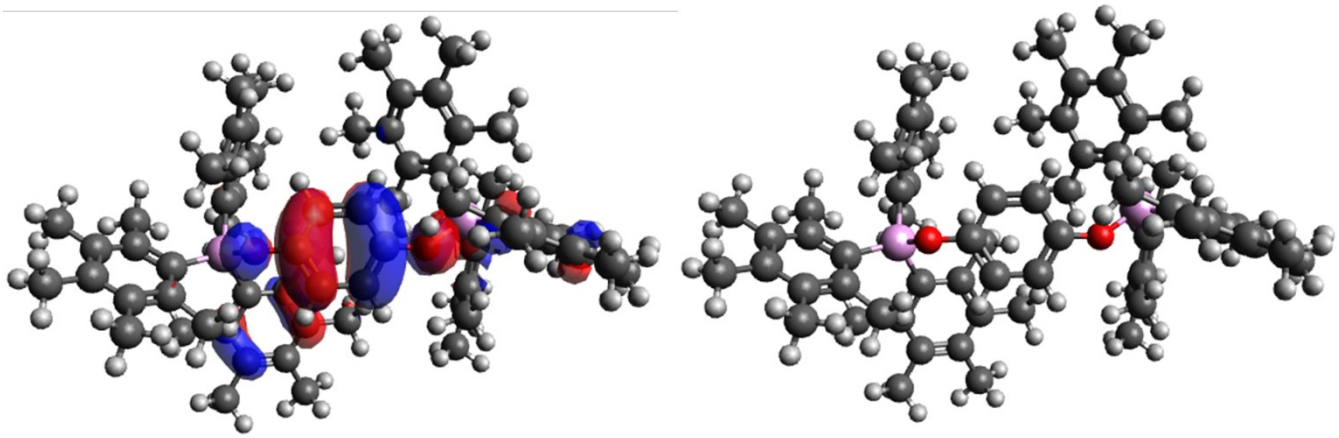


Figure S51. HOMO (left) and LUMO (right) images of **Si(C_6Me_5)$_3$-Q-Si(C_6Me_5)$_3$**. Isovalue = 0.02 e^-/a.u.

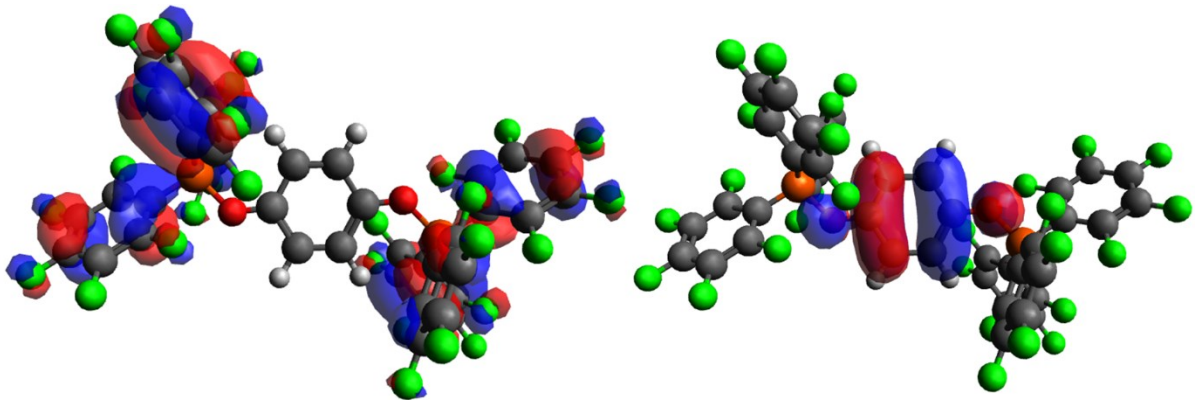


Figure S52. HOMO (left) and LUMO (right) images of **B(C_6F_5)$_3$-Q-B(C_6F_5)$_3$**. Isovalue = 0.02 e^-/a.u.

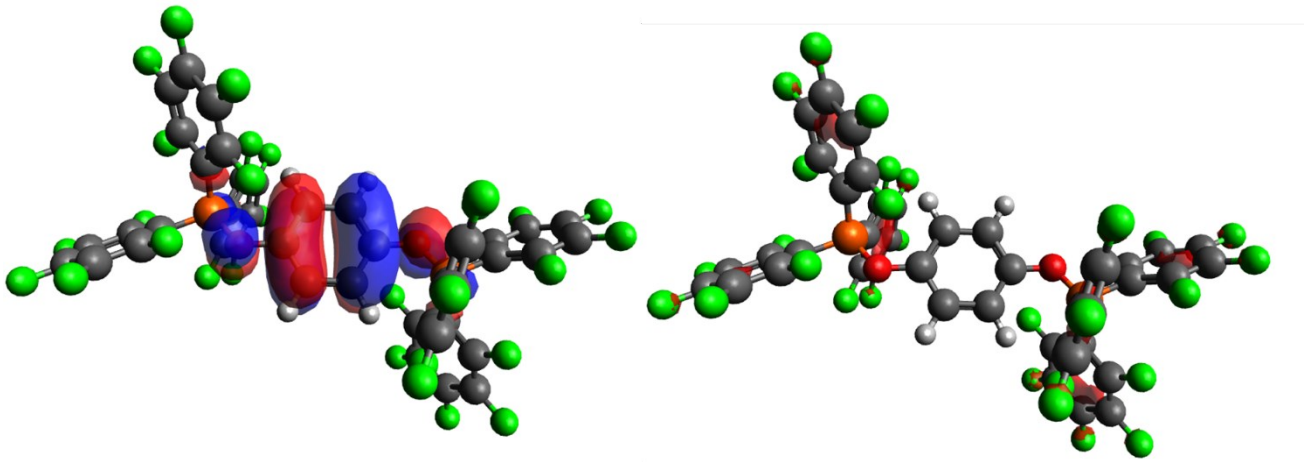


Figure S53. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-B(C_6F_5)$_3$]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

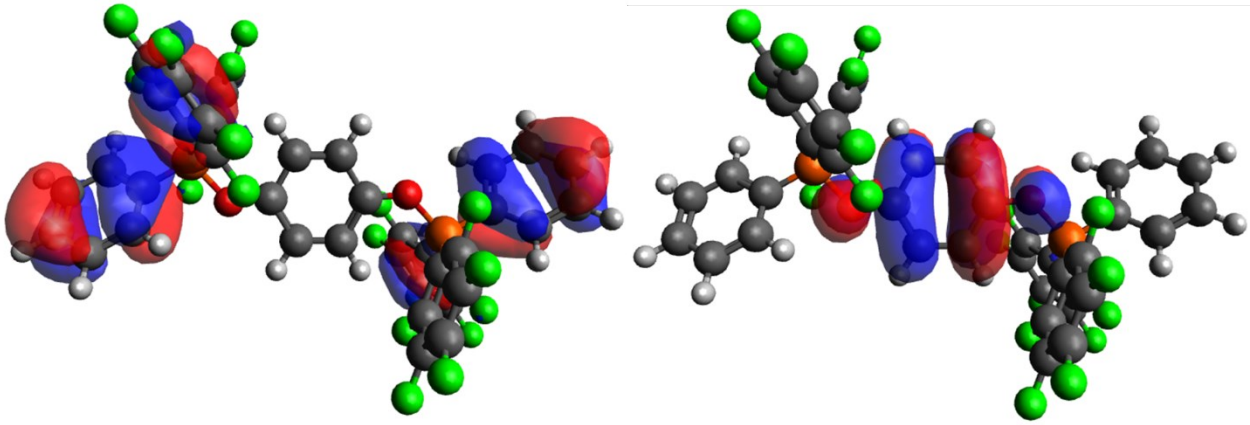


Figure S54. HOMO (left) and LUMO (right) images of **B(C_6F_5)$_2$Ph-Q-B(C_6F_5)$_2$Ph**. Isovalue = 0.02 e^-/a.u.

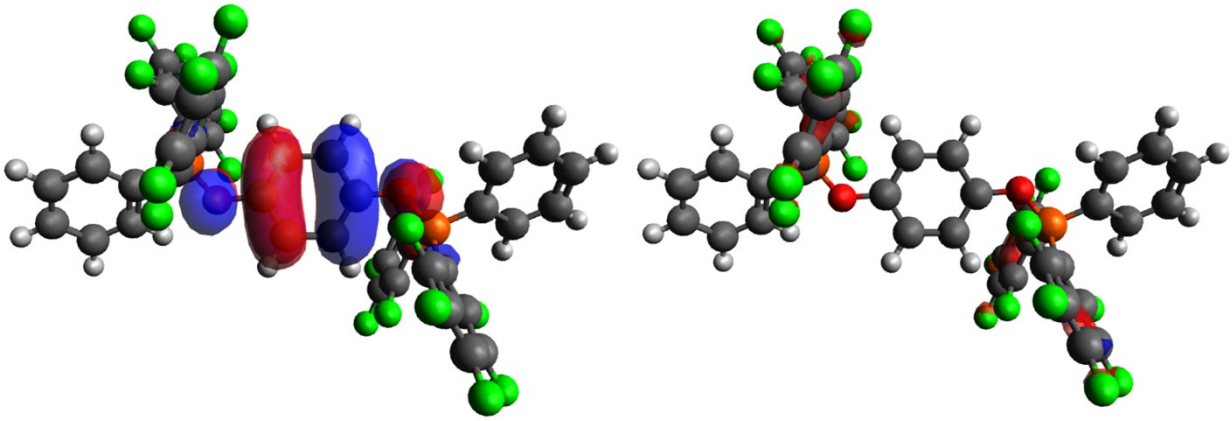


Figure S55. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_2$Ph-Q-B(C_6F_5)$_2$Ph]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

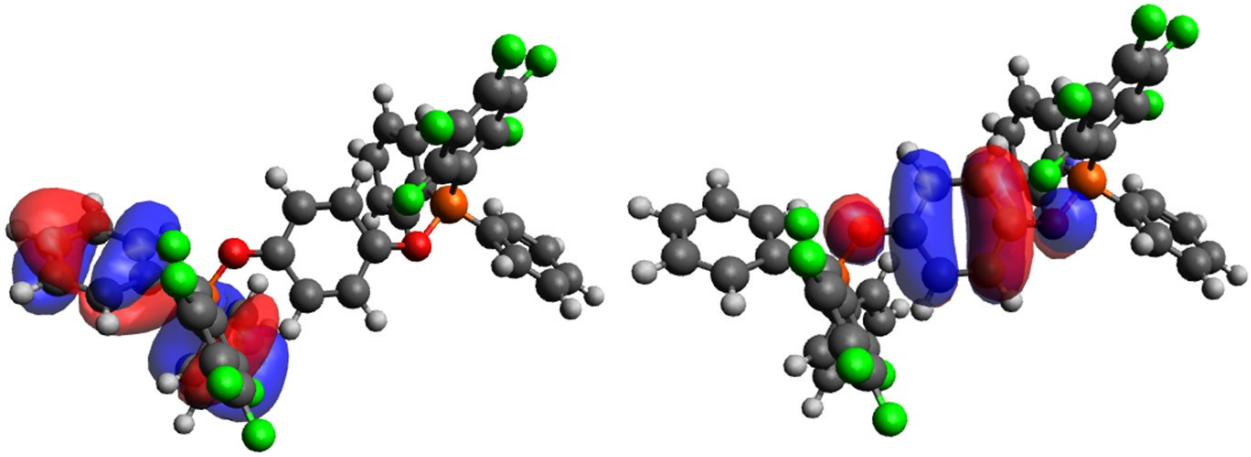


Figure S56. HOMO (left) and LUMO (right) images of **B(C_6F_5)Ph$_2$-Q-B(C_6F_5)Ph$_2$**. Isovalue = 0.02 e^-/a.u.

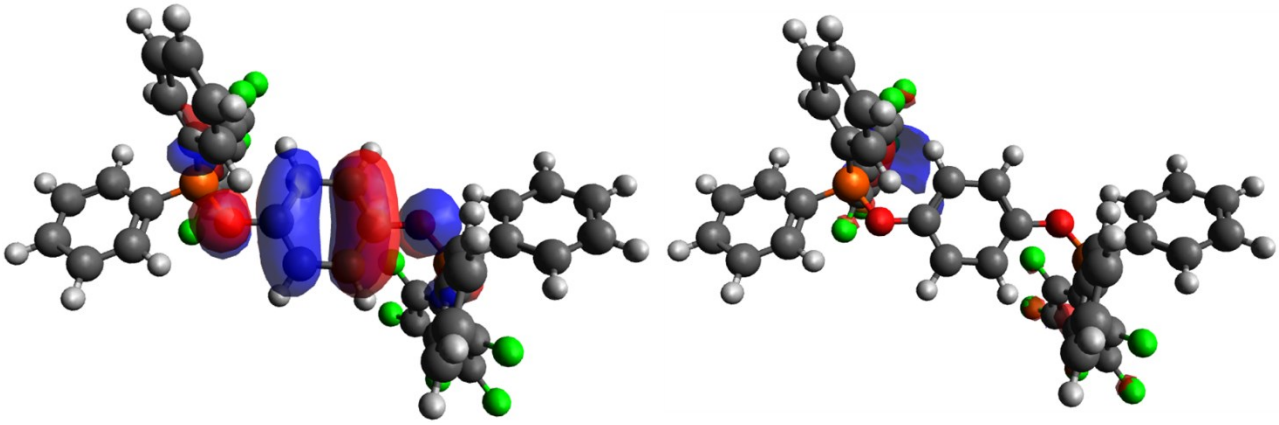


Figure S57. HOMO (left) and LUMO (right) images of **[B(C_6F_5)Ph_2-Q-B(C_6F_5)Ph_2]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

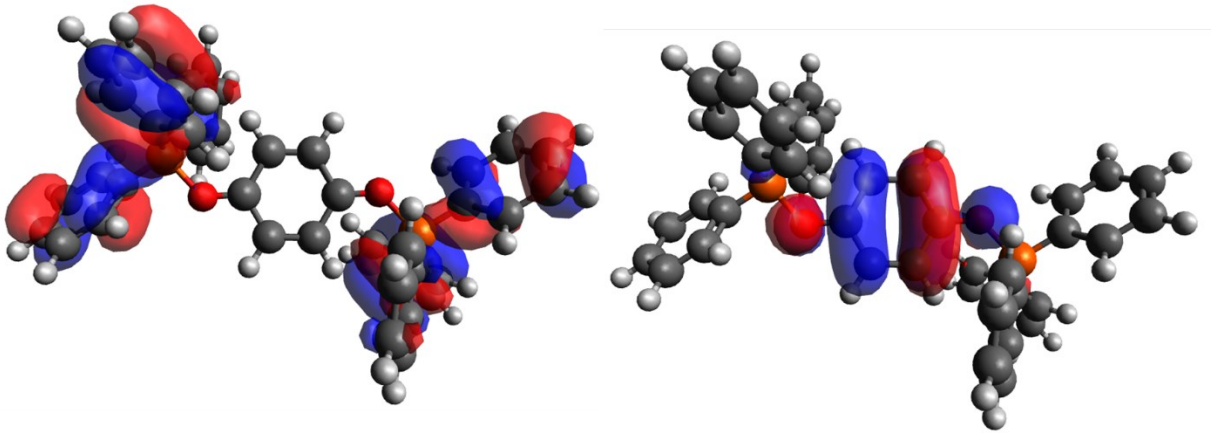


Figure S58. HOMO (left) and LUMO (right) images of **BPh_3-Q-BPh_3**. Isovalue = 0.02 e^-/a.u.

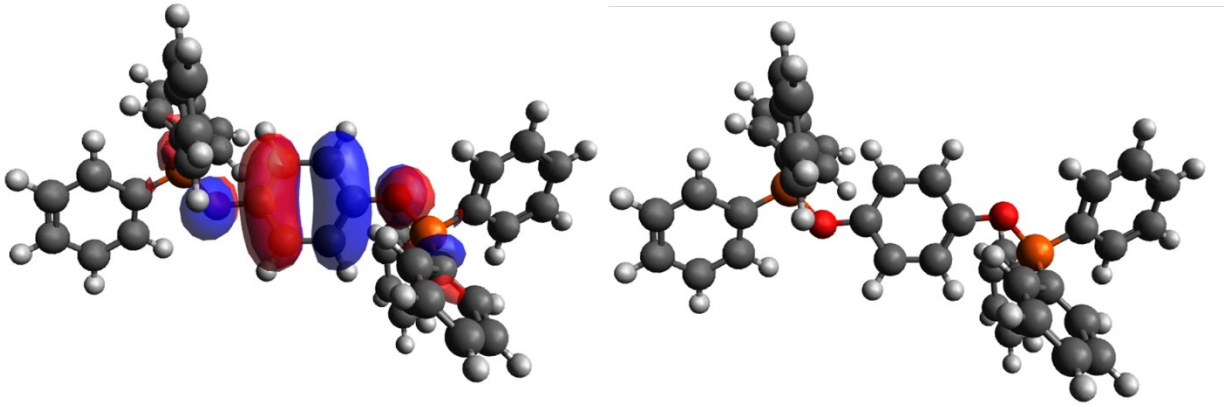


Figure S59. HOMO (left) and LUMO (right) images of **[BPh_3-Q-BPh_3]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

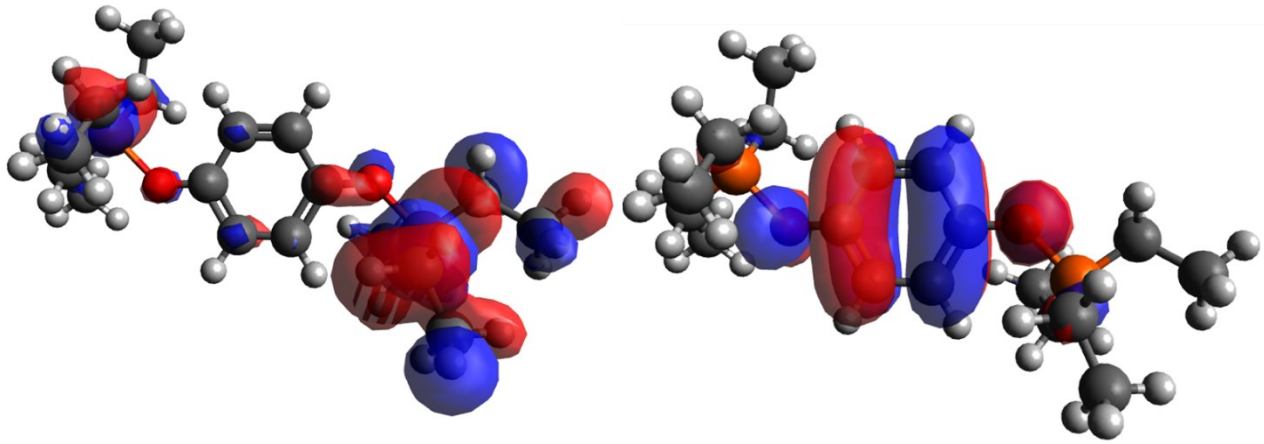


Figure S60. HOMO (left) and LUMO (right) images of **BEt_3-Q-BEt_3**. Isovalue = 0.02 e^-/a.u.

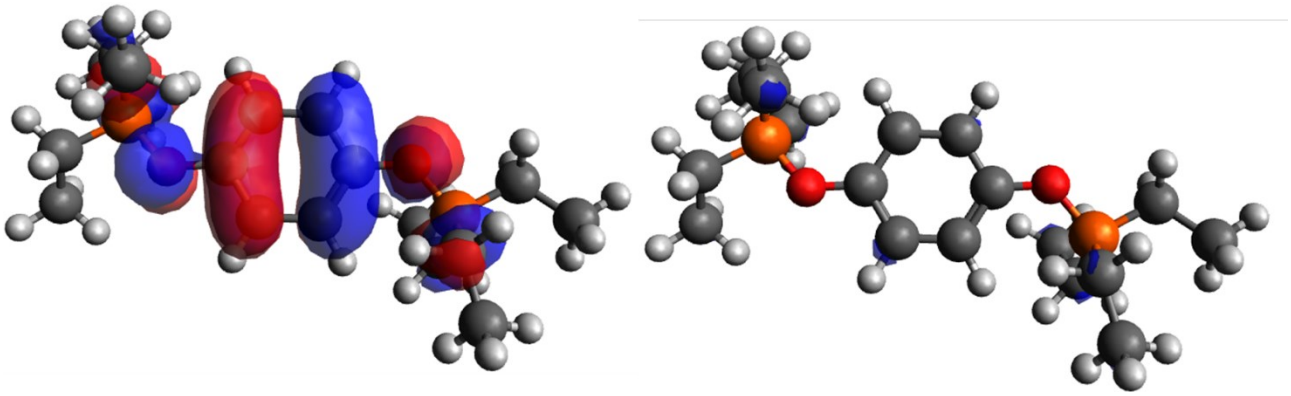


Figure S61. HOMO (left) and LUMO (right) images of **$[BEt_3$-Q-$BEt_3]^{2-}$**. Isovalue = 0.02 e^-/a.u.

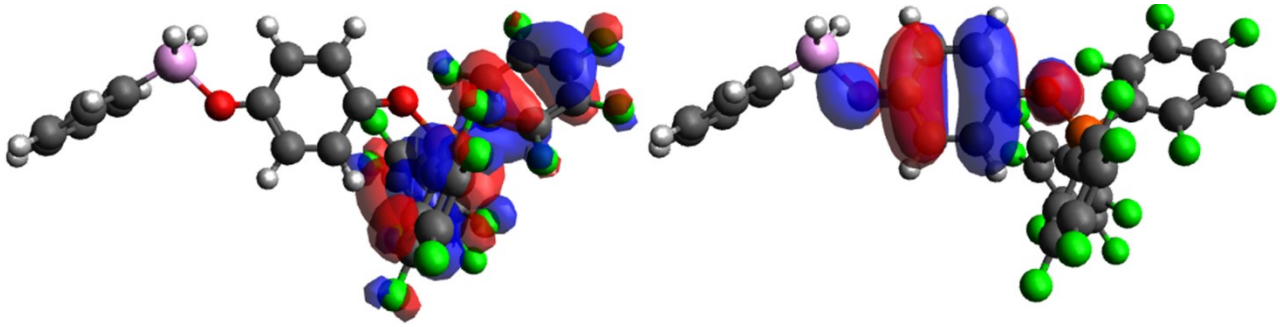


Figure S62. HOMO (left) and LUMO (right) images of **$[B(C_6F_5)_3$-Q-$SiH_2Ph]^+$**. Isovalue = 0.02 e^-/a.u.

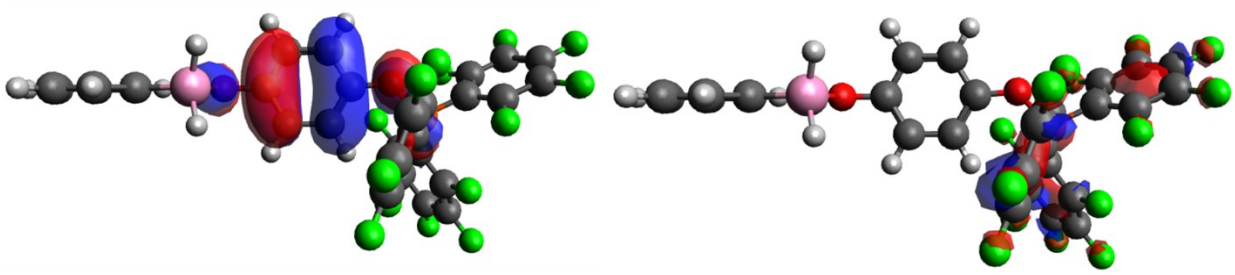


Figure S63. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-SiH_2Ph]$^-$**. Isovalue = 0.02 e$^-$/a.u.

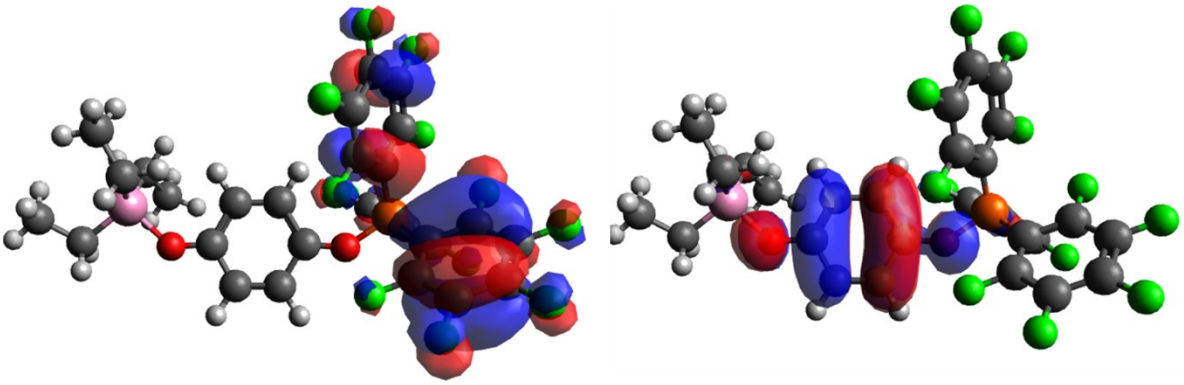


Figure S64. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-$SiEt_3$]$^+$**. Isovalue = 0.02 e$^-$/a.u.

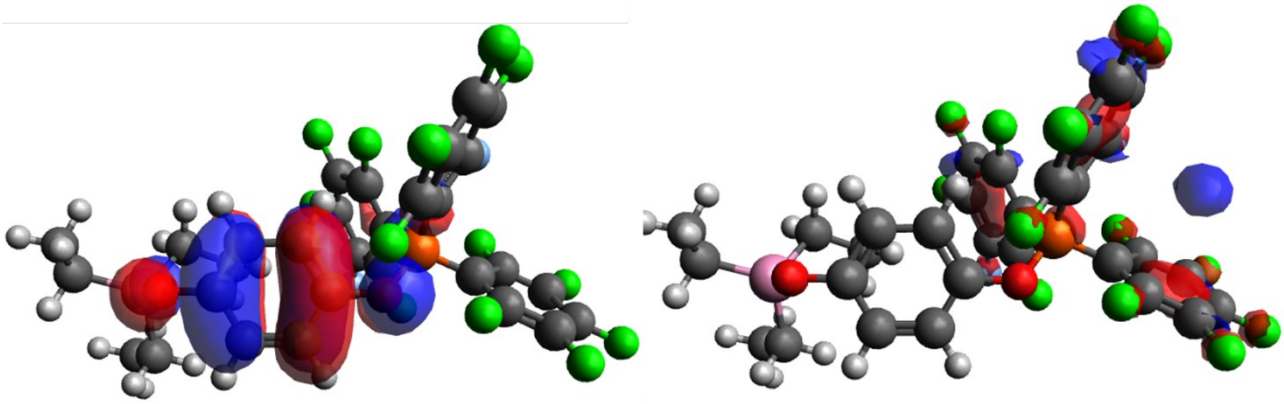


Figure S65. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-$SiEt_3$]$^-$**. Isovalue = 0.02 e$^-$/a.u.

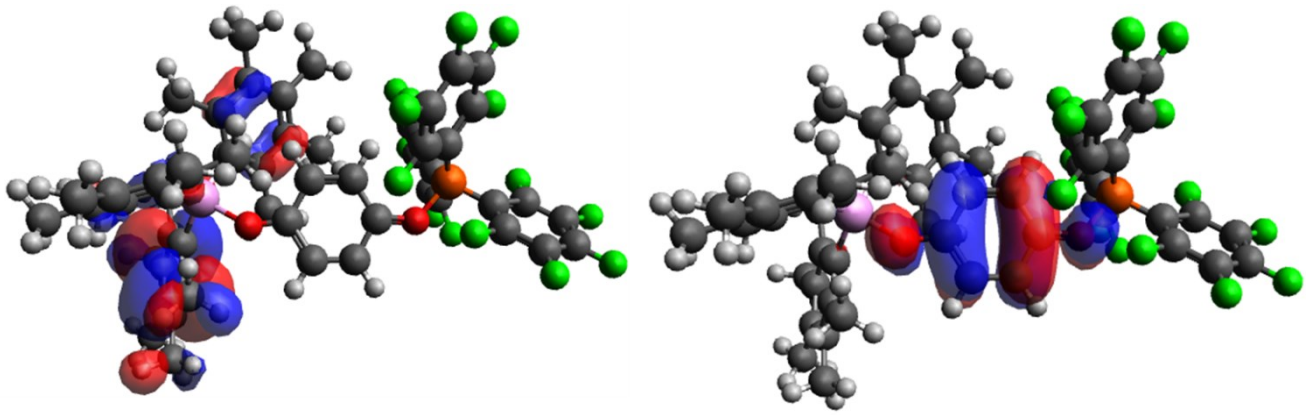


Figure S66. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-Si(C_6Me_5)$_3$]$^+$**. Isovalue = 0.02 e$^-$/a.u.

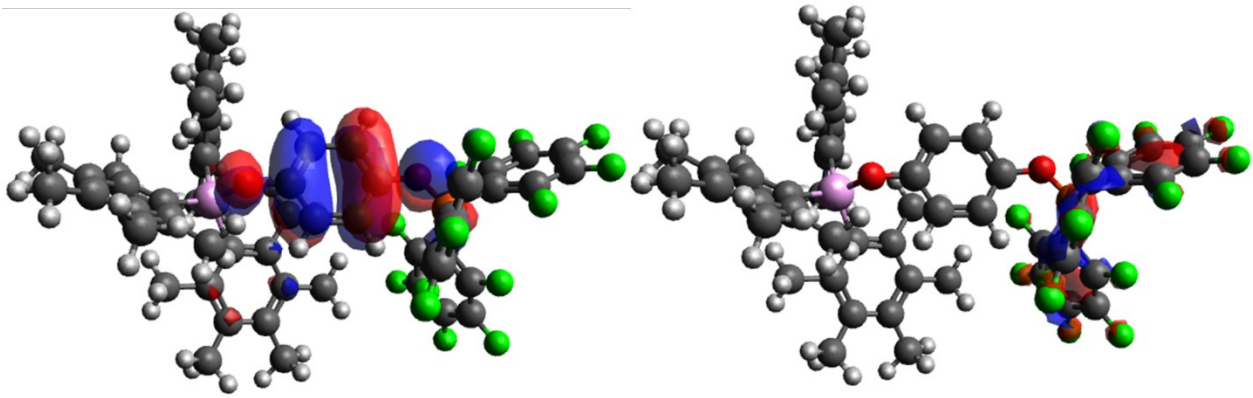


Figure S67. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-Si(C_6Me_5)$_3$]$^-$**. Isovalue = 0.02 e$^-$/a.u.

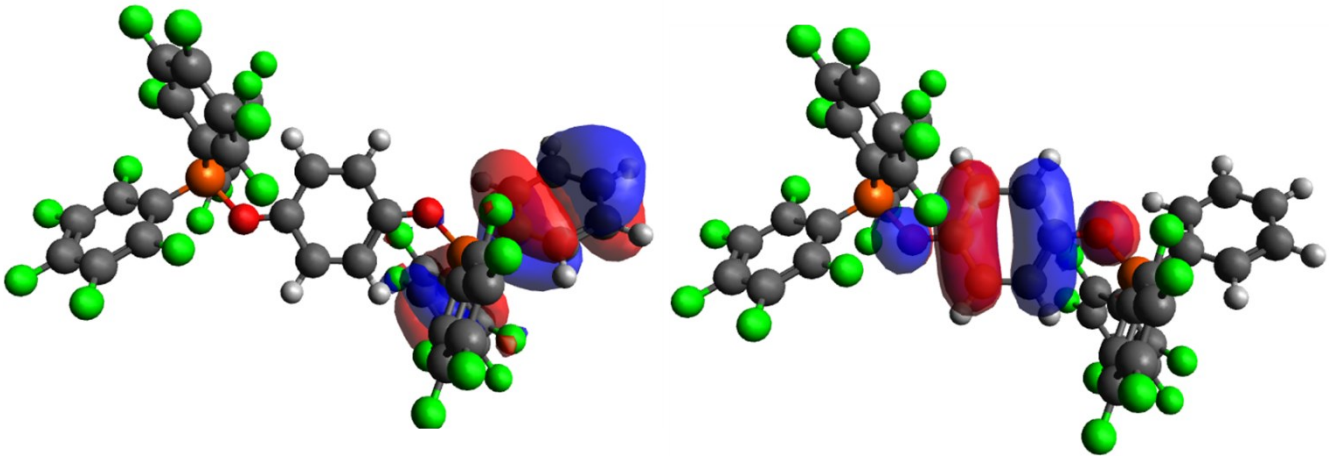


Figure S68. HOMO (left) and LUMO (right) images of **B(C_6F_5)$_3$-Q-B(C_6F_5)$_2$Ph**. Isovalue = 0.02 e$^-$/a.u.

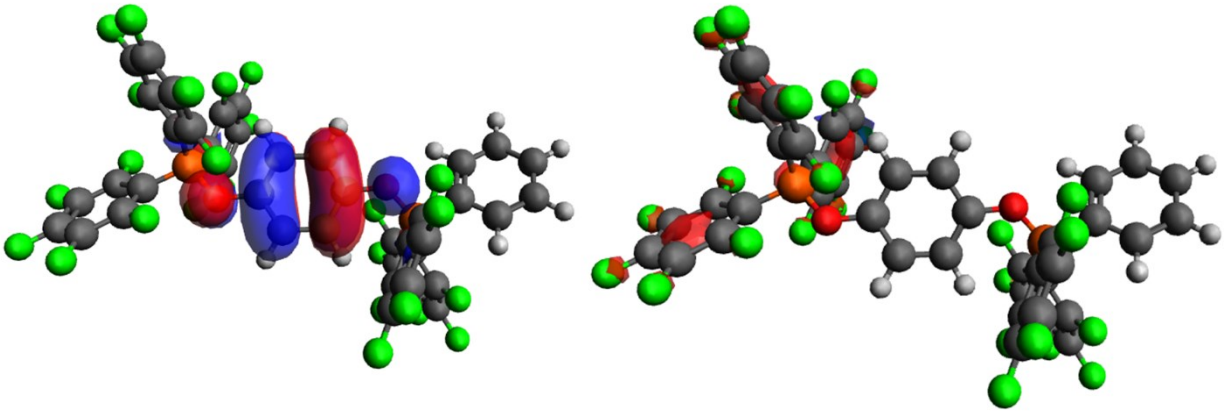


Figure S69. HOMO (left) and LUMO (right) images of **$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_2Ph]^{2-}$**. Isovalue = 0.02 e^-/a.u.

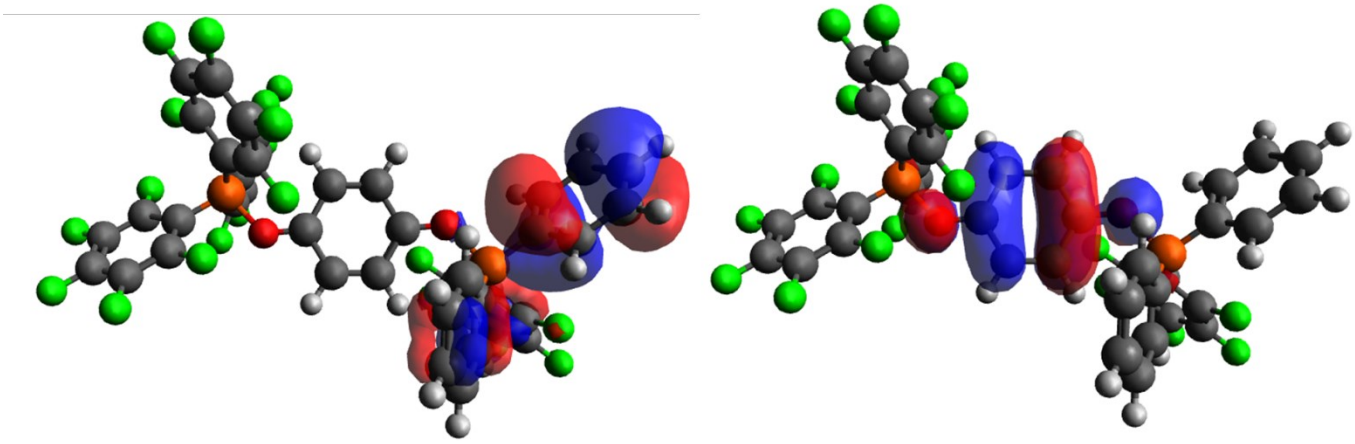


Figure S70. HOMO (left) and LUMO (right) images of **$B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)Ph_2$**. Isovalue = 0.02 e^-/a.u.

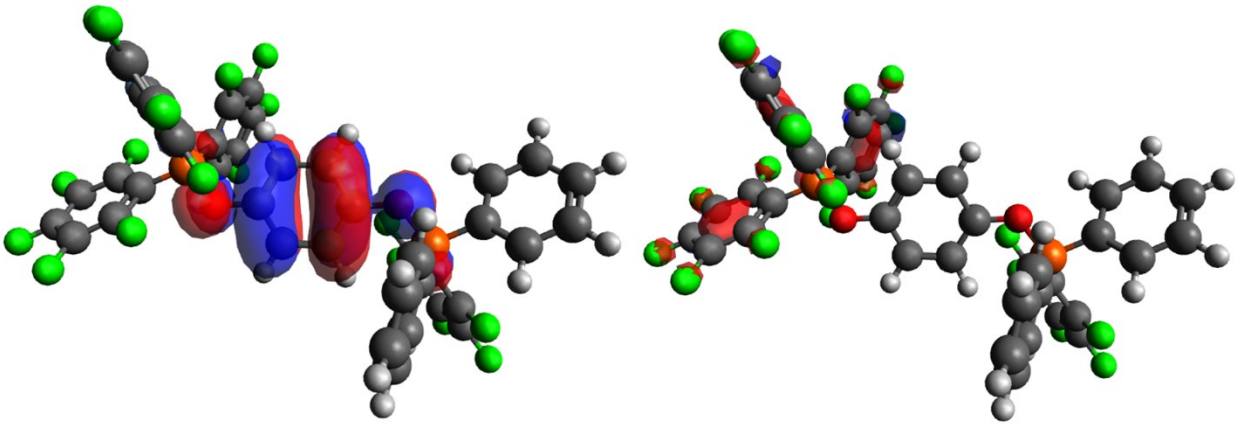


Figure S71. HOMO (left) and LUMO (right) images of **$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)Ph_2]^{2-}$**. Isovalue = 0.02 e^-/a.u.

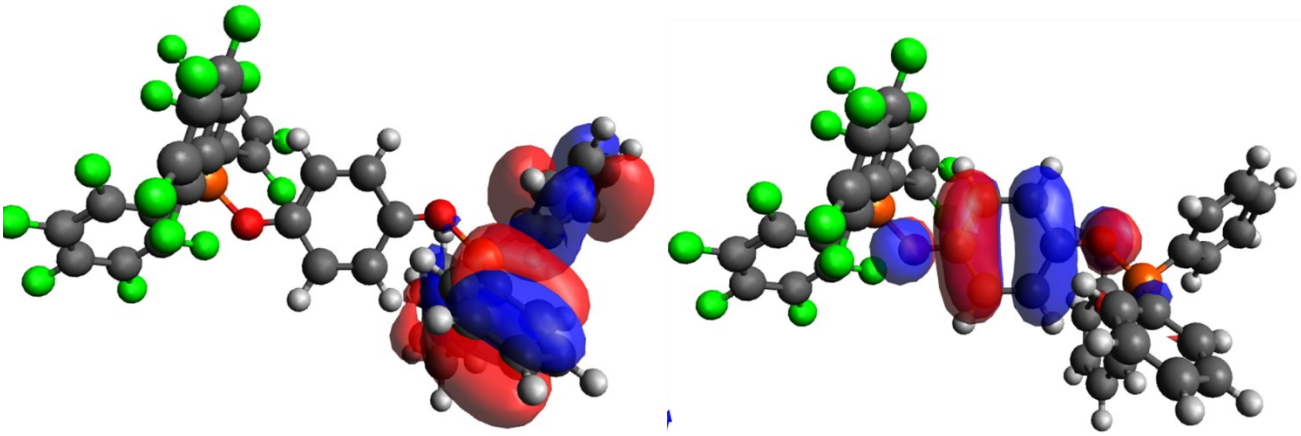


Figure S72. HOMO (left) and LUMO (right) images of **$B(C_6F_5)_3$-Q-BPh_3**. Isovalue = 0.02 e^-/a.u.

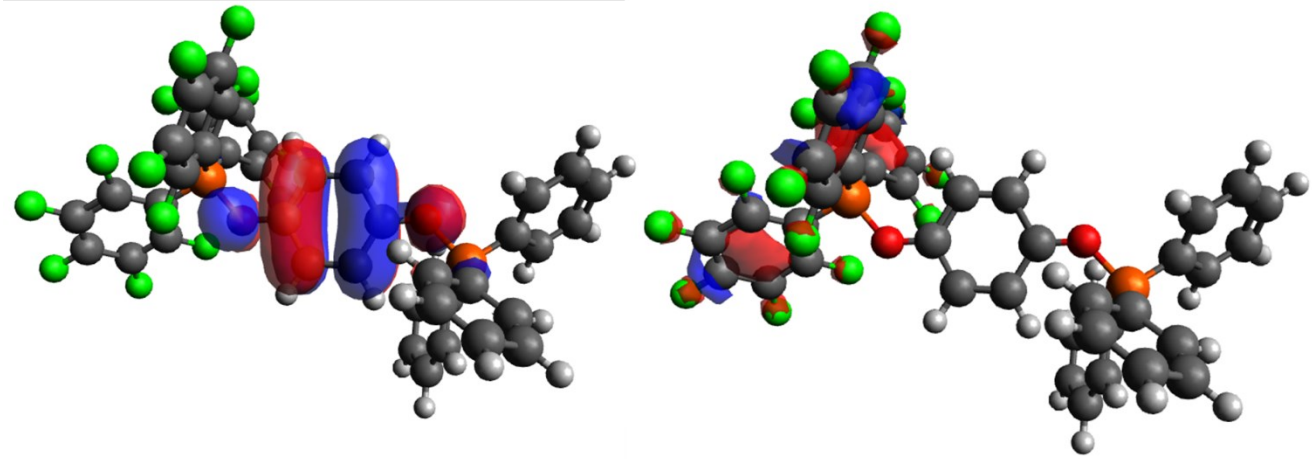


Figure S73. HOMO (left) and LUMO (right) images of **$[B(C_6F_5)_3$-Q-$BPh_3]^{2-}$**. Isovalue = 0.02 e^-/a.u.

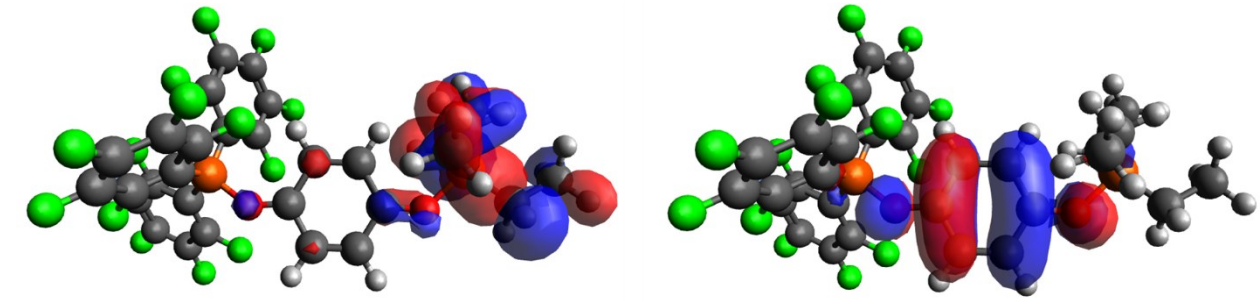


Figure S74. HOMO (left) and LUMO (right) images of **$B(C_6F_5)_3$-Q-BEt_3**. Isovalue = 0.02 e^-/a.u.

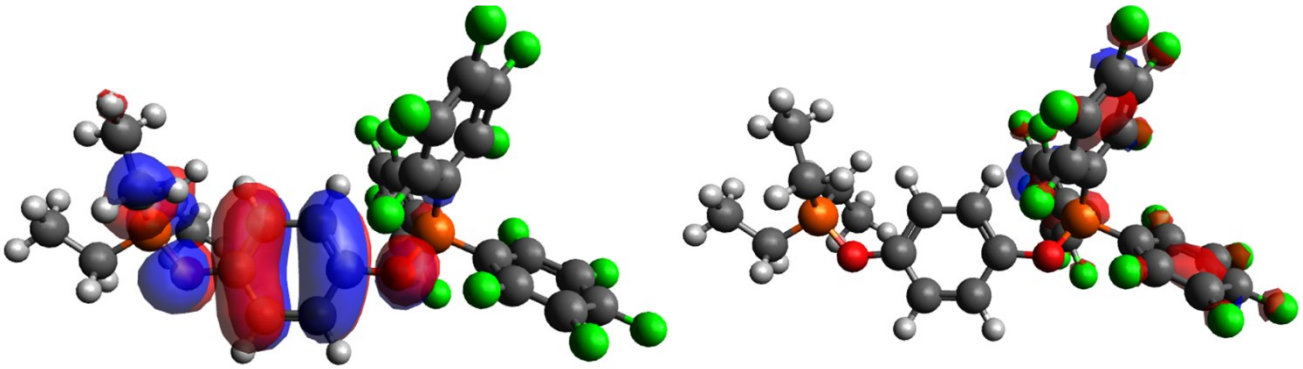


Figure S75. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-Q-BEt_3]$^{2-}$**. Isovalue = 0.02 e^-/a.u.

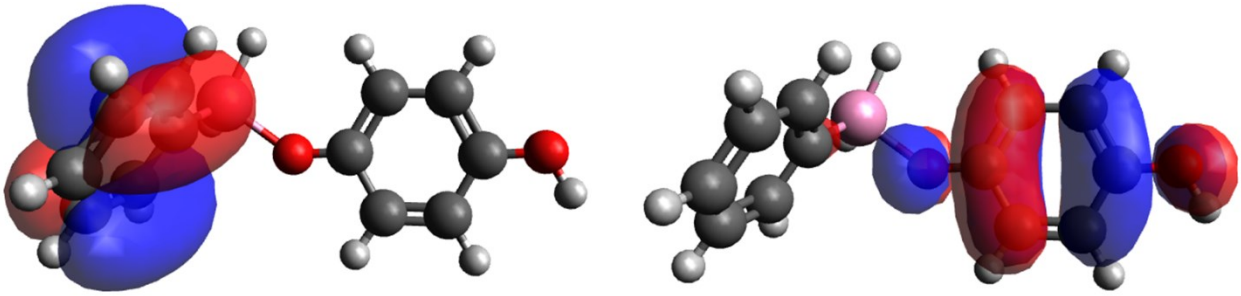


Figure S76. HOMO (left) and LUMO (right) images of **[SiH_2Ph-HQ]$^{2+}$**. Isovalue = 0.02 e^-/a.u.

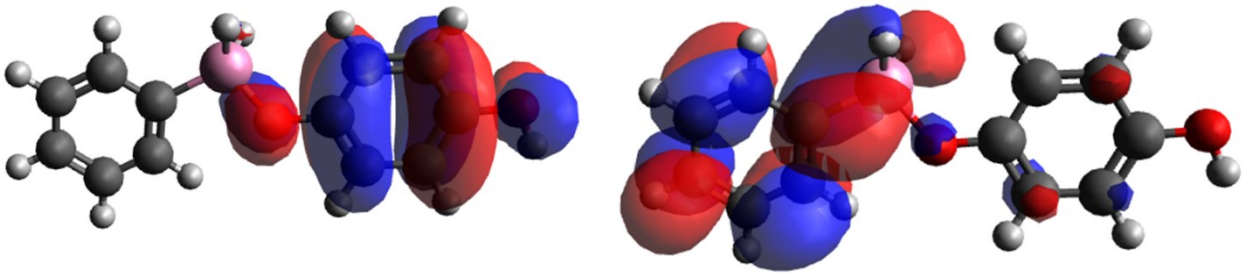


Figure S77. HOMO (left) and LUMO (right) images of **SiH_2Ph-HQ**. Isovalue = 0.02 e^-/a.u.

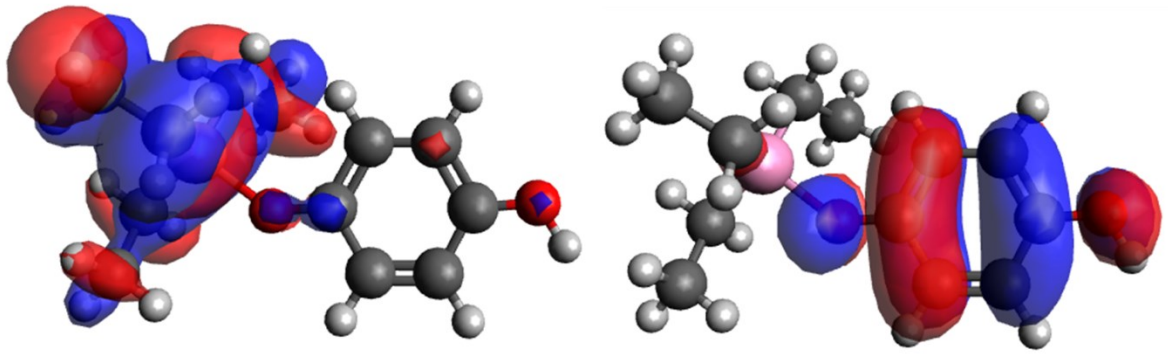


Figure S78. HOMO (left) and LUMO (right) images of **[SiEt$_3$-HQ]$^{2+}$**. Isovalue = 0.02 e$^-$/a.u.

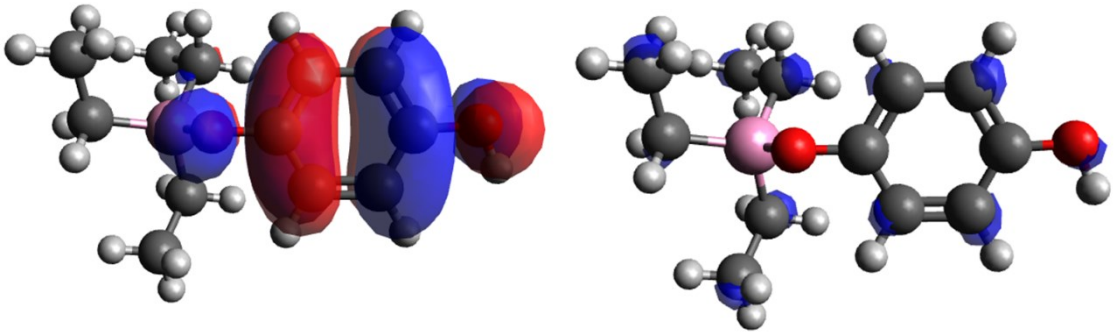


Figure S79. HOMO (left) and LUMO (right) images of **SiEt$_3$-HQ**. Isovalue = 0.02 e$^-$/a.u.

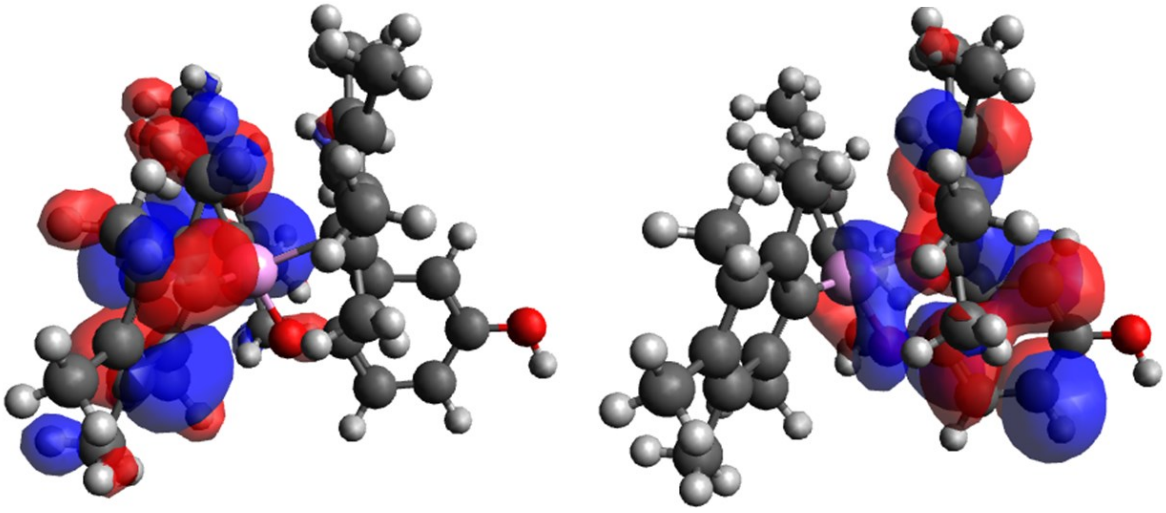


Figure S80. HOMO (left) and LUMO (right) images of **[Si(C$_6$Me$_5$)$_3$-HQ]$^{2+}$**. Isovalue = 0.02 e$^-$/a.u.

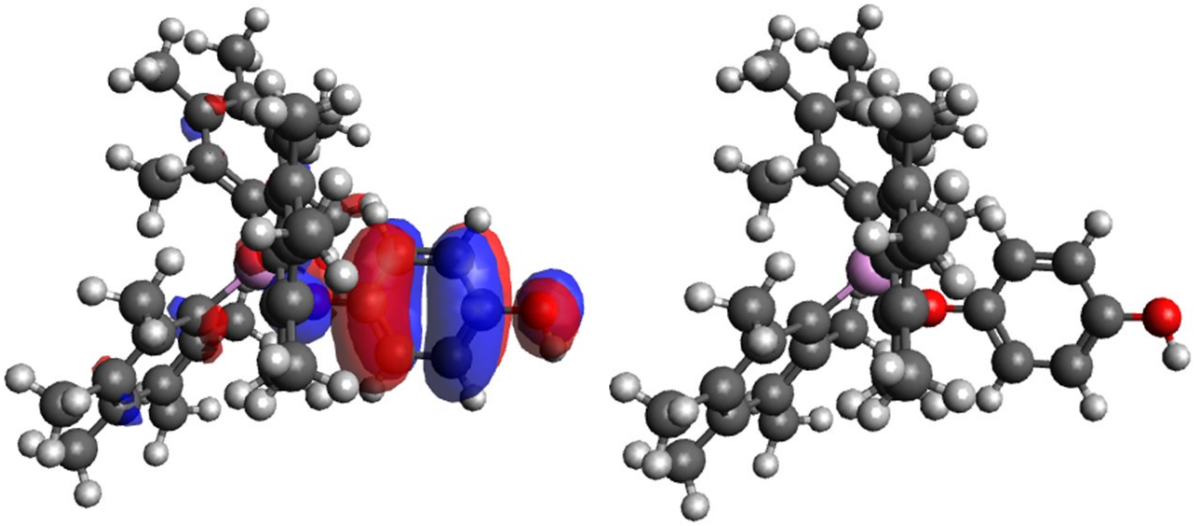


Figure S81. HOMO (left) and LUMO (right) images of **Si(C_6Me_5)$_3$-HQ**. Isovalue = 0.02 e^-/a.u.

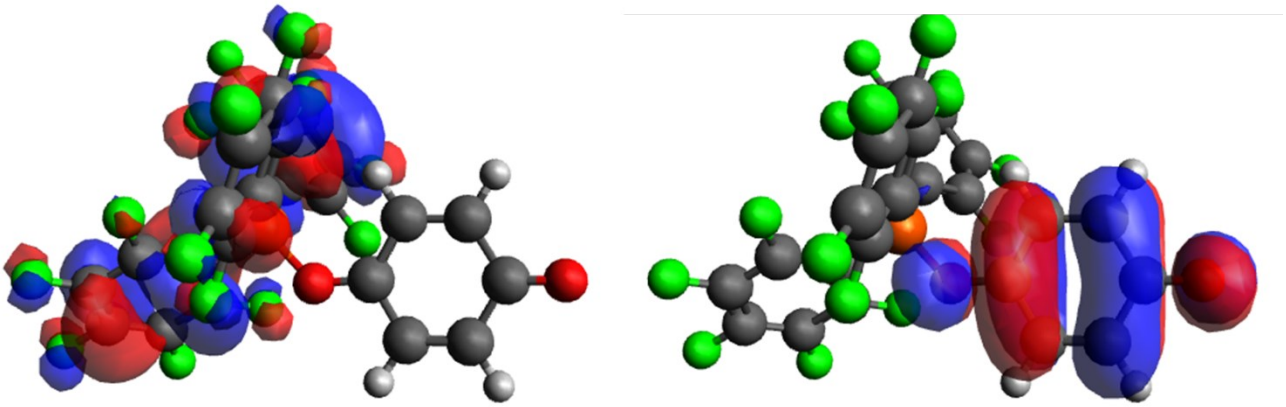


Figure S82. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-HQ]$^+$**. Isovalue = 0.02 e^-/a.u.

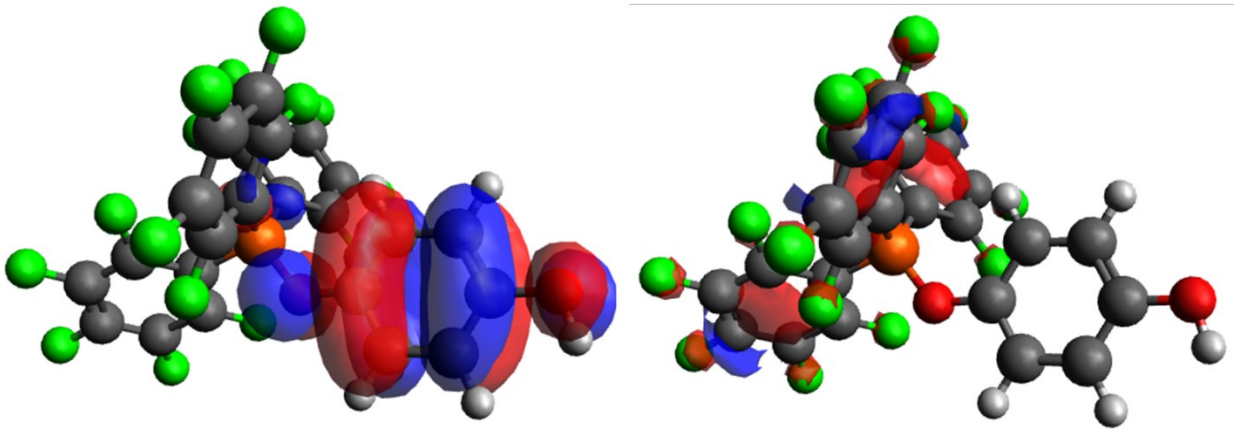


Figure S83. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_3$-HQ]$^-$**. Isovalue = 0.02 e$^-$/a.u.

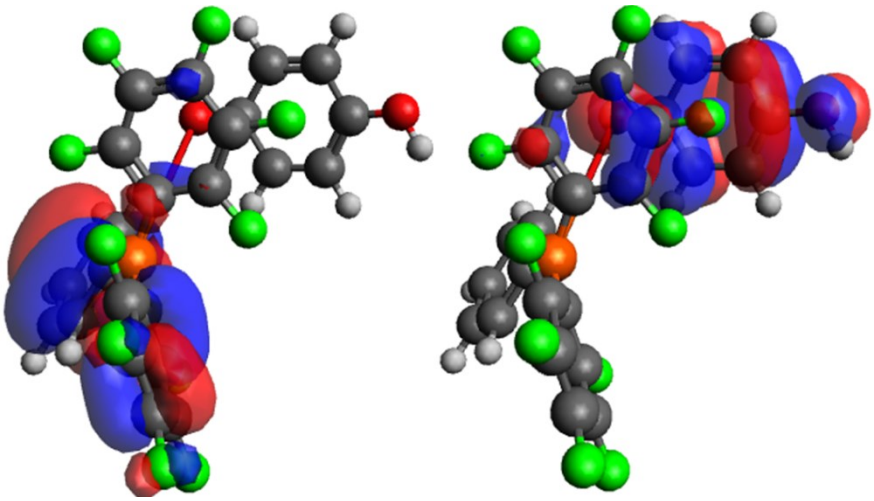


Figure S84. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_2$Ph-HQ]$^+$**. Isovalue = 0.02 e$^-$/a.u.

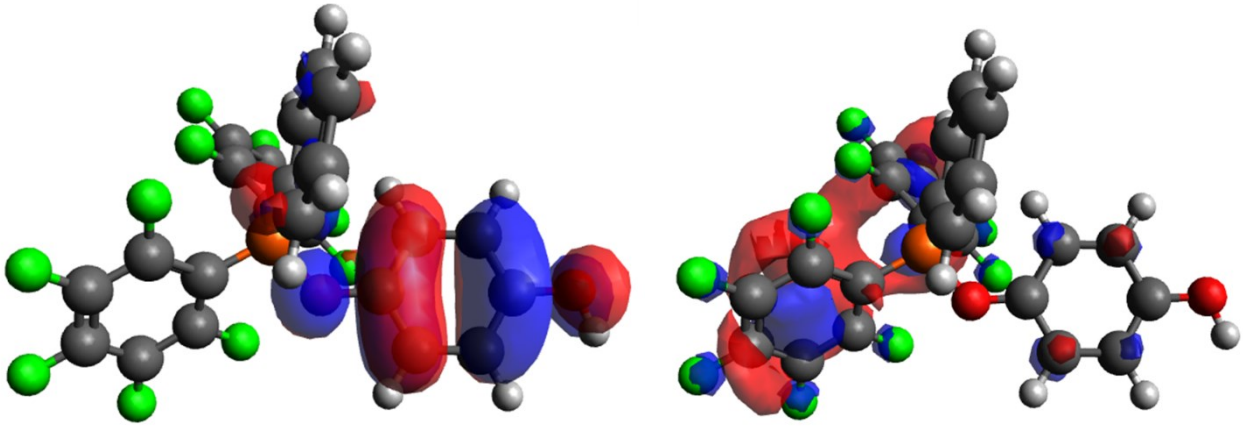


Figure S85. HOMO (left) and LUMO (right) images of **[B(C_6F_5)$_2$Ph-HQ]$^-$**. Isovalue = 0.02 e$^-$/a.u.

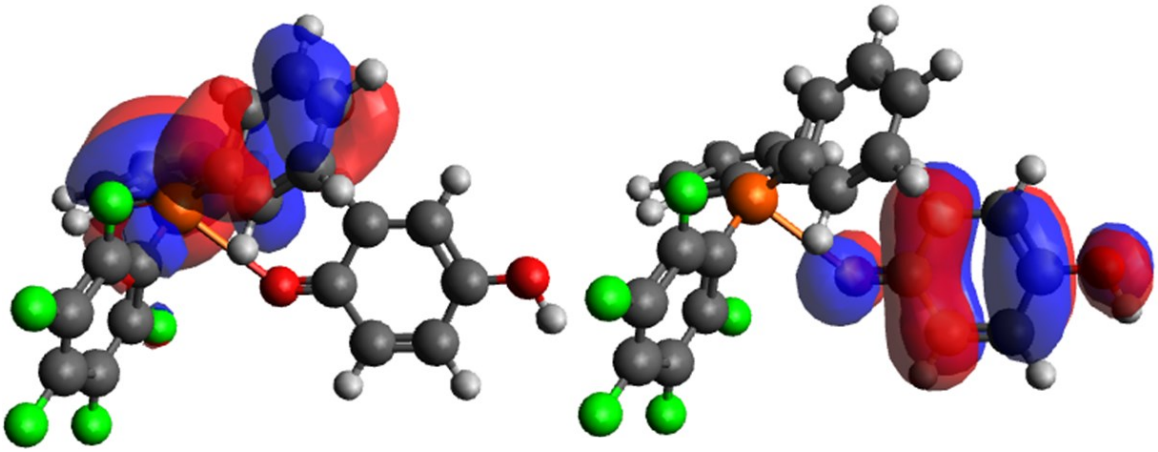


Figure S86. HOMO (left) and LUMO (right) images of **[B(C_6F_5)Ph_2-HQ]$^+$**. Isovalue = 0.02 e^-/a.u.

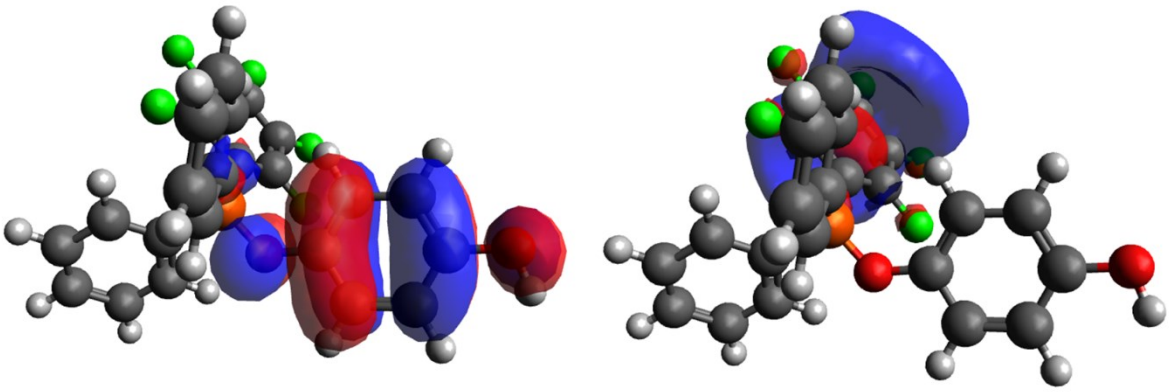


Figure S87. HOMO (left) and LUMO (right) images of **[B(C_6F_5)Ph_2-HQ]$^-$**. Isovalue = 0.02 e^-/a.u.

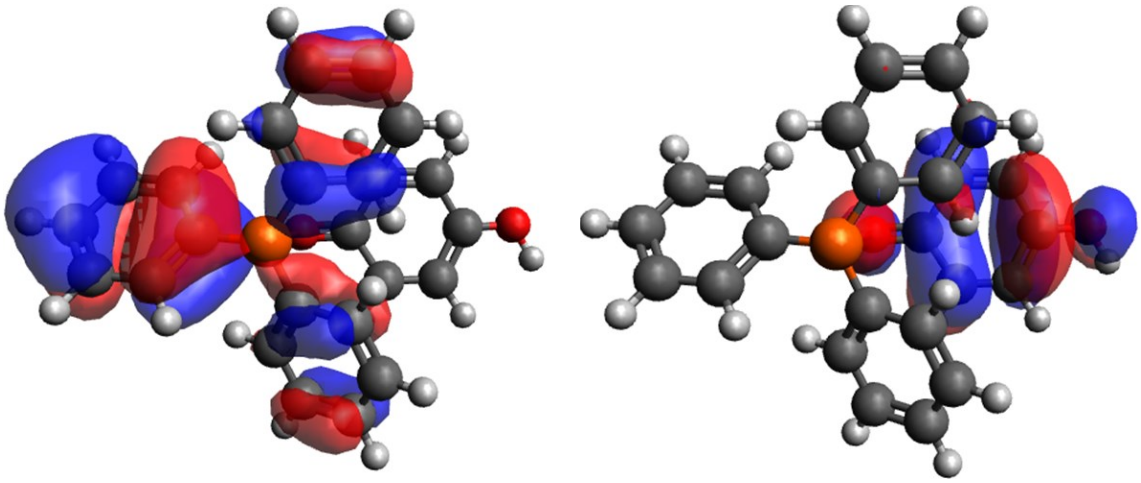


Figure S88. HOMO (left) and LUMO (right) images of **[BPh_3-HQ]$^+$**. Isovalue = 0.02 e^-/a.u.

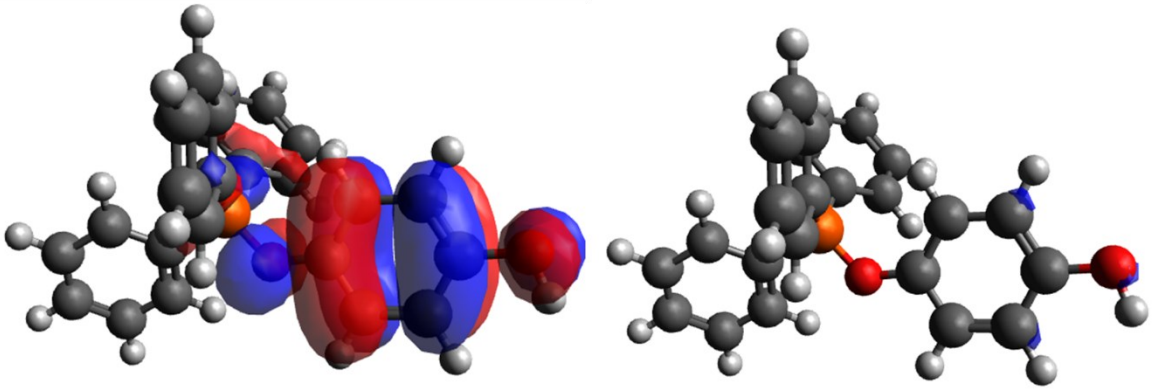


Figure S89. HOMO (left) and LUMO (right) images of **[BPh_3-HQ]$^-$**. Isovalue = 0.02 e^-/a.u.

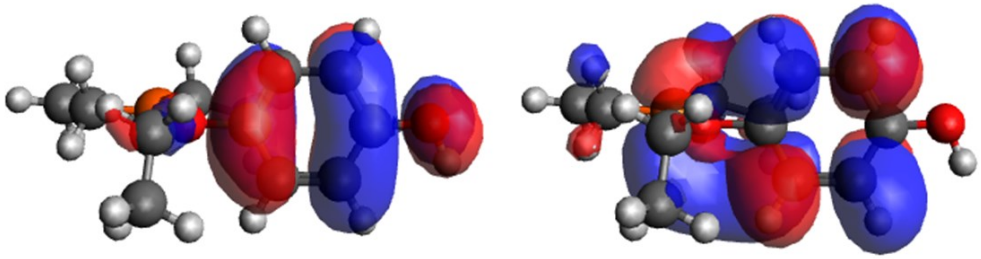


Figure S90. HOMO (left) and LUMO (right) images of **[BEt_3-HQ]$^+$**. Isovalue = 0.02 e^-/a.u.

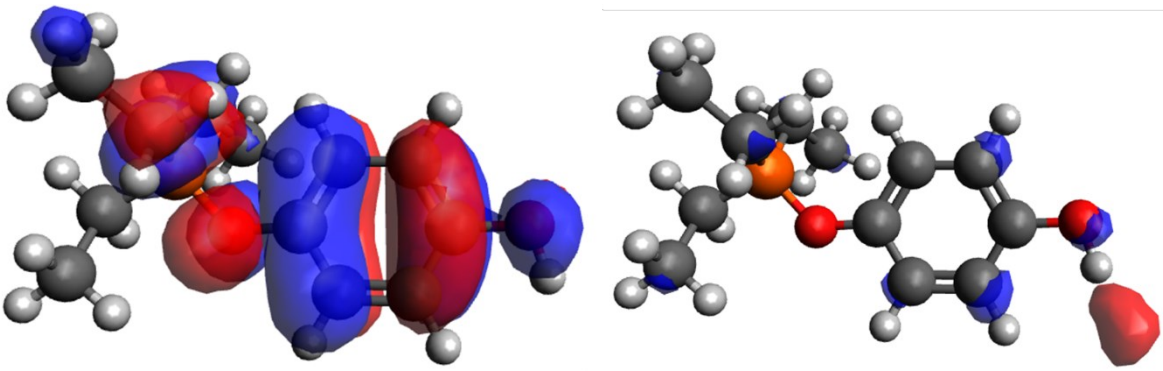
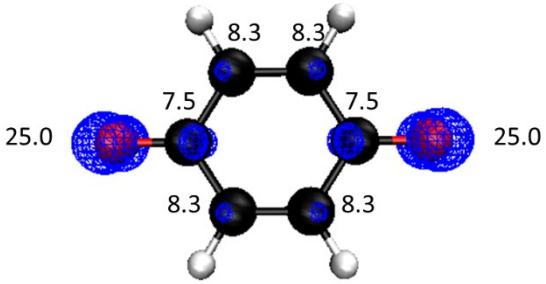


Figure S91. HOMO (left) and LUMO (right) images of **[BEt$_3$-HQ]**$^-$. Isovalue = 0.02 e$^-$/a.u.

18) Plots Showing the Locations of the Unpaired Spin Density

Figure S92. Unpaired spin density plot of semiquinone (**[Q]**$^{\bullet-}$) where the numbers show



the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

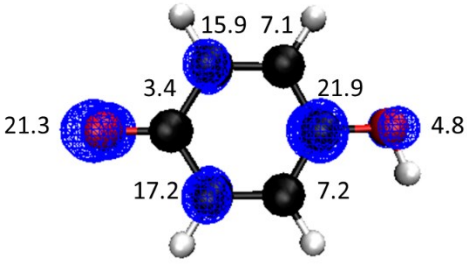


Figure S93. Unpaired spin density plot of **[HQ]**$^{\bullet}$ where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

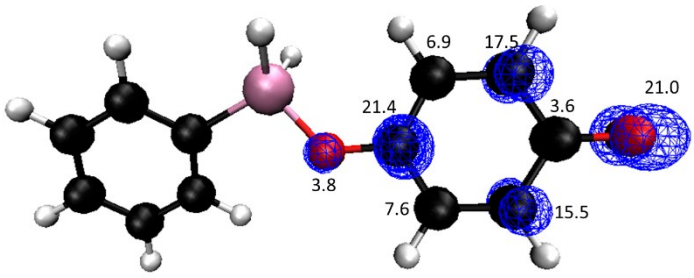


Figure S94. Unpaired spin density plot of **[SiH_2Ph-Q]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

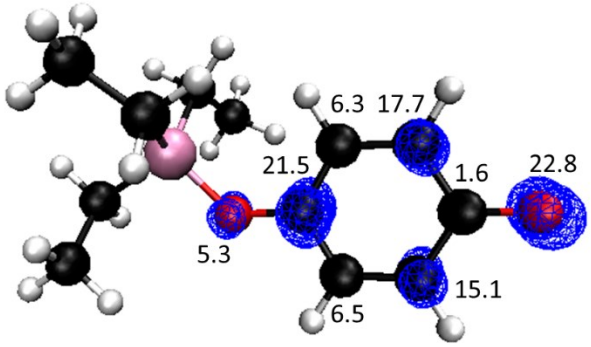


Figure S95. Unpaired spin density plot of **[$SiEt_3$-Q]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

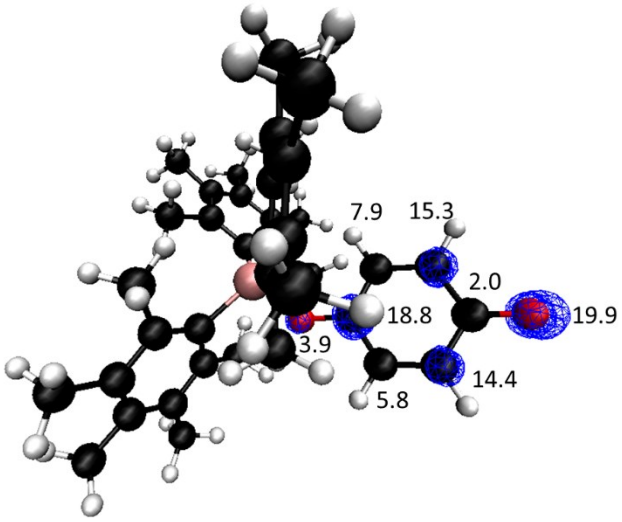


Figure S96. Unpaired spin density plot of **[Si(C_6Me_5)$_3$-Q]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

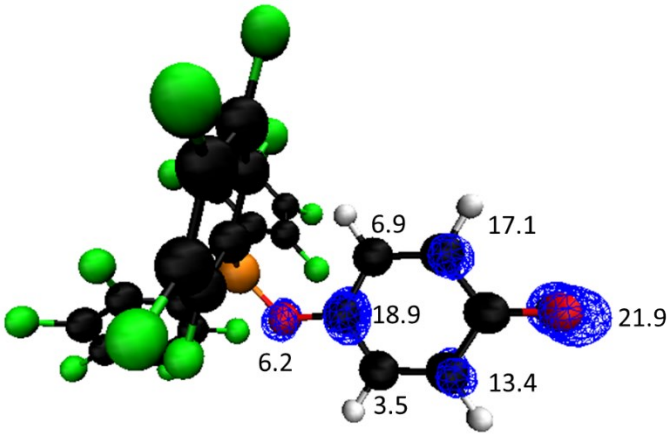


Figure S97. Unpaired spin density plot of **[B(C_6F_5)$_3$-Q]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

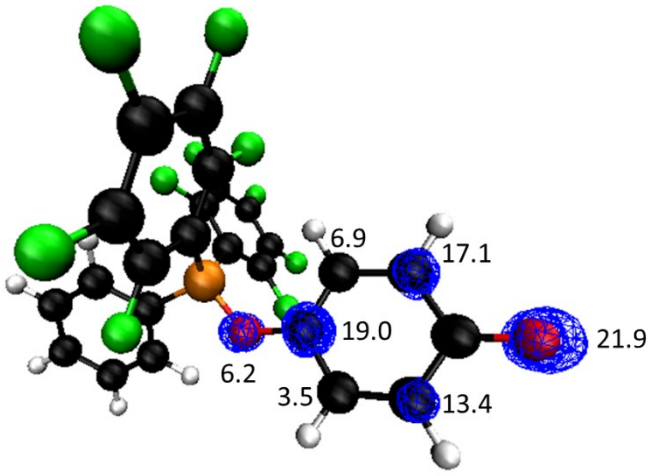


Figure S98. Unpaired spin density plot of **[B(C_6F_5)$_2$Ph-Q]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

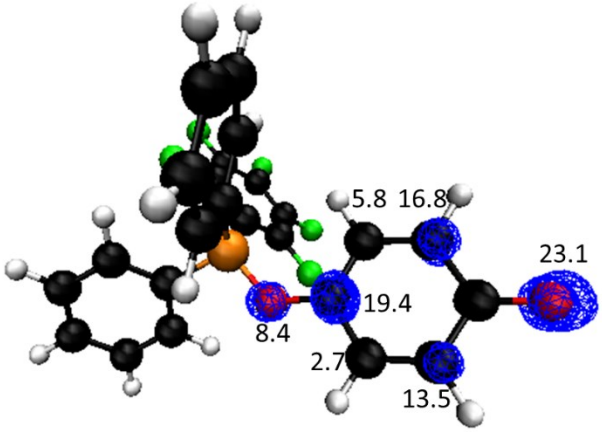


Figure S99. Unpaired spin density plot of **[B(C_6F_5)Ph$_2$-Q]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

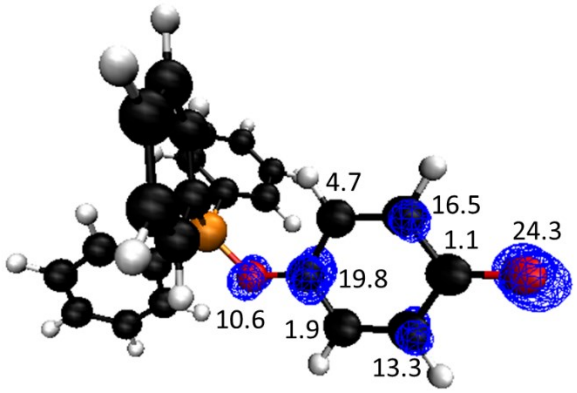


Figure S100. Unpaired spin density plot of **[BPh_3-Q]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

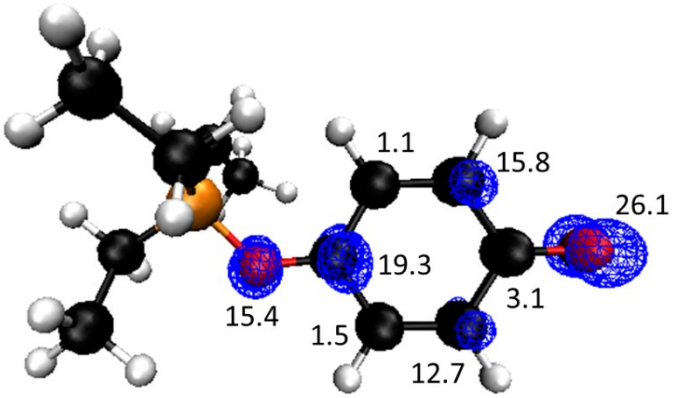


Figure S101. Unpaired spin density plot of **[BEt_3-Q]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

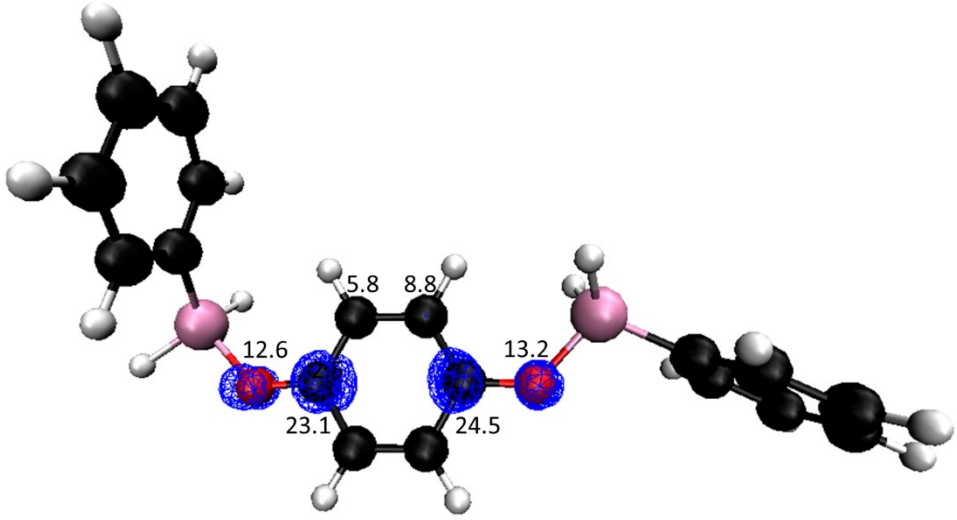


Figure S102. Unpaired spin density plot of **[SiH_2Ph-Q-SiH_2Ph]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

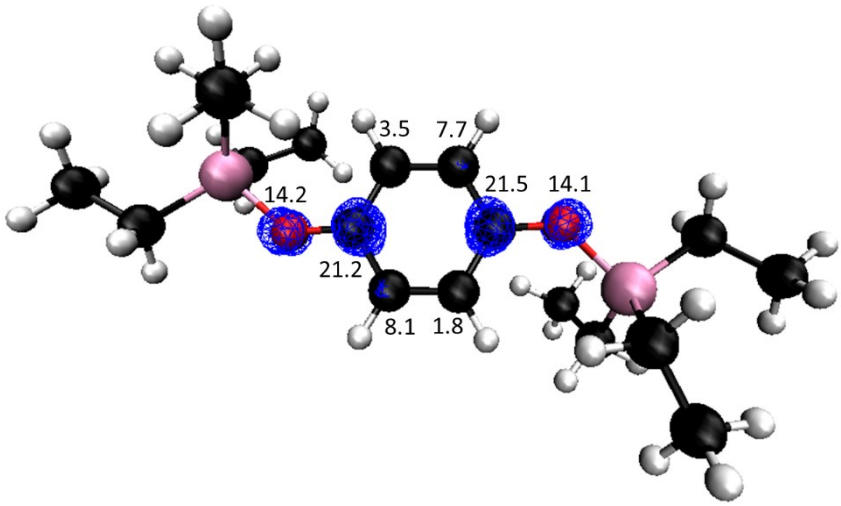


Figure S103. Unpaired spin density plot of **[$SiEt_3$-Q-$SiEt_3$]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

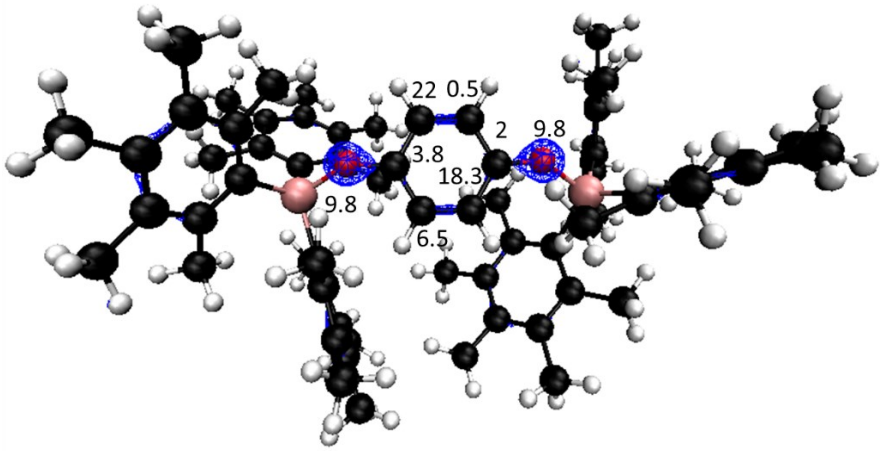


Figure S104. Unpaired spin density plot of **[Si(C_6Me_5)$_3$-Q-Si(C_6Me_5)$_3$]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.5 e^-/a.u.

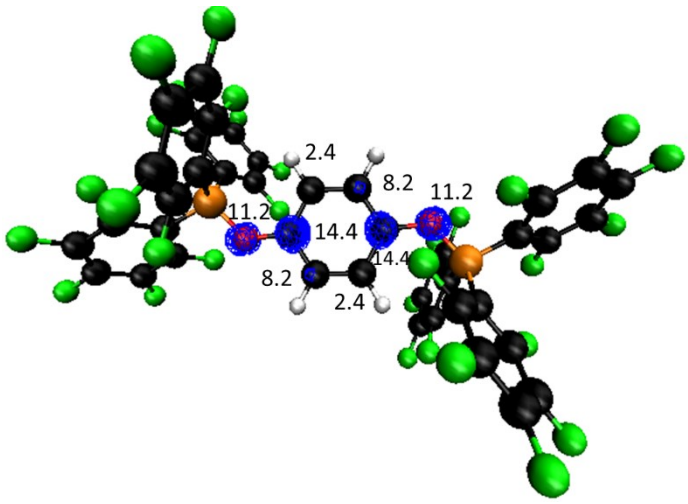


Figure S105. Unpaired spin density plot of **[B(C_6F_5)$_3$-Q-B(C_6F_5)$_3$]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

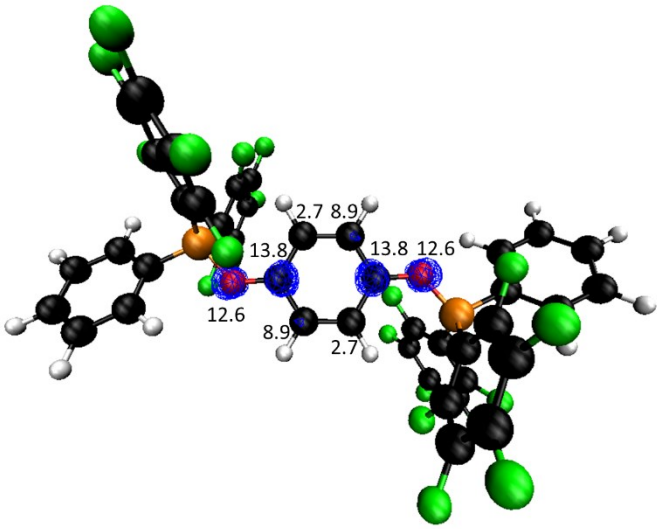


Figure S106. Unpaired spin density plot of **[B(C_6F_5)$_2$Ph-Q-B(C_6F_5)$_2$Ph]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

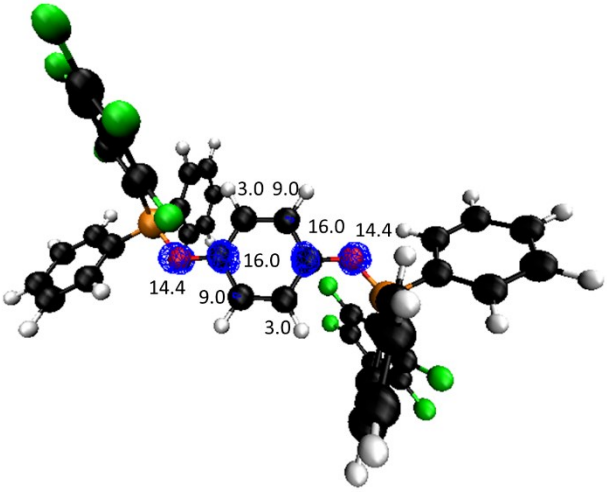


Figure S107. Unpaired spin density plot of **[B(C_6F_5)Ph$_2$-Q-B(C_6F_5)Ph$_2$]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

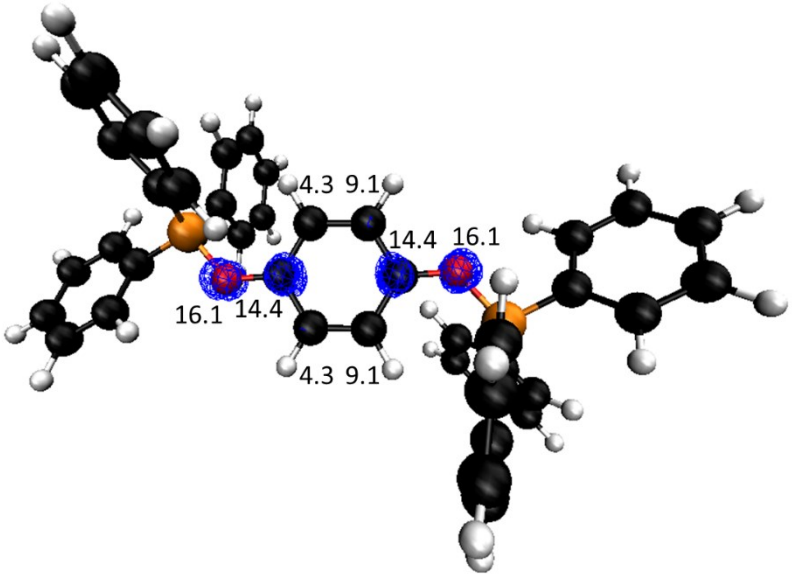


Figure S108. Unpaired spin density plot of **[BPh_3-Q-BPh_3]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

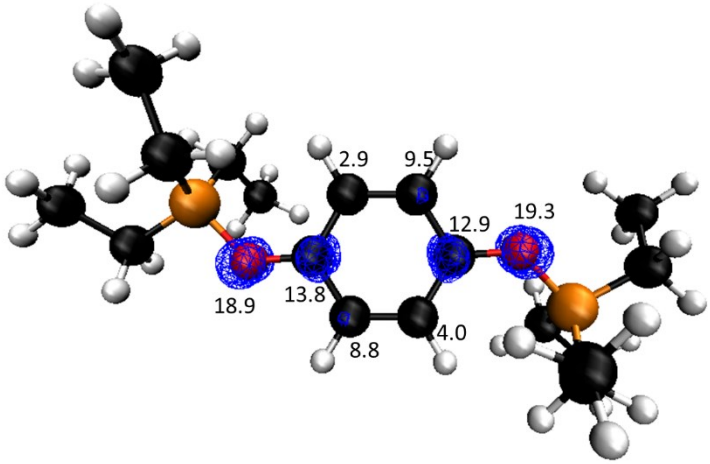


Figure S109. Unpaired spin density plot of **[BEt_3-Q-BEt_3]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

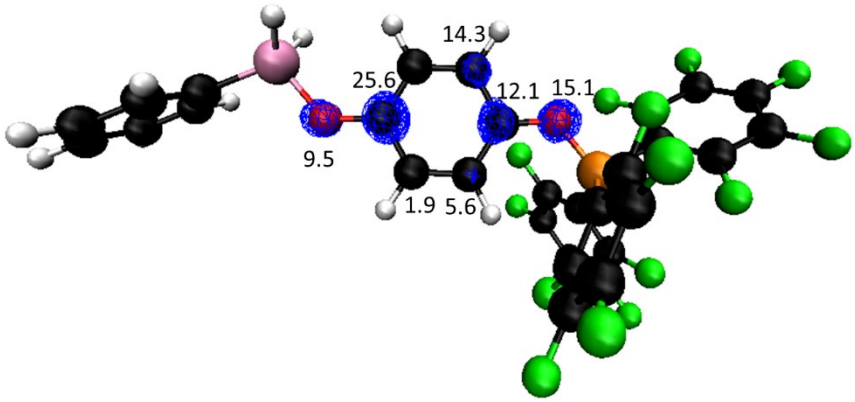


Figure S110. Unpaired spin density plot of **[B(C$_6$F$_5$)$_3$-Q-SiH$_2$Ph]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

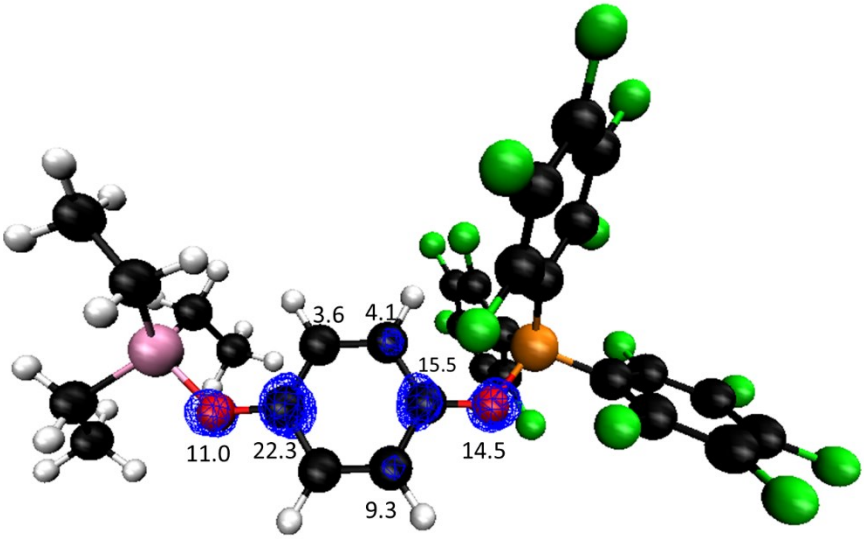


Figure S111. Unpaired spin density plot of **[B(C$_6$F$_5$)$_3$-Q-SiEt$_3$]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

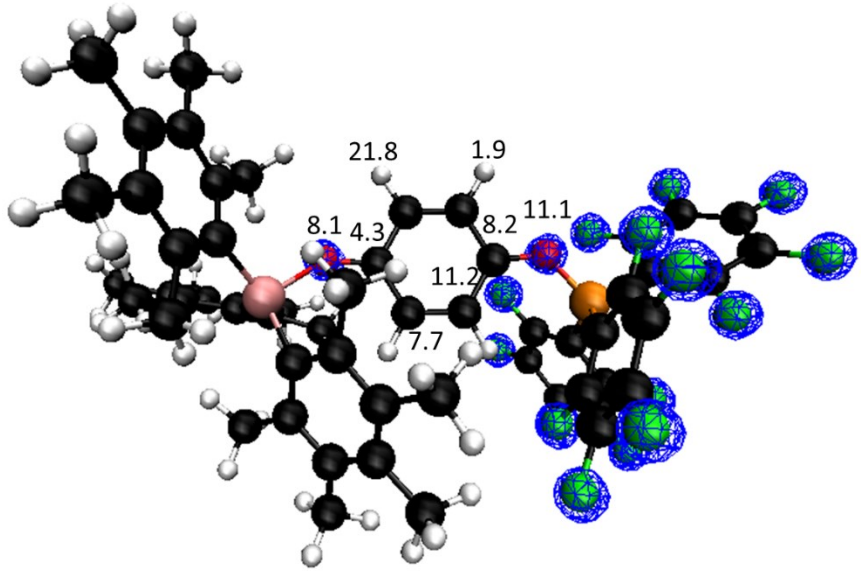


Figure S112. Unpaired spin density plot of **[B(C_6F_5)$_3$-Q-Si(C_6Me_5)$_3$]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.5 e^-/a.u.

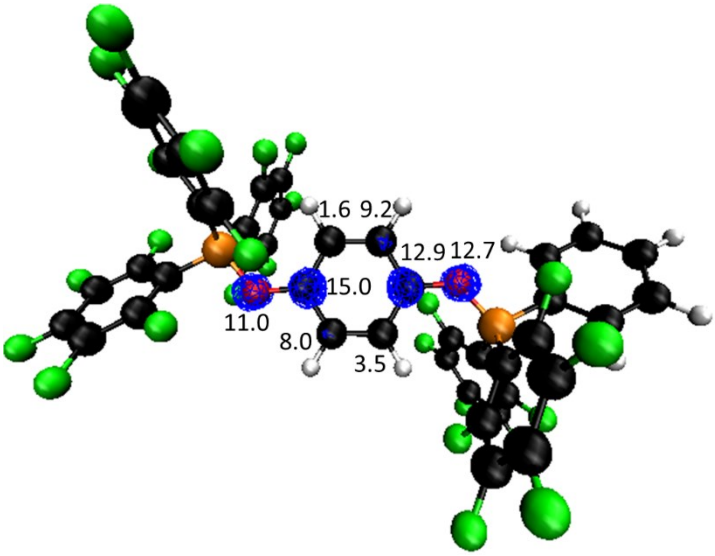


Figure S113. Unpaired spin density plot of **[B(C_6F_5)$_3$-Q-B(C_6F_5)$_2$Ph]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

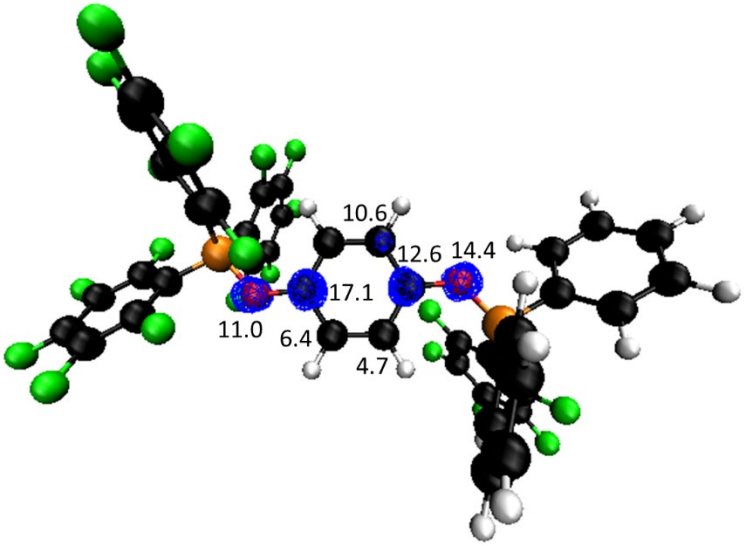


Figure S114. Unpaired spin density plot of **[B(C$_6$F$_5$)$_3$-Q-B(C$_6$F$_5$)Ph$_2$]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

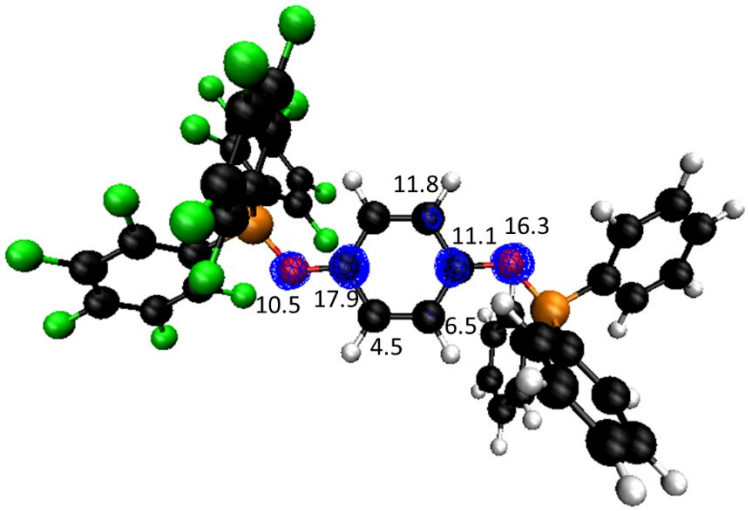


Figure S115. Unpaired spin density plot of **[B(C$_6$F$_5$)$_3$-Q-BPh$_3$]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

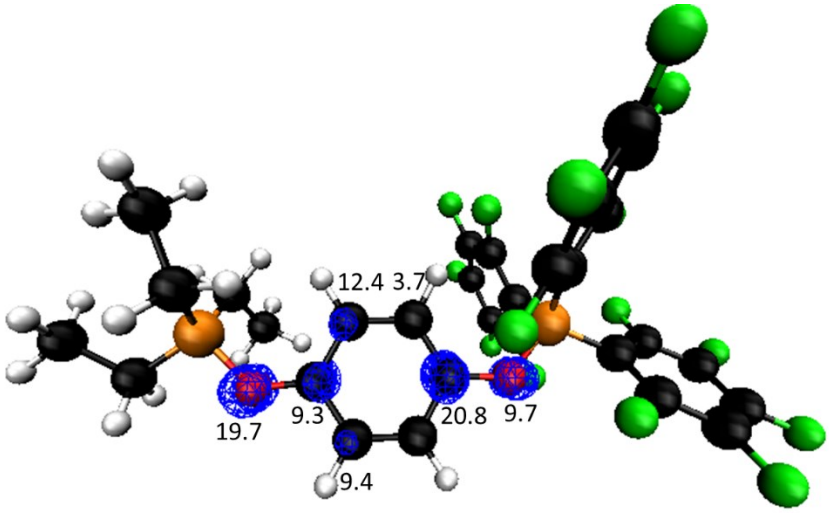


Figure S116. Unpaired spin density plot of **[B(C_6F_5)$_3$-Q-BEt_3]$^{\bullet-}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

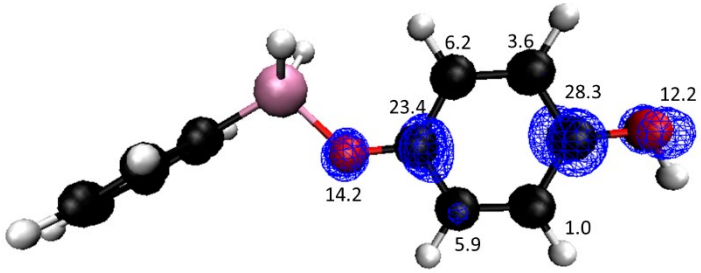


Figure S117. Unpaired spin density plot of **[SiH_2Ph-HQ]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

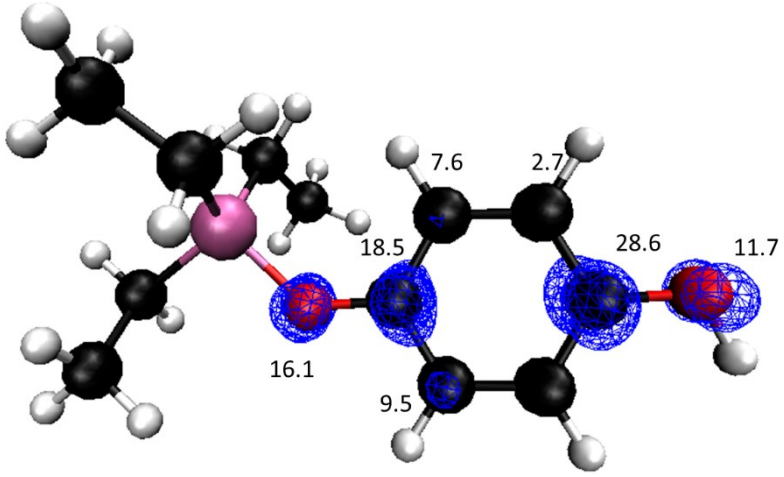


Figure S118. Unpaired spin density plot of **[$SiEt_3$-HQ]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

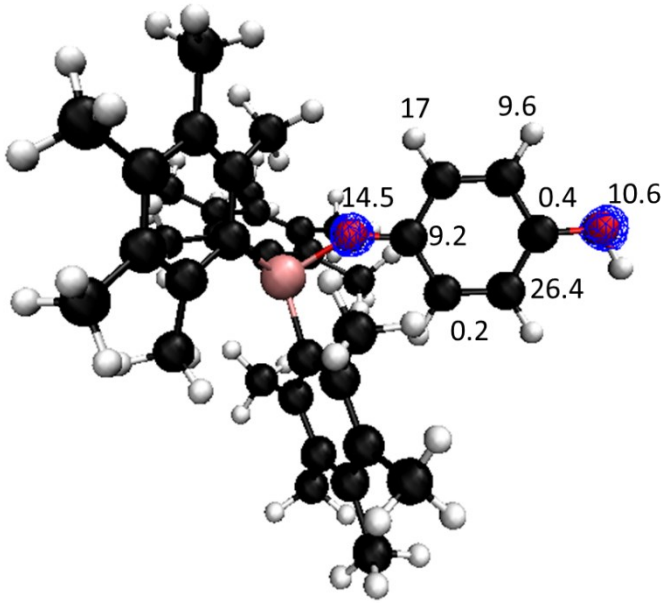


Figure S119. Unpaired spin density plot of **[Si(C_6Me_5)$_3$-HQ]$^{\bullet+}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.5 e^-/a.u.

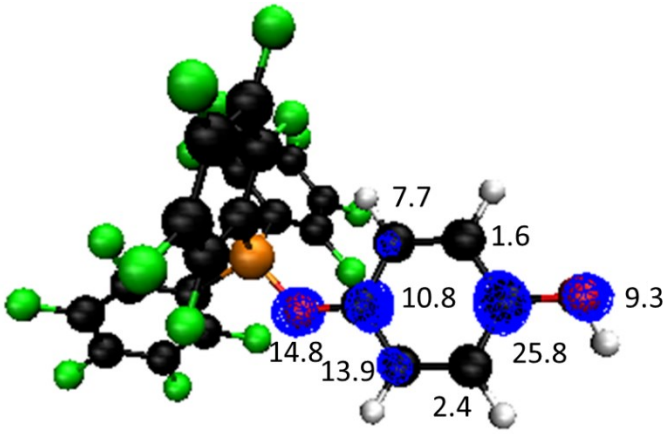


Figure S120. Unpaired spin density plot of **[B(C_6F_5)$_3$-HQ]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

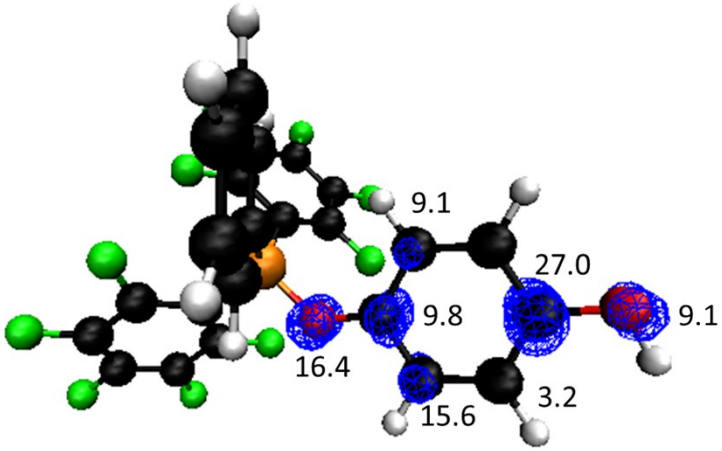


Figure S121. Unpaired spin density plot of **[B(C_6F_5)$_2$Ph-HQ]$^\bullet$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

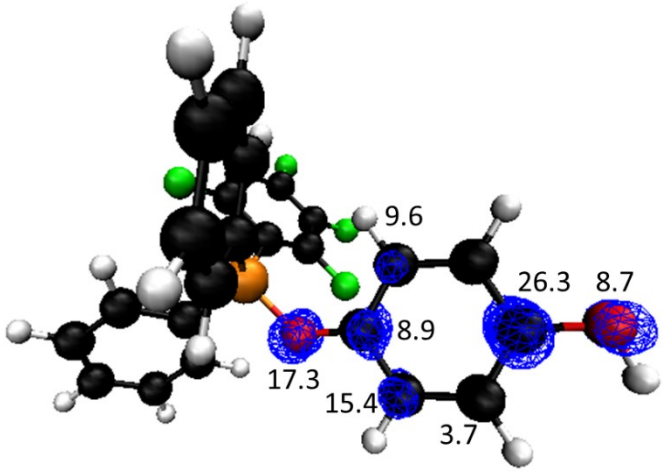


Figure S122. Unpaired spin density plot of **[B(C_6F_5)Ph$_2$-HQ]$^\bullet$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

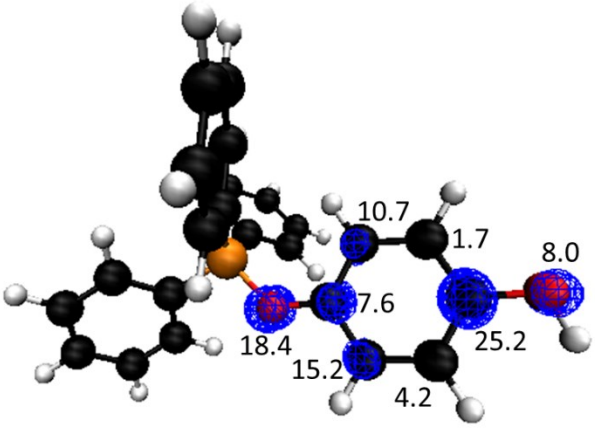


Figure S123. Unpaired spin density plot of **[BPh$_3$-HQ]$^\bullet$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e^-/a.u.

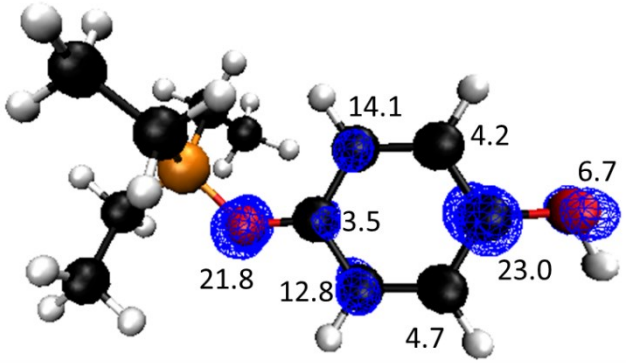


Figure S124. Unpaired spin density plot of **[BEt$_3$-HQ]$^{\bullet}$** where the numbers show the percentage of electron density residing on each atom. Isovalue = 0.01 e$^-$/a.u.

19) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms,followed by the complex name, and the 3D coordinates.

14
[SiPhH$_2$]$^+$

Si	-2.307320	-0.000050	-0.000060
H	-3.042560	-1.266470	-0.000790
H	-3.040870	1.267300	0.000970
C	-0.520980	-0.000550	0.000010
C	0.185450	1.223700	0.000070
C	0.186290	-1.224270	0.000110
C	1.571090	1.217380	-0.000070
H	-0.352740	2.167060	-0.000280
C	1.571870	-1.216910	0.000050
H	-0.351320	-2.167970	0.000440
C	2.257170	0.000480	-0.000050
H	2.120230	2.152240	0.000040
H	2.121690	-2.151370	-0.000150
H	3.342670	0.000830	-0.000110

15
SiPhH$_3$

Si	2.34012	0.00008	0.00586
H	2.87243	-0.12789	1.38488
H	2.85060	-1.14158	-0.79117
C	0.46581	0.00037	-0.01159
C	-0.25436	1.20210	-0.00962
C	-0.25426	-1.20208	-0.00962
C	-1.64668	1.20474	0.00301
H	0.27691	2.15076	-0.02299
C	-1.64589	-1.20541	0.00319
H	0.27673	-2.15116	-0.02318
C	-2.34370	-0.00020	0.01046
H	-2.18710	2.14608	0.00312
H	-2.18608	-2.14689	0.00354
H	-3.42914	-0.00056	0.01774
H	2.83834	1.27295	-0.56896

20
[SiPhH$_2$-NCMe]$^+$

Si	0.74879	1.51005	0.00009
N	2.15955	0.27574	0.00001
C	-0.79350	0.52734	0.00003
C	-1.39326	0.15118	-1.21336
C	-1.39321	0.15098	1.21339
C	-2.56508	-0.59586	-1.21052
C	-2.56504	-0.59606	1.21046
C	-3.14711	-0.96858	-0.00005
C	3.00418	-0.50445	-0.00004
C	4.07078	-1.48773	-0.00009
H	1.06453	2.23120	-1.23941
H	1.06454	2.23104	1.23967
H	-0.95451	0.45018	-2.16204

H	-0.95443	0.44982	2.16209
H	-3.02923	-0.87993	-2.14847
H	-3.02915	-0.88029	2.14839
H	-4.06529	-1.54654	-0.00008
H	5.03284	-0.96968	-0.00009
H	3.98214	-2.10873	-0.89471
H	3.98217	-2.10881	0.89447

22
$[SiEt_3]^+$

Si	-0.140300	-0.134490	-0.251900
C	1.307680	-1.207480	-0.636650
H	0.982450	-2.078000	-1.212630
H	2.022490	-0.642400	-1.244350
C	0.133080	1.630970	0.202280
H	-0.632590	2.223200	-0.316370
H	-0.127850	1.705580	1.269620
C	-1.830960	-0.860220	-0.158280
H	-2.033820	-1.304550	-1.142770
H	-1.748740	-1.718080	0.525580
C	1.971360	-1.651690	0.692050
H	1.294450	-2.255290	1.302200
H	2.848520	-2.260840	0.463540
H	2.305460	-0.798610	1.289160
C	-2.948410	0.097700	0.272410
H	-3.898420	-0.439280	0.320660
H	-2.754180	0.523420	1.260080
H	-3.065170	0.919530	-0.438190
C	1.544770	2.168690	-0.065090
H	1.617470	3.205110	0.271770
H	2.304050	1.590800	0.468660
H	1.784920	2.144420	-1.130660

23
$HSiEt_3$

Si	0.18357	-0.01320	0.57896
H	0.45617	0.46702	1.96546
C	-1.17890	-1.32124	0.63099
H	-0.81854	-2.18720	1.19881
H	-2.03031	-0.92407	1.19648
C	-0.39341	1.45718	-0.45801
H	0.35958	2.25163	-0.39580
H	-0.42678	1.15487	-1.51271
C	1.77733	-0.73301	-0.13401
H	2.09873	-1.56946	0.49814
H	1.56185	-1.16361	-1.11993
C	-1.63595	-1.75977	-0.76657
H	-0.80696	-2.18172	-1.34369
H	-2.42098	-2.51987	-0.71859
H	-2.03281	-0.91439	-1.33862
C	2.90258	0.30288	-0.25189
H	3.82795	-0.14142	-0.62973
H	2.62506	1.11214	-0.93424
H	3.12687	0.75626	0.71888
C	-1.76087	1.99522	-0.01857
H	-2.06425	2.86791	-0.60405
H	-2.54165	1.23606	-0.13240
H	-1.74855	2.29299	1.03486

28
$[SiEt_3\text{-}NCMe]^+$

Si	0.74490	0.00025	0.00047
N	-1.15236	-0.00036	-0.00103
C	1.10554	-1.79185	-0.35404
C	1.10286	0.58969	1.73011
C	1.10541	1.20338	-1.37402
C	0.70021	2.04963	1.98692
C	0.70438	0.69666	-2.76755
C	0.70439	-2.74529	0.78150
C	-2.30246	-0.00084	-0.00134
C	-3.75474	-0.00162	-0.00167
H	0.61253	-2.07077	-1.29279
H	2.18233	-1.86940	-0.55257
H	0.60945	-0.08387	2.44070
H	2.17959	0.45747	1.89776
H	0.61245	2.15587	-1.14633
H	2.18222	1.41403	-1.34192
H	0.90791	2.33250	3.02033
H	1.25163	2.73647	1.33997
H	-0.36832	2.21141	1.81224
H	0.91442	1.45004	-3.52873
H	1.25510	-0.20773	-3.03810
H	-0.36434	0.46590	-2.82233
H	0.91484	-3.78115	0.50979
H	1.25467	-2.52713	1.70021
H	-0.36444	-2.67754	1.00823
H	-4.11220	0.06088	1.02868
H	-4.11228	0.85908	-0.57146
H	-4.11126	-0.92563	-0.46258

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$[Si(C_6Me_5)_3]^+$

Si	-0.04398	-0.07210	0.00443
C	1.37039	-1.24737	0.02721
C	0.32636	1.72957	-0.00162
C	-1.79085	-0.64791	-0.01628
C	-2.27436	-1.48495	1.01238
C	-3.62105	-1.87035	1.00330
C	-4.45868	-1.45226	-0.04547
C	-3.98764	-0.57927	-1.04298
C	-2.64478	-0.18639	-1.04174
C	-0.19709	2.56284	1.01039

C	0.10378	3.93082	0.99478
C	0.89986	4.45727	-0.03745
C	1.46705	3.61756	-1.01267
C	1.16693	2.25058	-1.00942
C	2.33612	-1.10827	1.04768
C	3.46122	-1.93934	1.04414
C	3.59008	-2.93041	0.05355
C	2.64854	-3.04222	-0.98426
C	1.52342	-2.20710	-0.99510
C	1.15497	5.94351	-0.09660
C	-1.03820	2.00296	2.13626
C	2.38564	4.20009	-2.06155
C	1.71198	1.37576	-2.11843
C	-1.38033	-1.93440	2.14666
C	-4.18308	-2.72996	2.11181
C	-5.88411	-1.94464	-0.10116
C	-4.93218	-0.07857	-2.11075
C	-2.12578	0.67974	-2.16957
C	0.52007	-2.32472	-2.12085
C	2.86258	-4.06173	-2.07894
C	4.75695	-3.88614	0.10542
C	4.53305	-1.78318	2.09773
C	2.14837	-0.11296	2.17367
C	-0.41632	4.84983	2.07580
H	0.32593	6.50905	0.32884
H	2.05882	6.21192	0.46391
H	1.29345	6.28419	-1.12301
H	-1.29940	0.95043	1.99362
H	-0.51358	2.08015	3.09485
H	-1.98363	2.54236	2.23604
H	3.02999	4.96992	-1.63308
H	3.03588	3.44417	-2.50059
H	1.81982	4.66458	-2.87765
H	2.79145	1.22249	-2.01868
H	1.26109	0.37909	-2.14500
H	1.52813	1.82626	-3.09760
H	-0.32223	-1.72933	1.96180
H	-1.65336	-1.43995	3.08588
H	-1.45790	-3.01175	2.31119
H	-3.58076	-2.67556	3.01783
H	-5.19444	-2.41629	2.37692
H	-4.23485	-3.78335	1.81311
H	-5.98274	-2.93320	0.34747
H	-6.55797	-1.26838	0.43889
H	-6.24264	-2.01242	-1.12856
H	-5.92112	0.12220	-1.69482
H	-4.58010	0.84751	-2.56421
H	-5.05802	-0.81444	-2.91360
H	-2.45212	0.29566	-3.13942
H	-2.47721	1.71307	-2.08299
H	-1.03285	0.72375	-2.20919
H	0.18875	-3.35786	-2.25162
H	-0.38352	-1.73255	-1.94994
H	0.95276	-1.99796	-3.07311
H	3.91402	-4.11120	-2.36876
H	2.56643	-5.06506	-1.75188
H	2.29075	-3.82803	-2.97599
H	5.08591	-4.05943	1.13030
H	4.49963	-4.85390	-0.32534
H	5.61488	-3.49400	-0.45430
H	4.53234	-0.78381	2.53238
H	4.40327	-2.50185	2.91541
H	5.52490	-1.94802	1.67324
H	1.11742	0.24898	2.25522
H	2.38495	-0.56587	3.13937
H	2.78459	0.76994	2.05006
H	-0.72468	4.30567	2.96729
H	0.34789	5.56727	2.38177
H	-1.28164	5.42451	1.72625

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$HSi(C_6Me_5)_3$

Si	0.00474	0.00006	-0.58051
C	1.85123	-0.13115	-0.13966
C	-0.80785	1.66323	-0.13897
C	-1.03404	-1.53309	-0.14288
C	-0.63775	-2.48588	0.81702
C	-1.32594	-3.70440	0.93241
C	-2.45600	-3.95053	0.13879
C	-2.85847	-3.01043	-0.82058
C	-2.16572	-1.79515	-0.94340
C	-1.83222	1.79006	0.82055
C	-2.55206	2.99033	0.93445
C	-2.20800	4.09363	0.13966
C	-1.19053	3.97882	-0.81839
C	-0.47559	2.77637	-0.93937
C	2.47589	0.69208	0.81858
C	3.87531	0.71137	0.93212
C	4.65604	-0.14217	0.13877
C	4.04533	-0.96554	-0.81788
C	2.64649	-0.97884	-0.93919
C	-2.91483	5.41696	0.33707
C	-2.15351	0.66682	1.78444
C	-0.87945	5.14190	-1.73564
C	0.67900	2.71665	-1.91982
C	0.49900	-2.20991	1.77917
C	-0.83958	-4.76054	1.90163
C	-3.25820	-5.21789	0.33902
C	-4.02376	-3.31546	-1.73706
C	-2.68432	-0.76434	-1.92659
C	2.01506	-1.94759	-1.91941
C	4.89441	-1.82114	-1.73321

C	6.15531	-0.19592	0.33640
C	4.54414	1.66519	1.89869
C	1.66606	1.53628	1.78057
C	-3.71083	3.08959	1.90329
H	0.00622	0.00194	-2.06672
H	-3.80207	5.50758	-0.30205
H	-3.24189	5.54204	1.37033
H	-2.25749	6.25617	0.10495
H	-2.99485	0.05168	1.44243
H	-1.30882	-0.00940	1.91667
H	-2.40771	1.06316	2.77041
H	-0.11499	5.80698	-1.31435
H	-0.51250	4.79652	-2.70316
H	-1.76830	5.74509	-1.92739
H	1.21927	3.66605	-1.93976
H	1.40597	1.94761	-1.65402
H	0.33757	2.51049	-2.94153
H	0.66816	-1.14131	1.91308
H	0.28322	-2.62900	2.76484
H	1.44949	-2.63508	1.43406
H	0.24148	-4.70621	2.03733
H	-1.29983	-4.65568	2.89236
H	-1.06658	-5.76484	1.54026
H	-3.20621	-5.56119	1.37329
H	-4.31233	-5.06107	0.10584
H	-2.89863	-6.03611	-0.29747
H	-4.11030	-4.38663	-1.92614
H	-4.97923	-2.97721	-1.31646
H	-3.90437	-2.82829	-2.70576
H	-3.77673	-0.76228	-1.94460
H	-2.37320	0.24826	-1.66570
H	-2.33857	-0.96406	-2.94814
H	2.56122	-2.89376	-1.93444
H	0.98296	-2.18555	-1.65776
H	2.01441	-1.55160	-2.94225
H	5.86204	-1.35561	-1.92735
H	5.08651	-2.81470	-1.30872
H	4.41067	-1.96852	-2.69976
H	6.42756	0.02415	1.36971
H	6.55071	-1.18589	0.10439
H	6.67948	0.52572	-0.30262
H	3.95172	2.57093	2.03552
H	4.68906	1.21574	2.88933
H	5.52455	1.97623	1.53423
H	0.65816	1.14375	1.91632
H	2.13820	1.56238	2.76552
H	1.55385	2.57103	1.43424
H	-3.39275	3.43999	2.89345
H	-4.47276	3.78151	1.54073
H	-4.19636	2.12241	2.04067

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$[Si(C_6F_5)_3\text{-}NCMe]^+$

Si	-0.002294	-0.000176	0.084485
C	0.712187	1.713800	-0.184766
C	-1.843342	-0.240039	-0.185231
C	-2.527427	0.616676	-1.075721
C	-3.929212	0.602466	-1.120655
C	-4.646234	-0.327500	-0.350995
C	-3.970622	-1.203233	0.512719
C	-2.568660	-1.177524	0.583034
C	1.796241	1.875856	-1.075727
C	2.487413	3.095446	-1.121043
C	2.044121	4.181732	-0.349911
C	0.948194	4.036174	0.514484
C	0.265805	2.811145	0.583372
C	-1.788878	1.516781	-2.045465
C	-4.671374	1.587056	-1.996397
C	-6.149207	-0.411533	-0.482559
C	-4.762009	-2.172924	1.361950
C	-1.883814	-2.228238	1.435427
C	-0.986406	2.746475	1.436077
C	0.508131	5.206358	1.365894
C	2.725129	5.524200	-0.481430
C	3.709720	3.243813	-1.999095
C	2.203661	0.786633	-2.047173
N	-0.005844	0.001413	1.994805
C	-0.009213	0.003388	3.142810
C	-0.013176	0.004579	4.595384
H	-0.777406	1.164018	-2.255953
H	-2.312376	1.550057	-3.002797
H	-1.696298	2.545937	-1.679001
H	-4.100270	2.504261	-2.141988
H	-5.623933	1.870735	-1.546991
H	-4.886657	1.170515	-2.987796
H	-6.653375	0.245189	0.236742
H	-6.508974	-1.425944	-0.308896
H	-6.477703	-0.118689	-1.480000
H	-5.017036	-3.082914	0.805548
H	-4.213806	-2.479081	2.252715
H	-5.698432	-1.725485	1.699084
H	-2.317576	-3.211588	1.235017
H	-0.815710	-2.315453	1.232455
H	-2.016959	-2.043059	2.509133
H	-1.617157	3.617160	1.237753
H	-1.600019	1.868452	1.231074
H	-0.759193	2.765965	2.509801
H	1.365818	5.790174	1.703913
H	-0.150471	5.885407	0.811124
H	-0.031706	4.884916	2.256363
H	3.138358	5.663968	-1.480591
H	2.029007	6.343892	-0.302317

H	3.549733	5.629115	0.234047
H	4.217856	2.290167	-2.143964
H	3.454855	3.636974	-2.990650
H	4.432808	3.927388	-1.552303
H	1.390540	0.090012	-2.259897
H	2.496325	1.224341	-3.003478
H	3.046532	0.188559	-1.681287
H	-0.419573	-0.943851	4.952942
H	-0.632926	0.830689	4.950519
H	1.010257	0.128345	4.955699
C	1.127120	-1.474849	-0.180577
C	0.731527	-2.495151	-1.073686
C	1.448416	-3.699853	-1.120276
C	2.610269	-3.855025	-0.347200
C	3.025042	-2.833462	0.521200
C	2.299409	-1.633609	0.591382
C	3.439272	-5.111368	-0.480297
C	-0.416504	-2.307266	-2.044730
C	4.257256	-3.033944	1.375220
C	2.862553	-0.516435	1.448302
C	0.972653	-4.833138	-2.001476
H	3.356842	-5.538140	-1.480092
H	4.495997	-4.912560	-0.300344
H	3.121918	-5.880724	0.233997
H	-0.616382	-1.255310	-2.257844
H	-0.183280	-2.779589	-3.000876
H	-1.354359	-2.740579	-1.677714
H	5.174657	-2.795310	0.823737
H	4.242882	-2.409597	2.268361
H	4.339264	-4.069610	1.708880
H	3.932231	-0.401461	1.253971
H	2.406310	0.452823	1.243784
H	2.762840	-0.725495	2.521243
H	-0.107524	-4.802313	-2.146380
H	1.440412	-4.803649	-2.992975
H	1.208442	-5.801004	-1.557253

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$B(C_6F_5)_3$

B	-0.000120	-0.000030	-0.000360
C	1.314780	-0.853570	-0.000240
C	1.398460	-2.096160	0.636440
C	2.483810	-0.423980	-0.636770
C	2.554550	-2.860580	0.654850
C	3.652860	-1.168430	-0.654800
C	3.686770	-2.392930	0.000090
C	0.081750	1.565510	-0.000340
C	-0.875380	2.363520	-0.635580
C	1.116850	2.258990	0.635350
C	-0.814950	3.748190	-0.653290
C	1.201070	3.642390	0.654090
C	0.229340	4.389470	0.000650
C	-1.396730	-0.712110	-0.000120
C	-2.515050	-0.162630	0.635400
C	-1.608950	-1.939930	-0.635640
C	-3.755220	-0.781430	0.653510
C	-2.838270	-2.580000	-0.653830
C	-3.915990	-1.996430	-0.000130
F	-1.899060	1.803740	-1.282120
F	-1.741300	4.462730	-1.283100
F	0.298490	5.711060	0.000910
F	2.196970	4.255930	1.284270
F	2.076860	1.595290	1.281250
F	2.510170	0.741980	-1.284160
F	4.734350	-0.723870	-1.285770
F	4.796880	-3.113400	0.000230
F	2.588780	-4.029240	1.286080
F	0.344280	-2.595000	1.283880
F	-0.612250	-2.546490	-1.282150
F	-2.420330	1.000420	1.281640
F	-4.784870	-0.226130	1.283440
F	-5.095050	-2.597460	-0.000200
F	-2.993670	-3.739480	-1.283780

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$[HB(C_6F_5)_3]^-$

B	-0.07624	-0.06040	-0.97638
C	0.37095	1.40393	-0.38536
C	-1.61404	-0.46576	-0.59673
C	1.05767	-1.10242	-0.43322
C	1.49136	2.02243	-0.93553
C	1.98959	3.24572	-0.50679
C	1.35968	3.90415	0.53865
C	0.25023	3.32421	1.13158
C	-0.21162	2.09526	0.67067
C	-2.63938	0.43506	-0.88078
C	-3.98504	0.18217	-0.66324
C	-4.36734	-1.04266	-0.13499
C	-3.39187	-1.97749	0.16207
C	-2.05232	-1.67625	-0.07298
C	2.01819	-1.68494	-1.24871
C	3.03713	-2.49932	-0.75906
C	3.11982	-2.74790	0.60055
C	2.18479	-2.18086	1.45691
C	1.19116	-1.37423	0.92456
F	2.16057	1.42522	-1.93381
F	3.06944	3.79404	-1.07999
F	1.82091	5.08409	0.97123
F	-0.35859	3.95054	2.14716
F	-1.28217	1.60183	1.31178
F	-2.33969	1.64105	-1.39003
F	-4.91845	1.09718	-0.95702

F	-5.66035	-1.31495	0.07993
F	-3.74602	-3.16673	0.66739
F	-1.18821	-2.65853	0.23586
F	2.00929	-1.49187	-2.57423
F	3.94040	-3.04436	-1.58562
F	4.09191	-3.52903	1.08735
F	2.26300	-2.41884	2.77284
F	0.30939	-0.84328	1.78693
H	-0.01545	-0.00191	-2.18162

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$B(C_6F_5)_3$-NCMe

B	0.07219	-0.06470	0.60582
C	-0.30292	1.41763	0.04344
C	1.58732	-0.55841	0.28941
C	-1.12390	-1.07614	0.18266
C	-1.40980	2.08395	0.56122
C	-1.84574	3.32034	0.10891
C	-1.15910	3.93500	-0.92902
C	-0.05962	3.30205	-1.48988
C	0.34671	2.06439	-1.00240
C	2.64357	0.27148	0.65852
C	3.97698	-0.02923	0.43783
C	4.29893	-1.22894	-0.18465
C	3.28498	-2.09304	-0.56465
C	1.95728	-1.75157	-0.31990
C	-2.07314	-1.67226	1.00004
C	-3.11585	-2.45078	0.50626
C	-3.23551	-2.64641	-0.85959
C	-2.31016	-2.06372	-1.71833
C	-1.29133	-1.29417	-1.18308
F	-2.11780	1.51825	1.55750
F	-2.90674	3.91405	0.65364
F	-1.55458	5.11933	-1.38349
F	0.59734	3.88336	-2.49056
F	1.40586	1.51249	-1.60072
F	2.37329	1.43953	1.26688
F	4.94233	0.80635	0.81719
F	5.56988	-1.54738	-0.40412
F	3.58572	-3.25008	-1.15010
F	1.04663	-2.65423	-0.69856
F	-2.03371	-1.53166	2.33890
F	-3.99791	-3.00249	1.33893
F	-4.22514	-3.38759	-1.34668
F	-2.41617	-2.24726	-3.03178
F	-0.41222	-0.74816	-2.03392
N	0.06065	0.08365	2.18752
C	0.02746	0.19886	3.32479
C	-0.06521	0.31790	4.76975
H	-0.85927	-0.34643	5.11690
H	-0.30735	1.34920	5.03110
H	0.88454	0.03297	5.22442

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$B(C_6F_5)_2Ph$

B	0.000020	0.755480	-0.000050
C	1.346700	-0.053560	0.103210
C	2.504990	0.327180	-0.578200
C	1.442470	-1.225990	0.856260
C	3.688150	-0.396910	-0.511680
C	2.610520	-1.965450	0.958960
C	3.739410	-1.545660	0.265960
C	0.000060	2.303110	-0.000030
C	-1.061040	3.030010	-0.568390
C	1.061220	3.029940	0.568340
C	-1.058090	4.418620	-0.582990
H	-1.892950	2.494630	-1.018440
C	1.058350	4.418540	0.582970
H	1.893080	2.494500	1.018380
C	0.000150	5.113340	-0.000010
H	-1.879340	4.960880	-1.039690
H	1.879630	4.960750	1.039680
H	0.000190	6.198960	0.000000
C	-1.346710	-0.053490	-0.103250
C	-1.442600	-1.225860	-0.856380
C	-2.504930	0.327260	0.578270
C	-2.610690	-1.965260	-0.959030
C	-3.688120	-0.396780	0.511800
C	-3.739500	-1.545460	-0.265920
F	2.506000	1.404870	-1.363930
F	4.764780	-0.005000	-1.186410
F	4.863270	-2.243520	0.345350
F	2.660980	-3.065290	1.703980
F	0.382870	-1.671930	1.536700
F	-0.383060	-1.671800	-1.536930
F	-2.505820	1.404890	1.364090
F	-4.764680	-0.004870	1.186650
F	-4.863400	-2.243270	-0.345260
F	-2.661260	-3.065050	-1.704130

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$[HB(C_6F_5)_2Ph]^-$

B	-0.02561	0.67634	-1.02415
C	1.28851	-0.16687	-0.50258
C	0.07481	2.26138	-0.68936
C	-1.35963	-0.02948	-0.38390
C	1.63283	-1.36525	-1.12449
C	2.72586	-2.14286	-0.76150
C	3.53278	-1.72914	0.28705
C	3.22689	-0.55195	0.95026
C	2.12005	0.19399	0.55503
C	1.15333	3.00359	-1.19997

C	1.28833	4.37002	-0.98311
C	0.32763	5.05747	-0.24114
C	-0.75585	4.35341	0.27239
C	-0.87137	2.98056	0.04991
C	-2.41635	-0.50647	-1.15222
C	-3.54274	-1.11908	-0.60981
C	-3.64370	-1.27173	0.76359
C	-2.61861	-0.80862	1.57525
C	-1.51284	-0.20589	0.98869
F	0.88884	-1.83837	-2.13669
F	3.00979	-3.28522	-1.40461
F	4.59219	-2.46111	0.65666
F	3.99844	-0.15266	1.97139
F	1.89222	1.30532	1.26477
F	-2.40448	-0.39472	-2.48753
F	-4.53390	-1.56269	-1.39632
F	-4.72124	-1.85649	1.30270
F	-2.71255	-0.94941	2.90470
F	-0.55780	0.22815	1.82644
H	-0.06631	0.54228	-2.22708
H	1.91040	2.48230	-1.78468
H	2.14195	4.90460	-1.39358
H	0.42454	6.12603	-0.06825
H	-1.51467	4.87303	0.85298
H	-1.73085	2.45632	0.46310

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$B(C_6F_5)_2Ph$-NCMe

B	0.01437	0.74255	0.47842
C	-1.31884	-0.15474	0.19732
C	-0.03718	2.26462	-0.05756
C	1.33877	-0.09263	0.03524
C	-1.60955	-1.26701	0.98315
C	-2.69702	-2.10126	0.76978
C	-3.54506	-1.83891	-0.29686
C	-3.28477	-0.75736	-1.12468
C	-2.18464	0.05740	-0.87365
C	-1.14107	3.07236	0.25173
C	-1.20770	4.40136	-0.14815
C	-0.15773	4.95978	-0.87624
C	0.94771	4.17881	-1.19340
C	1.00412	2.84692	-0.78328
C	2.39268	-0.52481	0.83060
C	3.47102	-1.25239	0.33776
C	3.52149	-1.57266	-1.00937
C	2.49385	-1.15858	-1.84690
C	1.43561	-0.43856	-1.31204
F	-0.80492	-1.58331	2.01616
F	-2.92875	-3.14365	1.56822
F	-4.59463	-2.62252	-0.52554
F	-4.08845	-0.50970	-2.15727
F	-1.99083	1.06039	-1.72909
F	2.43338	-0.25249	2.14944
F	4.45327	-1.63948	1.15134
F	4.54634	-2.26500	-1.49699
F	2.53409	-1.45623	-3.14349
F	0.47014	-0.05536	-2.15617
N	0.06374	0.91950	2.06151
C	0.13176	1.07870	3.19224
C	0.26541	1.24888	4.62926
H	-1.97516	2.64327	0.80633
H	-2.07858	5.00140	0.09814
H	-0.20547	5.99613	-1.19570
H	1.76887	4.60412	-1.76230
H	1.87960	2.25426	-1.03614
H	-0.49873	0.65854	5.13706
H	0.15521	2.30294	4.88755
H	1.25634	0.89663	4.92320

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$B(C_6F_5)Ph_2$

B	0.897430	0.000030	0.000140
C	-0.686060	-0.000010	0.000070
C	-1.425950	-0.930390	-0.730670
C	-1.426060	0.930330	0.730750
C	-2.814250	-0.941240	-0.748550
C	-2.814360	0.941100	0.748520
C	-3.508980	-0.000090	-0.000040
C	1.645050	-1.351100	0.200340
C	2.926390	-1.569830	-0.336160
C	1.049780	-2.406070	0.914530
C	3.583630	-2.783760	-0.166280
H	3.402600	-0.781360	-0.912070
C	1.710520	-3.612160	1.110910
H	0.055000	-2.270000	1.331760
C	2.979110	-3.802790	0.565800
H	4.565510	-2.936430	-0.602630
H	1.237160	-4.407040	1.678150
H	3.493500	-4.748380	0.706940
C	1.644980	1.351190	-0.200220
C	1.049580	2.406090	-0.914390
C	2.926360	1.570000	0.336140
C	1.710240	3.612210	-1.110900
H	0.054750	2.269950	-1.331510
C	3.583520	2.783960	0.166140
H	3.402660	0.781580	0.912050
C	2.978870	3.802920	-0.565930
H	1.236780	4.407040	-1.678130
H	4.565440	2.936690	0.602380
H	3.493200	4.748530	-0.707170
F	-0.803360	-1.844470	-1.477880
F	-3.482240	-1.835910	-1.472270

F	-4.835920	-0.000130	-0.000100
F	-3.482460	1.835740	1.472180
F	-0.803580	1.844450	1.477990

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$[HB(C_6F_5)Ph_2]^-$

B	-0.86819	-0.10161	-0.95830
C	0.69143	0.08314	-0.45665
C	-1.78319	1.19317	-0.58803
C	-1.41769	-1.49689	-0.31169
C	1.79165	-0.07402	-1.29308
C	3.11098	0.03667	-0.86186
C	3.37351	0.31801	0.46860
C	2.31240	0.48226	1.34679
C	1.01330	0.35667	0.87109
C	-1.26456	2.45941	-0.27897
C	-2.07877	3.56533	-0.03765
C	-3.46391	3.44090	-0.09330
C	-4.01476	2.19696	-0.39638
C	-3.18564	1.10454	-0.63680
C	-1.17698	-2.71716	-0.96249
C	-1.58200	-3.94001	-0.43210
C	-2.25632	-3.98160	0.78657
C	-2.51184	-2.78844	1.45831
C	-2.09541	-1.57371	0.91543
F	1.63566	-0.35353	-2.59758
F	4.13388	-0.12438	-1.71577
F	4.63687	0.42998	0.90293
F	2.55939	0.75387	2.63696
F	0.03630	0.52240	1.77734
H	-0.85015	-0.22472	-2.16962
H	-0.18443	2.58774	-0.23009
H	-1.62941	4.52731	0.19924
H	-4.10460	4.29788	0.09818
H	-5.09526	2.07900	-0.44338
H	-3.63524	0.14002	-0.86646
H	-2.30499	-0.65163	1.45309
H	-0.65389	-2.69530	-1.91733
H	-1.37647	-4.86273	-0.97054
H	-2.57985	-4.93096	1.20591
H	-3.03683	-2.80511	2.41096

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$B(C_6F_5)Ph_2$-NCMe

B	0.80429	-0.09401	0.29710
C	-0.81254	0.08379	0.17181
C	1.64985	1.26541	0.05700
C	1.28016	-1.39243	-0.54480
C	-1.78281	-0.18893	1.12762
C	-3.14790	-0.05790	0.89439
C	-3.59007	0.36024	-0.34988
C	-2.65987	0.63887	-1.34281
C	-1.30836	0.49003	-1.06700
C	1.05501	2.52882	-0.02715
C	1.81628	3.68546	-0.18459
C	3.20342	3.60324	-0.25570
C	3.82158	2.35780	-0.16769
C	3.05006	1.20984	-0.01357
C	0.99147	-2.68752	-0.09375
C	1.34099	-3.81498	-0.83060
C	1.98493	-3.66823	-2.05708
C	2.26653	-2.39159	-2.53440
C	1.91718	-1.26973	-1.78509
F	-1.44599	-0.61361	2.36347
F	-4.02899	-0.33285	1.85754
F	-4.89180	0.49353	-0.59167
F	-3.07357	1.03899	-2.54404
F	-0.45470	0.76380	-2.06060
N	1.12697	-0.44478	1.82606
C	1.41595	-0.66406	2.91202
C	1.74281	-0.94071	4.30198
H	-0.02728	2.61574	0.03167
H	1.32485	4.65134	-0.25391
H	3.79922	4.50209	-0.38131
H	4.90343	2.28198	-0.22587
H	3.54385	0.24112	0.03989
H	0.46839	-2.81965	0.85336
H	1.10666	-4.80633	-0.45392
H	2.25915	-4.54310	-2.63844
H	2.75968	-2.26756	-3.49392
H	2.13995	-0.27834	-2.16994
H	0.81350	-1.03159	4.86748
H	2.34089	-0.12208	4.70505
H	2.30488	-1.87357	4.36552

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BPh_3

B	0.000460	-0.000110	-0.000260
C	-0.732810	-1.384860	0.000040
C	-0.171710	-2.509190	-0.631650
C	-1.978220	-1.552010	0.631740
C	-0.826110	-3.736650	-0.645500
H	0.789710	-2.411220	-1.128920
C	-2.626180	-2.782860	0.645940
H	-2.437140	-0.701410	1.128810
C	-2.052620	-3.876020	0.000290
H	-0.379560	-4.585670	-1.153520
H	-3.579460	-2.890130	1.153940
H	-2.560920	-4.835460	0.000390
C	1.566310	0.057680	0.000170
C	2.258850	1.105420	-0.632860
C	2.334340	-0.936170	0.632930

C	3.649030	1.152980	-0.647190
H	1.692790	1.888230	-1.130820
C	3.724240	-0.881280	0.646660
H	1.827620	-1.758530	1.131080
C	4.383550	0.161500	-0.000440
H	4.160560	1.963810	-1.156300
H	4.294290	-1.652310	1.155450
H	5.468590	0.201410	-0.000700
C	-0.832580	1.327120	-0.000280
C	-2.085940	1.403100	-0.633750
C	-0.356470	2.488860	0.633520
C	-2.822530	2.583050	-0.647600
H	-2.480480	0.521660	-1.132360
C	-1.099380	3.664850	0.647890
H	0.608890	2.461200	1.132040
C	-2.331840	3.714560	0.000290
H	-3.780300	2.620690	-1.157090
H	-0.717190	4.543730	1.157610
H	-2.909290	4.634040	0.000560

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$[HBPh_3]^-$

B	-0.00016	-0.00007	0.90791
C	-1.53050	-0.26993	0.40251
C	-1.86705	-1.12188	-0.66044
C	-2.60490	0.40574	1.00827
C	-3.18325	-1.29517	-1.09239
H	-1.07015	-1.66995	-1.16003
C	-3.92321	0.24646	0.59121
H	-2.38603	1.07929	1.83564
C	-4.22187	-0.61148	-0.46750
H	-3.39843	-1.96783	-1.92030
H	-4.72314	0.78861	1.09172
H	-5.24923	-0.74419	-0.79785
C	0.99861	-1.19065	0.40252
C	1.91313	-1.05340	-0.65278
C	0.94229	-2.46198	1.00130
C	2.72164	-2.10676	-1.08386
H	1.99589	-0.08699	-1.14693
C	1.73954	-3.52414	0.58501
H	0.24263	-2.61148	1.82242
C	2.64056	-3.35099	-0.46591
H	3.41845	-1.95458	-1.90576
H	1.66338	-4.49033	1.07997
H	3.26924	-4.17451	-0.79573
C	0.53155	1.46034	0.40295
C	-0.04790	2.18690	-0.64830
C	1.66413	2.04429	0.99825
C	0.46005	3.41405	-1.07870
H	-0.92873	1.77764	-1.13984
C	2.18552	3.26587	0.58242
H	2.14615	1.51052	1.81610
C	1.58164	3.96288	-0.46437
H	-0.02279	3.94394	-1.89742
H	3.06318	3.68050	1.07447
H	1.98060	4.91918	-0.79378
H	-0.00012	-0.00026	2.13669

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BPh_3-NCMe

B	0.00032	-0.00021	0.16893
C	1.46747	-0.56916	-0.21469
C	2.31194	0.09202	-1.11355
C	1.92598	-1.78540	0.31585
C	3.55702	-0.43012	-1.46446
C	3.16857	-2.31296	-0.01981
C	3.99181	-1.63162	-0.91498
C	-0.24055	1.55514	-0.21336
C	-1.23180	1.95562	-1.11629
C	0.58012	2.56077	0.32157
C	-1.40189	3.29504	-1.46698
C	0.41583	3.90077	-0.01377
C	-0.58218	4.27273	-0.91313
C	-1.22652	-0.98571	-0.21449
C	-1.07804	-2.04550	-1.11619
C	-2.50806	-0.77569	0.31887
C	-2.15360	-2.86165	-1.46710
C	-3.58701	-1.58700	-0.01672
C	-3.41045	-2.63851	-0.91473
N	0.00053	-0.00132	1.79881
C	0.00036	-0.00246	2.94543
C	0.00033	-0.00399	4.40178
H	1.98868	1.03454	-1.54735
H	1.28340	-2.34141	0.99806
H	4.18856	0.10496	-2.16768
H	3.49442	-3.25638	0.40896
H	4.96192	-2.03838	-1.18402
H	-1.88378	1.20411	-1.55352
H	1.38019	2.28264	1.00715
H	-2.17817	3.57417	-2.17350
H	1.06726	4.65499	0.41849
H	-0.71478	5.31634	-1.18191
H	-0.10098	-2.23591	-1.55222
H	-2.66687	0.05722	1.00336
H	-2.00745	-3.67448	-2.17253
H	-4.56613	-1.39836	0.41431
H	-4.24841	-3.27446	-1.18370
H	0.96300	-0.36882	4.76313
H	-0.79667	-0.65587	4.76272
H	-0.16543	1.01156	4.76454

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BEt_3

B	-0.007510	-0.004080	-0.694580
C	0.380220	1.527080	-0.642750
H	1.066860	1.752730	-1.471360
H	-0.485760	2.191890	-0.751930
C	-1.526710	-0.434400	-0.637150
H	-1.669460	-1.515780	-0.756720
H	-2.069630	0.055410	-1.458480
C	1.126010	-1.104050	-0.652590
H	0.956650	-1.834280	-1.456660
H	2.130780	-0.688400	-0.798960
C	1.106740	1.838920	0.681750
H	2.009020	1.227150	0.789600
H	1.408180	2.889520	0.738350
H	0.465670	1.633210	1.546670
C	1.069120	-1.852180	0.695420
H	0.091110	-2.322560	0.843930
H	1.828700	-2.638060	0.752440
H	1.237040	-1.170870	1.537410
C	-2.153880	0.025380	0.694950
H	-2.071190	1.110950	0.815980
H	-3.215130	-0.235880	0.752040
H	-1.654270	-0.439030	1.552800

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$[HBEt_3]^-$

B	-0.00021	0.00001	0.29919
H	-0.00070	0.00014	1.54564
C	-1.50720	0.42388	-0.22448
H	-1.79938	1.39912	0.19794
H	-1.50873	0.57147	-1.32075
C	0.38630	-1.51735	-0.22368
H	-0.31155	-2.25790	0.19996
H	0.25818	-1.59330	-1.31977
C	1.12098	1.09306	-0.22351
H	2.11095	0.85859	0.20058
H	1.25123	1.02002	-1.31955
C	1.81074	-1.95835	0.12674
H	2.03837	-3.00318	-0.13624
H	2.55259	-1.32969	-0.38023
H	1.98794	-1.84264	1.20387
C	0.79097	2.54723	0.12686
H	1.58213	3.26662	-0.13620
H	-0.12436	2.87550	-0.38006
H	0.60223	2.64291	1.20400
C	-2.60163	-0.58848	0.12721
H	-3.62016	-0.26347	-0.13664
H	-2.42817	-1.54617	-0.37810
H	-2.59041	-0.79803	1.20469

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BEt_3-NCMe

B	-0.32882	-0.13269	0.01506
N	1.28384	-0.27870	0.12227
C	-0.55404	0.79928	-1.30052
C	-0.71930	0.57545	1.42997
C	-0.85974	-1.66871	-0.16467
C	-2.22368	0.82771	1.56928
C	-2.22039	-1.77541	-0.86513
C	0.01746	2.21652	-1.21533
C	2.42552	-0.36306	0.20267
C	3.87552	-0.47105	0.30508
H	-0.15926	0.29456	-2.19509
H	-1.63765	0.86718	-1.46711
H	-0.18740	1.53091	1.54653
H	-0.38979	-0.05344	2.27010
H	-0.13933	-2.25878	-0.75055
H	-0.91820	-2.16386	0.81557
H	-2.47106	1.37074	2.48754
H	-2.60832	1.41412	0.72699
H	-2.77961	-0.11500	1.58910
H	-2.58475	-2.80764	-0.89950
H	-2.15732	-1.41553	-1.89685
H	-2.98547	-1.17358	-0.36486
H	-0.11881	2.78303	-2.14235
H	-0.46072	2.78472	-0.41084
H	1.09384	2.20570	-0.99923
H	4.34188	0.21849	-0.40017
H	4.18243	-1.49169	0.07185
H	4.18871	-0.21992	1.31953

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Q

C	-1.297754	0.603643	-0.131806
C	-1.047532	-0.494437	-0.850958
C	0.269687	-1.183746	-0.775123
C	1.297751	-0.603646	0.131810
C	1.047531	0.494434	0.850962
C	-0.269706	1.183713	0.775166
O	-0.497283	2.181859	1.429176
O	0.497289	-2.181849	-1.429190
H	-2.247465	1.128127	-0.165525
H	-1.776015	-0.940757	-1.520497
H	2.247473	-1.128112	0.165505
H	1.776024	0.940771	1.520478

12

$[Q]^{\bullet-}$

C	-1.253600	0.613810	-0.104004
C	-0.997726	-0.508975	-0.839392
C	0.274767	-1.205688	-0.789688
C	1.253600	-0.613809	0.104003

C	0.997726	0.508975	0.839392
C	-0.274767	1.205688	0.789688
O	-0.510408	2.239692	1.466927
O	0.510408	-2.239693	-1.466926
H	-2.216949	1.117540	-0.159625
H	-1.749685	-0.932831	-1.502553
H	2.216949	-1.117540	0.159624
H	1.749685	0.932832	1.502553

12
$[Q]^{2-}$

C	-1.220339	0.626678	-0.079072
C	-0.957779	-0.525246	-0.833654
C	0.282941	-1.241249	-0.813145
C	1.220342	-0.626673	0.079065
C	0.957783	0.525252	0.833647
C	-0.282936	1.241256	0.813135
O	-0.525767	2.307389	1.511101
O	0.525752	-2.307413	-1.511070
H	-2.201131	1.109496	-0.158439
H	-1.737161	-0.926103	-1.491866
H	2.201133	-1.109492	0.158435
H	1.737163	0.926105	1.491862

13
$[HQ]^{+}$

C	-1.310352	0.635392	-0.110930
C	-1.066759	-0.468331	-0.839422
C	0.259630	-1.157980	-0.762395
C	1.295760	-0.582523	0.146445
C	1.036886	0.521600	0.868235
C	-0.263406	1.141101	0.748893
O	-0.435428	2.192930	1.469058
O	0.476919	-2.149374	-1.415534
H	-2.263231	1.156527	-0.147220
H	-1.802416	-0.907581	-1.507080
H	2.248955	-1.101488	0.185141
H	1.750238	0.982776	1.542958
H	-1.313424	2.607313	1.385132

13
$[HQ]^{\cdot}$

C	-1.265625	0.642619	-0.085838
C	-1.020489	-0.482102	-0.828734
C	0.258181	-1.165764	-0.767412
C	1.256087	-0.593811	0.120022
C	0.999982	0.528768	0.856405
C	-0.261804	1.157563	0.761142
O	-0.450329	2.258153	1.511150
O	0.485718	-2.189858	-1.441961
H	-2.227688	1.147288	-0.139544
H	-1.771191	-0.902473	-1.488938
H	2.213842	-1.100307	0.170224
H	1.736925	0.964732	1.522186
H	-1.340237	2.605555	1.374578

13
$[HQ]^{-}$

C	-1.231894	0.649503	-0.066641
C	-0.989573	-0.491610	-0.821995
C	0.265266	-1.203040	-0.792039
C	1.230995	-0.604113	0.100893
C	0.976990	0.535272	0.850261
C	-0.257608	1.177946	0.776827
O	-0.471418	2.325826	1.549283
O	0.496446	-2.240532	-1.474178
H	-2.204299	1.146472	-0.131739
H	-1.764578	-0.887853	-1.474380
H	2.199946	-1.094313	0.169162
H	1.736692	0.950667	1.510885
H	-1.373593	2.606137	1.366941

26
$[SiPhH_2\text{-}Q]^{+}$

C	1.971548	-0.547860	1.578338
C	3.023320	-1.316192	1.903653
C	3.399140	-2.502239	1.073648
C	2.565964	-2.801825	-0.126899
C	1.517360	-2.026933	-0.442020
C	1.188445	-0.881617	0.395781
O	0.185981	-0.193637	0.039700
O	4.346731	-3.189380	1.372017
Si	-0.586539	1.276166	0.740738
C	-1.994777	1.677543	-0.346020
C	-3.264912	1.134095	-0.090770
C	-4.334933	1.435545	-0.924423
C	-4.147065	2.284226	-2.013986
C	-2.894075	2.836556	-2.274074
C	-1.821237	2.537844	-1.443059
H	1.686831	0.315685	2.170813
H	3.646760	-1.121636	2.771241
H	2.857167	-3.667107	-0.714256
H	0.880220	-2.200448	-1.302391
H	-0.932567	0.807102	2.094030
H	0.533847	2.232974	0.720458
H	-3.423047	0.480528	0.763378
H	-5.314530	1.016409	-0.722985
H	-4.984806	2.522526	-2.660971
H	-2.757194	3.503019	-3.118439
H	-0.850229	2.982194	-1.646579

26

[SiPhH$_2$-Q]$^{\cdot}$

C	1.748926	-0.792702	1.649590
C	2.896996	-1.471106	1.966538
C	3.623269	-2.241991	0.974769
C	3.067380	-2.256895	-0.367038
C	1.922161	-1.576098	-0.670794
C	1.249737	-0.834515	0.328624
O	0.128445	-0.190943	-0.042345
O	4.668410	-2.859025	1.261800
Si	-0.819057	0.854643	0.881995
C	-2.138365	1.447754	-0.279111
C	-3.368550	1.897355	0.217843
C	-4.352451	2.375184	-0.642310
C	-4.119309	2.401884	-2.015022
C	-2.904766	1.950210	-2.525397
C	-1.920383	1.477390	-1.662770
H	1.218778	-0.225326	2.409853
H	3.304541	-1.458137	2.971575
H	3.603541	-2.832453	-1.113880
H	1.496056	-1.579632	-1.668385
H	-1.406625	0.136129	2.036666
H	0.060065	1.932720	1.391834
H	-3.568846	1.868092	1.286818
H	-5.301358	2.719580	-0.244165
H	-4.886971	2.770424	-2.688013
H	-2.725933	1.964598	-3.595694
H	-0.978288	1.116401	-2.066057

26

[SiPhH$_2$-Q]$^{-}$

C	1.179812	-1.881441	1.262977
C	2.344833	-2.447369	1.751508
C	3.657249	-2.127602	1.230901
C	3.627778	-1.164676	0.150335
C	2.456852	-0.604653	-0.330826
C	1.223114	-0.955075	0.219848
O	0.022959	-0.402370	-0.299009
O	4.718669	-2.637844	1.672615
Si	-0.448511	0.989516	0.438284
C	-2.039273	1.491193	-0.434418
C	-2.746729	2.645891	-0.076193
C	-3.921887	3.005501	-0.729701
C	-4.412818	2.208213	-1.761805
C	-3.724433	1.056455	-2.132954
C	-2.548327	0.702545	-1.474123
H	0.209443	-2.155649	1.676095
H	2.303830	-3.168997	2.563813
H	4.585466	-0.887811	-0.283771
H	2.476083	0.110546	-1.152771
H	-0.732976	0.819171	1.886830
H	0.539144	2.091065	0.299172
H	-2.375815	3.279252	0.728422
H	-4.455617	3.905165	-0.436599
H	-5.329602	2.485260	-2.274433
H	-4.104418	0.432751	-2.937094
H	-2.007425	-0.195497	-1.760181

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[SiEt$_3$-Q]$^{+}$

C	1.736597	-0.726559	1.212037
C	2.900775	-1.216412	1.665089
C	3.692876	-2.195239	0.859246
C	3.144841	-2.606097	-0.465892
C	1.980243	-2.110406	-0.908815
C	1.236994	-1.159868	-0.089102
O	0.145284	-0.737929	-0.561837
O	4.740239	-2.633297	1.272497
Si	-1.138346	0.417531	0.021227
C	-1.942438	-0.467603	1.450876
C	-0.231926	1.997377	0.448223
C	-2.190279	0.518094	-1.505398
C	-2.870745	-0.812036	-1.863834
C	0.941633	2.332948	-0.485900
C	-3.192112	0.313060	1.903549
H	1.148855	-0.013355	1.780237
H	3.323731	-0.932894	2.624122
H	3.736945	-3.316713	-1.034129
H	1.540484	-2.378169	-1.863377
H	-2.221982	-1.481054	1.141543
H	-1.243186	-0.575271	2.288207
H	0.089390	1.996991	1.496409
H	-0.988063	2.790872	0.380868
H	-2.942418	1.300292	-1.342301
H	-1.569922	0.873036	-2.336985
H	-3.455422	-0.714879	-2.780302
H	-3.551443	-1.138223	-1.072288
H	-2.136688	-1.607144	-2.023742
H	1.349509	3.319192	-0.257984
H	0.633848	2.338591	-1.535209
H	1.762022	1.614492	-0.384657
H	-3.677339	-0.187312	2.743359
H	-2.940780	1.327554	2.227558
H	-3.928492	0.390014	1.098082

34

[SiEt$_3$-Q]$^{\cdot}$

C	1.738926	-0.728508	1.152121
C	2.887293	-1.262023	1.676022
C	3.657016	-2.264149	0.962418
C	3.144602	-2.664787	-0.336445
C	1.998732	-2.125217	-0.848336
C	1.274128	-1.153013	-0.115680

O	0.163469	-0.668021	-0.684230
O	4.701194	-2.751298	1.439311
Si	-1.041216	0.359544	-0.047312
C	-1.866394	-0.487140	1.409779
C	-0.277734	2.014779	0.419779
C	-2.222823	0.535141	-1.487205
C	-2.888611	-0.790790	-1.878197
C	0.873607	2.424013	-0.510397
C	-3.107666	0.288404	1.877205
H	1.182811	0.026193	1.700357
H	3.265622	-0.952640	2.644462
H	3.714193	-3.411829	-0.878891
H	1.606873	-2.417469	-1.816845
H	-2.144330	-1.505729	1.114381
H	-1.154251	-0.594961	2.235945
H	0.060970	2.003890	1.462745
H	-1.078068	2.765016	0.377345
H	-2.982423	1.285009	-1.232943
H	-1.665832	0.944963	-2.338361
H	-3.540468	-0.674365	-2.747925
H	-3.499794	-1.183348	-1.058978
H	-2.137619	-1.547665	-2.121602
H	1.258895	3.415399	-0.259003
H	0.550138	2.450104	-1.555485
H	1.704820	1.715800	-0.444103
H	-3.584826	-0.192987	2.734518
H	-2.852656	1.310568	2.176185
H	-3.855891	0.356699	1.080741

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[$SiEt_3$-Q]$^-$

C	1.047020	-2.413445	0.915105
C	2.118349	-2.799461	1.704217
C	3.435011	-2.209497	1.593274
C	3.518558	-1.187798	0.572370
C	2.438953	-0.810208	-0.210158
C	1.189531	-1.411329	-0.046466
O	0.092110	-1.024010	-0.848611
O	4.410352	-2.553054	2.310912
Si	-0.841322	0.213255	-0.250709
C	-1.516696	-0.194023	1.461502
C	0.129772	1.828488	-0.200730
C	-2.279406	0.368702	-1.464492
C	-3.207503	-0.851244	-1.432117
C	0.518871	2.328156	-1.597262
C	-2.557821	0.815807	1.959196
H	0.072971	-2.890059	1.027201
H	1.994975	-3.582261	2.449001
H	4.487064	-0.713088	0.433683
H	2.550237	-0.041081	-0.975211
H	-1.952879	-1.200258	1.423475
H	-0.674761	-0.265129	2.159068
H	1.030460	1.645308	0.397292
H	-0.450902	2.595252	0.329031
H	-2.843416	1.288093	-1.256553
H	-1.857364	0.488603	-2.469903
H	-4.007067	-0.788158	-2.178369
H	-3.681616	-0.960569	-0.450418
H	-2.640346	-1.767197	-1.622093
H	1.153952	3.219305	-1.555732
H	-0.367148	2.581475	-2.189879
H	1.067050	1.555184	-2.145118
H	-2.941593	0.557823	2.951770
H	-2.135356	1.824089	2.027269
H	-3.417354	0.871916	1.280830

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[$Si(C_6Me_5)_3$-Q]$^+$

C	1.28284	2.16784	1.75112
C	1.60007	3.32105	2.35835
C	0.88903	3.77461	3.58888
C	-0.16543	2.87969	4.14799
C	-0.46844	1.72253	3.54431
C	0.21506	1.33920	2.30994
O	-0.15686	0.25823	1.78539
O	1.16470	4.82650	4.11852
Si	-0.02098	-0.43180	0.07719
C	-1.64977	-1.37690	0.03424
C	-0.05323	1.21228	-0.86161
C	1.56430	-1.45113	0.01716
C	-2.60085	-1.22294	-1.00383
C	-3.87451	-1.80048	-0.87246
C	-4.19671	-2.56094	0.26282
C	0.97044	1.62115	-1.75330
C	0.75928	2.71183	-2.61562
C	-0.40637	3.48251	-2.50761
C	1.80522	-2.06066	-1.23680
C	3.05802	-2.61682	-1.53345
C	4.06505	-2.62803	-0.55751
C	-3.26031	-2.71719	1.29442
C	-1.97621	-2.16827	1.16019
C	3.84009	-2.02537	0.69034
C	2.58375	-1.47594	1.00030
C	-1.40515	3.12105	-1.59006
C	-1.23377	1.99822	-0.76369
C	-5.54035	-3.24706	0.35049
C	-3.63515	-3.47953	2.54610
C	-0.94932	-2.50407	2.22128
C	-4.91065	-1.61187	-1.95814
C	-2.30561	-0.51157	-2.31020
C	2.38274	-0.99647	2.42568
C	4.96882	-1.95864	1.69686

C	5.37908	-3.32250	-0.83357
C	3.33322	-3.16689	-2.91553
C	-2.67518	3.93966	-1.51299
C	-0.56897	4.72934	-3.34633
C	1.79360	3.06081	-3.66370
C	2.35883	1.00757	-1.77080
C	-2.35626	1.72518	0.22460
C	0.73048	-2.11264	-2.30126
H	1.79196	1.81861	0.86044
H	2.38707	3.97416	1.99490
H	-0.65948	3.22127	5.05204
H	-1.23114	1.04045	3.90489
H	-6.30450	-2.58564	0.77635
H	-5.49409	-4.14071	0.97244
H	-5.88970	-3.55812	-0.63469
H	-3.06006	-3.14458	3.40980
H	-3.46513	-4.55722	2.43511
H	-4.68891	-3.33833	2.79006
H	-1.03656	-1.86858	3.11107
H	0.06857	-2.42459	1.83817
H	-1.06730	-3.53827	2.55001
H	-5.91840	-1.58697	-1.54188
H	-4.87878	-2.42729	-2.69108
H	-4.76548	-0.67992	-2.50402
H	-1.26112	-0.24222	-2.43630
H	-2.58202	-1.15624	-3.15028
H	-2.88228	0.41492	-2.41286
H	1.34989	-1.08690	2.75161
H	2.70876	0.04197	2.57623
H	2.97156	-1.60590	3.11189
H	4.97706	-2.82894	2.36430
H	4.90089	-1.06653	2.32049
H	5.93666	-1.92130	1.19689
H	5.81110	-3.73115	0.08009
H	6.11643	-2.63958	-1.27218
H	5.24798	-4.15486	-1.52498
H	3.00864	-4.20950	-3.01429
H	4.39576	-3.12849	-3.15375
H	2.81520	-2.58866	-3.68267
H	-2.59225	4.74837	-0.77630
H	-3.53592	3.33334	-1.23156
H	-2.90935	4.39765	-2.47383
H	-1.11049	5.50390	-2.80211
H	-1.12596	4.52441	-4.26833
H	0.39496	5.15010	-3.63093
H	2.51235	3.80747	-3.30434
H	1.31888	3.46832	-4.55688
H	2.36014	2.18363	-3.97627
H	3.10170	1.79077	-1.93673
H	2.49343	0.26869	-2.56937
H	2.61768	0.50939	-0.83825
H	-2.15894	0.92987	0.93720
H	-3.27989	1.43830	-0.28947
H	-2.57922	2.63647	0.79031
H	-0.26845	-2.17181	-1.86804
H	0.76674	-1.24247	-2.97104
H	0.83695	-3.00164	-2.92350

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[Si(C_6Me_5)$_3$-Q]$^{\cdot}$

C	1.39520	2.14575	1.83472
C	1.74744	3.33812	2.40740
C	0.98847	3.91170	3.50456
C	-0.15828	3.14828	3.96462
C	-0.49829	1.95705	3.38600
C	0.26394	1.43998	2.31080
O	-0.11666	0.25707	1.81074
O	1.30692	4.99939	4.02523
Si	-0.01537	-0.34588	0.21120
C	-1.63755	-1.34820	0.10634
C	-0.05285	1.23943	-0.84433
C	1.54224	-1.43244	0.01942
C	-2.60378	-1.21920	-0.91948
C	-3.85948	-1.83945	-0.79043
C	-4.15354	-2.62163	0.33472
C	0.95494	1.62299	-1.75925
C	0.72919	2.67737	-2.66309
C	-0.44323	3.43872	-2.58172
C	1.73772	-2.04108	-1.24364
C	2.95389	-2.65597	-1.57178
C	3.97403	-2.73996	-0.61327
C	-3.20636	-2.75421	1.35805
C	-1.94102	-2.16103	1.22342
C	3.79864	-2.14536	0.64275
C	2.57998	-1.52389	0.97851
C	-1.42423	3.10930	-1.63540
C	-1.22948	2.02733	-0.76182
C	-5.47396	-3.35528	0.42169
C	-3.55113	-3.52728	2.61299
C	-0.90882	-2.46527	2.29029
C	-4.90557	-1.66205	-1.86984
C	-2.35002	-0.48194	-2.22084
C	2.45419	-1.02309	2.40494
C	4.93808	-2.15712	1.63972
C	5.24473	-3.50262	-0.91952
C	3.18216	-3.18522	-2.97194
C	-2.70139	3.91731	-1.56394
C	-0.62740	4.64933	-3.47038
C	1.76152	2.99657	-3.72366
C	2.34799	1.02120	-1.75966
C	-2.32255	1.78933	0.26526
C	0.64436	-2.02440	-2.28880

H	1.97313	1.72573	1.01672
H	2.60983	3.89924	2.06374
H	-0.72955	3.56785	4.78584
H	-1.35422	1.37821	3.71877
H	-6.26062	-2.73116	0.86346
H	-5.39016	-4.25702	1.02889
H	-5.81919	-3.66534	-0.56581
H	-3.01304	-3.13915	3.47864
H	-3.30375	-4.59259	2.52384
H	-4.61575	-3.45549	2.84047
H	-1.00206	-1.80425	3.15894
H	0.10702	-2.37029	1.90722
H	-1.01196	-3.49558	2.63727
H	-5.91449	-1.71670	-1.45893
H	-4.82425	-2.43314	-2.64660
H	-4.81366	-0.69547	-2.36596
H	-1.31868	-0.17133	-2.34899
H	-2.61249	-1.12545	-3.06743
H	-2.96121	0.42453	-2.30398
H	1.42288	-0.90992	2.72007
H	2.95319	-0.05689	2.54791
H	2.92789	-1.73001	3.09007
H	4.88681	-3.02162	2.31364
H	4.93311	-1.26126	2.26155
H	5.90448	-2.19051	1.13569
H	5.66133	-3.95353	-0.01809
H	6.01830	-2.85670	-1.35273
H	5.05958	-4.31337	-1.62499
H	2.77459	-4.19460	-3.10682
H	4.24395	-3.22307	-3.21547
H	2.70952	-2.54147	-3.71663
H	-2.62951	4.72201	-0.82157
H	-3.55379	3.29737	-1.28279
H	-2.94049	4.37518	-2.52407
H	-1.15171	5.44743	-2.94253
H	-1.20977	4.41176	-4.36910
H	0.32929	5.05748	-3.79606
H	2.47412	3.76181	-3.39086
H	1.28669	3.36529	-4.63424
H	2.33779	2.11273	-3.99906
H	3.08602	1.81162	-1.91818
H	2.49923	0.27751	-2.55172
H	2.59502	0.53325	-0.81986
H	-2.07353	1.04712	1.01749
H	-3.25509	1.45826	-0.20656
H	-2.53879	2.72512	0.79094
H	-0.34061	-2.09515	-1.82950
H	0.67199	-1.11215	-2.90039
H	0.72698	-2.87408	-2.96719

$[Si(C_6Me_5)_3\text{-}Q]^-$

C	1.71942	1.96575	1.88845
C	2.23217	3.14641	2.40062
C	1.54933	3.93427	3.40375
C	0.28359	3.36463	3.81324
C	-0.21815	2.18341	3.29303
C	0.48896	1.47151	2.32432
O	-0.05329	0.26095	1.85539
O	2.01064	5.00613	3.87399
Si	-0.04091	-0.28723	0.29236
C	-1.75557	-1.16689	0.17134
C	0.05677	1.25475	-0.83208
C	1.37416	-1.56523	0.00435
C	-2.73323	-0.95019	-0.82794
C	-4.03359	-1.46961	-0.68260
C	-4.36889	-2.24153	0.43613
C	1.06557	1.50923	-1.78635
C	0.91198	2.54523	-2.72657
C	-0.17928	3.41759	-2.64341
C	1.46705	-2.19004	-1.26246
C	2.58301	-2.96040	-1.61794
C	3.59803	-3.19198	-0.67871
C	-3.41418	-2.46034	1.43709
C	-2.10794	-1.96749	1.28438
C	3.52418	-2.58913	0.58171
C	2.41039	-1.80167	0.94063
C	-1.14677	3.22542	-1.64734
C	-1.02707	2.16174	-0.73955
C	-5.74180	-2.87157	0.54268
C	-3.79675	-3.20873	2.69705
C	-1.08948	-2.35576	2.33757
C	-5.08126	-1.18192	-1.73755
C	-2.45326	-0.21458	-2.12527
C	2.39120	-1.27880	2.36365
C	4.66233	-2.76545	1.56478
C	4.74878	-4.11855	-1.01203
C	2.71762	-3.49583	-3.02906
C	-2.32667	4.16674	-1.54506
C	-0.28184	4.60815	-3.57314
C	1.94341	2.72595	-3.82107
C	2.39918	0.78636	-1.78561
C	-2.08493	2.06540	0.34253
C	0.36619	-2.02082	-2.28585
H	2.27903	1.41132	1.13237
H	3.18982	3.52247	2.04957
H	-0.27670	3.91036	4.56867
H	-1.17515	1.78532	3.62948
H	-6.46854	-2.20191	1.02023
H	-5.71207	-3.79219	1.12738
H	-6.13562	-3.13154	-0.44165
H	-3.23476	-2.84073	3.55656

H	-3.60371	-4.28666	2.61779
H	-4.85554	-3.08033	2.92864
H	-1.09546	-1.66333	3.18533
H	-0.07763	-2.36119	1.93405
H	-1.28601	-3.36509	2.70744
H	-6.08798	-1.19833	-1.31721
H	-5.05327	-1.91308	-2.55648
H	-4.93678	-0.19705	-2.18405
H	-1.40183	0.00168	-2.27839
H	-2.80133	-0.81339	-2.97485
H	-2.97755	0.74764	-2.17059
H	1.41134	-0.92961	2.66911
H	3.07804	-0.43496	2.49456
H	2.70757	-2.06873	3.05200
H	4.48899	-3.60603	2.24945
H	4.79317	-1.87394	2.17884
H	5.60863	-2.94659	1.05275
H	5.10901	-4.63547	-0.12117
H	5.60161	-3.58181	-1.44687
H	4.44613	-4.88687	-1.72534
H	2.16654	-4.43321	-3.17840
H	3.76072	-3.68225	-3.28730
H	2.33570	-2.77662	-3.75714
H	-2.14403	4.95708	-0.80638
H	-3.22955	3.63986	-1.23037
H	-2.54737	4.64684	-2.49961
H	-0.65858	5.48458	-3.04207
H	-0.96063	4.41868	-4.41469
H	0.68875	4.88162	-3.98720
H	2.72558	3.44219	-3.53807
H	1.48255	3.08968	-4.74184
H	2.43814	1.78380	-4.06096
H	3.20138	1.50723	-1.96544
H	2.47903	0.01085	-2.55846
H	2.60582	0.31059	-0.83094
H	-1.85657	1.32796	1.10591
H	-3.07062	1.82146	-0.07465
H	-2.16589	3.02846	0.85597
H	-0.60860	-1.99158	-1.80219
H	0.48366	-1.09603	-2.86701
H	0.33841	-2.85268	-2.99118

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$B(C_6F_5)_3$-Q

C	1.554664	-1.299016	1.616872
C	2.361157	-2.008203	2.416387
C	3.473043	-2.840698	1.873983
C	3.674084	-2.843020	0.397915
C	2.866390	-2.139373	-0.402121
C	1.760380	-1.355945	0.163065
O	1.029303	-0.772447	-0.659151
B	-0.267148	0.119197	-0.378508
C	0.133489	1.401251	0.537950
C	-1.321834	-0.943529	0.256585
C	-0.642866	0.689580	-1.847066
C	-0.907764	2.239692	0.930932
C	-0.719688	3.432856	1.608712
C	0.574877	3.842151	1.907893
C	1.645614	3.049859	1.526491
C	1.407025	1.860223	0.845974
C	-1.797278	-0.944237	1.563106
C	-2.694838	-1.885965	2.053550
C	-3.150622	-2.890733	1.214506
C	-2.693224	-2.945791	-0.095843
C	-1.795567	-1.986369	-0.538706
C	0.358416	1.291344	-2.605210
C	0.140705	1.859936	-3.851422
C	-1.144174	1.855697	-4.376989
C	-2.178880	1.287508	-3.648915
C	-1.915513	0.723891	-2.405459
F	-2.166105	1.880386	0.646556
F	-1.753598	4.188054	1.968237
F	0.782149	4.982220	2.557031
F	2.890833	3.428931	1.807197
F	2.501644	1.147984	0.509248
F	-1.358629	-0.037502	2.454186
F	1.610736	1.348109	-2.121195
F	1.140510	2.412389	-4.536615
F	-1.381095	2.396014	-5.567721
F	-3.414281	1.286740	-4.144814
F	-2.963747	0.202785	-1.758482
F	-1.379670	-2.089004	-1.806976
F	-3.113168	-3.914401	-0.905367
F	-4.003206	-3.803482	1.664064
F	-3.103642	-1.837246	3.319327
O	4.188164	-3.486201	2.608405
H	0.755280	-0.677720	2.005044
H	2.253866	-2.006793	3.496297
H	4.498952	-3.440856	0.024680
H	2.966658	-2.107128	-1.481436

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$[B(C_6F_5)_3$-Q$]^{\bullet-}$

C	1.598324	-1.339278	1.590827
C	2.366843	-2.112897	2.417697
C	3.387672	-3.013394	1.914769
C	3.551537	-3.036839	0.471771
C	2.783246	-2.263355	-0.347844
C	1.780895	-1.400368	0.180750
O	1.089670	-0.699773	-0.692409
B	-0.133888	0.101265	-0.393029
C	0.161881	1.437293	0.519506

C	-1.240602	-0.935091	0.250719
C	-0.598423	0.719565	-1.846766
C	-0.911429	2.245960	0.883272
C	-0.780388	3.454234	1.547911
C	0.492083	3.914261	1.860405
C	1.594633	3.157521	1.502530
C	1.415193	1.947311	0.835318
C	-1.734161	-0.932713	1.548381
C	-2.618148	-1.887720	2.040613
C	-3.043167	-2.911664	1.212102
C	-2.573276	-2.966907	-0.092260
C	-1.690386	-1.993693	-0.535514
C	0.360865	1.370327	-2.620878
C	0.088862	1.960331	-3.848324
C	-1.206516	1.931423	-4.342193
C	-2.200784	1.319199	-3.597435
C	-1.884434	0.737774	-2.373602
F	-2.158947	1.850424	0.581530
F	-1.850610	4.183533	1.880961
F	0.648311	5.078025	2.497607
F	2.822122	3.600545	1.792698
F	2.535858	1.290161	0.514771
F	-1.345245	-0.000667	2.437095
F	1.620974	1.480283	-2.179749
F	1.052382	2.567190	-4.549959
F	-1.493429	2.495426	-5.518884
F	-3.455122	1.296130	-4.061174
F	-2.913526	0.182119	-1.718351
F	-1.286378	-2.095173	-1.809199
F	-2.979059	-3.950767	-0.901154
F	-3.891452	-3.838754	1.662927
F	-3.051728	-1.831118	3.304004
O	4.083653	-3.720809	2.674729
H	0.854442	-0.666293	2.003199
H	2.241625	-2.075037	3.495314
H	4.313917	-3.700974	0.076575
H	2.897513	-2.275880	-1.427055

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$[B(C_6F_5)_3\text{-}Q]^{2-}$

C	1.741194	-1.316222	1.581409
C	2.408795	-2.216929	2.405742
C	3.217690	-3.302744	1.912726
C	3.247691	-3.363846	0.472354
C	2.570422	-2.466557	-0.342503
C	1.807706	-1.423374	0.188477
O	1.196520	-0.550058	-0.696421
B	-0.021514	0.144512	-0.395408
C	0.157553	1.529597	0.521716
C	-1.124422	-0.908779	0.260595
C	-0.550176	0.780948	-1.848352
C	-0.954931	2.295380	0.852672
C	-0.895564	3.518841	1.501586
C	0.346737	4.039582	1.833481
C	1.488340	3.326534	1.510659
C	1.381527	2.097614	0.858907
C	-1.611706	-0.917994	1.559416
C	-2.456332	-1.903511	2.061840
C	-2.839637	-2.952212	1.245964
C	-2.373294	-2.997020	-0.059025
C	-1.532023	-1.992259	-0.512791
C	0.368157	1.501076	-2.612845
C	0.064284	2.083424	-3.837964
C	-1.221532	1.976053	-4.343902
C	-2.177060	1.295744	-3.610049
C	-1.829930	0.727062	-2.387441
F	-2.184013	1.846414	0.533754
F	-2.007872	4.210780	1.802891
F	0.438449	5.225893	2.456583
F	2.688726	3.839416	1.822719
F	2.535002	1.496224	0.573856
F	-1.285774	0.048788	2.436295
F	1.614184	1.704692	-2.171109
F	0.989597	2.765193	-4.532272
F	-1.538018	2.534283	-5.523279
F	-3.429615	1.198893	-4.085936
F	-2.836568	0.109913	-1.748153
F	-1.145953	-2.084505	-1.794102
F	-2.754544	-4.002612	-0.862547
F	-3.661202	-3.908136	1.706010
F	-2.904023	-1.849886	3.326255
O	3.835479	-4.119253	2.662765
H	1.149718	-0.517793	2.029871
H	2.335060	-2.114106	3.487272
H	3.835854	-4.166198	0.028250
H	2.618421	-2.551726	-1.427766

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$B(C_6F_5)_2Ph\text{-}Q$

C	1.487592	-1.463674	1.538039
C	2.240747	-2.284282	2.279778
C	3.358734	-3.072237	1.689225
C	3.629011	-2.899034	0.234112
C	2.874540	-2.082862	-0.508520
C	1.753882	-1.349262	0.097141
O	1.076102	-0.650435	-0.676241
B	-0.265473	0.196426	-0.370622
C	0.119938	1.475732	0.560162
C	-1.278954	-0.875284	0.280729
C	-0.651618	0.730439	-1.851192
C	-0.907425	2.381238	0.825481
C	-0.734545	3.554163	1.545659

C	0.530331	3.874788	2.022065
C	1.589055	3.017009	1.769388
C	1.366981	1.851745	1.043518
C	-1.948291	-0.677889	1.493126
C	-2.777605	-1.658368	2.035871
C	-2.956411	-2.867293	1.371795
C	-2.304091	-3.086961	0.160117
C	-1.480412	-2.101031	-0.372047
C	0.323267	1.339689	-2.638146
C	0.076618	1.856672	-3.901070
C	-1.212523	1.791239	-4.413399
C	-2.222714	1.218890	-3.655559
C	-1.932397	0.707331	-2.393957
F	-2.139285	2.123536	0.366433
F	-1.757271	4.373249	1.775630
F	0.722350	4.992244	2.714822
F	2.808343	3.313115	2.216003
F	2.455182	1.081618	0.836103
F	1.576325	1.457559	-2.167785
F	1.050685	2.419016	-4.616528
F	-1.476450	2.281652	-5.620911
F	-3.462795	1.167083	-4.139409
F	-2.958881	0.193061	-1.714113
O	4.028380	-3.820680	2.367583
H	0.670486	-0.884415	1.950246
H	2.082890	-2.411856	3.345655
H	4.460192	-3.466159	-0.171729
H	3.029045	-1.919776	-1.569556
H	-1.820851	0.256874	2.033629
H	-3.285583	-1.475097	2.977789
H	-3.602242	-3.632016	1.791453
H	-2.444167	-4.023505	-0.371098
H	-0.989288	-2.281114	-1.327473

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$[B(C_6F_5)_2Ph\text{-}Q]^{\bullet-}$

C	1.601705	-1.310129	1.623922
C	2.390833	-2.039615	2.471815
C	3.484270	-2.868644	2.000381
C	3.696126	-2.872217	0.563322
C	2.908159	-2.143147	-0.277418
C	1.835945	-1.346000	0.220267
O	1.136265	-0.681898	-0.670118
B	-0.120438	0.096924	-0.414190
C	0.153494	1.420041	0.536783
C	-1.246779	-0.956125	0.182223
C	-0.576546	0.700486	-1.852827
C	-0.912039	2.187730	1.000676
C	-0.768979	3.380267	1.692607
C	0.505420	3.874555	1.931949
C	1.600483	3.163312	1.473502
C	1.407690	1.968540	0.784299
C	-1.775451	-0.998532	1.467611
C	-2.716470	-1.931306	1.889624
C	-3.164975	-2.893711	1.000641
C	-2.655594	-2.912545	-0.288521
C	-1.714482	-1.961871	-0.664454
C	0.395406	1.012329	-2.812239
C	0.058753	1.589291	-4.034257
C	-1.272071	1.875280	-4.329292
C	-2.255620	1.578203	-3.389536
C	-1.906957	1.001349	-2.170305
F	-2.173758	1.776950	0.785959
F	-1.836555	4.062945	2.122093
F	0.671000	5.024950	2.592432
F	2.833402	3.636128	1.687986
F	2.528699	1.367456	0.356581
F	-1.367814	-0.133192	2.414006
F	-1.255156	-2.059715	-1.916842
F	-3.072916	-3.846263	-1.150528
F	-4.069243	-3.799346	1.383477
F	-3.185202	-1.914764	3.142207
O	4.199393	-3.535087	2.779937
H	0.800771	-0.692219	2.013468
H	2.225919	-2.019541	3.544683
H	4.511707	-3.484310	0.190616
H	3.058000	-2.142709	-1.352582
H	1.435628	0.787584	-2.590059
H	0.836042	1.815419	-4.759898
H	-1.540051	2.323657	-5.282038
H	-3.298332	1.793980	-3.608051
H	-2.688280	0.776645	-1.447715

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$[B(C_6F_5)_2\text{-}Q]^{2-}$

C	1.716219	-1.276767	1.626365
C	2.464390	-2.081765	2.482801
C	3.448605	-3.031509	2.033861
C	3.570892	-3.064096	0.597530
C	2.817941	-2.262703	-0.249732
C	1.875985	-1.352051	0.239166
O	1.197113	-0.577871	-0.681797
B	-0.039687	0.113695	-0.426644
C	0.130480	1.475683	0.545321
C	-1.185743	-0.946874	0.170358
C	-0.544868	0.737507	-1.859186
C	-0.959763	2.191736	1.029697
C	-0.869005	3.392326	1.719077
C	0.380219	3.950526	1.938094
C	1.500977	3.291860	1.463376
C	1.361609	2.085795	0.778083
C	-1.687681	-1.027311	1.464457

C	-2.612342	-1.979268	1.882007
C	-3.068456	-2.926366	0.982137
C	-2.586989	-2.906680	-0.316358
C	-1.662505	-1.937203	-0.687468
C	0.397483	0.952200	-2.874806
C	0.045664	1.524838	-4.095243
C	-1.274032	1.900435	-4.341009
C	-2.230655	1.692619	-3.350173
C	-1.864934	1.122819	-2.131506
F	-2.213885	1.729244	0.844963
F	-1.967149	4.027058	2.166401
F	0.498770	5.117703	2.593585
F	2.712168	3.837572	1.659723
F	2.503163	1.552964	0.336672
F	-1.301880	-0.163895	2.420088
F	-1.246764	-1.998165	-1.959496
F	-3.025941	-3.822359	-1.196464
F	-3.967781	-3.848909	1.360593
F	-3.071223	-1.993251	3.143960
O	4.135073	-3.763170	2.813257
H	0.994642	-0.578910	2.047112
H	2.314809	-2.004679	3.558850
H	4.296615	-3.763642	0.183413
H	2.942687	-2.322603	-1.330922
H	1.421177	0.641862	-2.683511
H	0.802848	1.675514	-4.862545
H	-1.553909	2.345407	-5.293439
H	-3.266989	1.973374	-3.528732
H	-2.625947	0.968445	-1.369719

46

$B(C_6F_5)Ph_2$-Q

C	1.492063	-1.457488	1.535256
C	2.220801	-2.299868	2.276775
C	3.336477	-3.095538	1.693018
C	3.635303	-2.902311	0.246175
C	2.909288	-2.059788	-0.495160
C	1.786532	-1.318460	0.100977
O	1.137043	-0.590570	-0.666597
B	-0.247128	0.243074	-0.389026
C	0.133185	1.512342	0.565668
C	-1.258690	-0.835439	0.259269
C	-0.627335	0.742824	-1.868878
C	-0.899658	2.407578	0.849908
C	-0.734323	3.568077	1.591684
C	0.526310	3.888747	2.078897
C	1.588394	3.039158	1.817100
C	1.372970	1.884779	1.071080
C	-1.912323	-0.665674	1.486067
C	-2.759494	-1.643270	2.005652
C	-2.973661	-2.825317	1.303662
C	-2.341088	-3.018227	0.077270
C	-1.501680	-2.032601	-0.433300
C	0.349355	1.319927	-2.692642
C	0.045937	1.789080	-3.966298
C	-1.260403	1.701210	-4.444104
C	-2.249599	1.143848	-3.640003
C	-1.931948	0.669719	-2.368253
F	-2.133872	2.149876	0.400839
F	-1.763731	4.375591	1.836574
F	0.709778	4.995887	2.792103
F	2.805322	3.329877	2.276682
F	2.470799	1.123195	0.863459
O	3.982920	-3.865610	2.370255
H	0.679228	-0.869375	1.943007
H	2.044791	-2.439683	3.338270
H	4.462221	-3.478963	-0.154971
H	3.083062	-1.886457	-1.551668
H	-1.755648	0.247144	2.056677
H	-3.253760	-1.479786	2.958586
H	-3.632768	-3.588592	1.705285
H	-2.509134	-3.932964	-0.483304
H	-1.031152	-2.185658	-1.403260
H	1.372064	1.401959	-2.326854
H	0.823090	2.227440	-4.585473
H	-1.504447	2.068483	-5.436242
H	-3.270748	1.076662	-4.003238
H	-2.712940	0.236298	-1.748721

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$[B(C_6F_5)Ph_2$-Q$]^{\bullet-}$

C	1.588083	-1.399668	1.563261
C	2.360218	-2.192697	2.366100
C	3.437759	-3.014611	1.846494
C	3.650195	-2.935947	0.411991
C	2.877953	-2.141746	-0.384014
C	1.819746	-1.353875	0.158100
O	1.140761	-0.616816	-0.685303
B	-0.141370	0.141623	-0.400969
C	0.144215	1.465925	0.557336
C	-1.237372	-0.895702	0.218203
C	-0.592995	0.719008	-1.857328
C	-0.919619	2.287936	0.928308
C	-0.782495	3.461019	1.658193
C	0.484226	3.880376	2.035015
C	1.580015	3.116275	1.671998
C	1.393866	1.944274	0.943168
C	-1.862898	-0.789048	1.465663
C	-2.771723	-1.742608	1.922867
C	-3.082684	-2.844694	1.132990
C	-2.472999	-2.981971	-0.112548
C	-1.569019	-2.020506	-0.553899

C	0.381949	1.134486	-2.775788
C	0.043664	1.666280	-4.017306
C	-1.296124	1.801722	-4.376141
C	-2.283779	1.398739	-3.481630
C	-1.931600	0.865888	-2.242300
F	-2.174636	1.964774	0.575878
F	-1.850589	4.195854	1.991665
F	0.644284	5.009134	2.734325
F	2.808692	3.517988	2.018197
F	2.522201	1.293771	0.620578
O	4.139430	-3.740441	2.584906
H	0.790952	-0.795087	1.980046
H	2.194157	-2.234054	3.438294
H	4.454092	-3.540632	0.003038
H	3.031660	-2.079047	-1.457019
H	-1.629196	0.057134	2.109387
H	-3.235342	-1.624862	2.898896
H	-3.789792	-3.591052	1.484410
H	-2.703531	-3.840100	-0.738618
H	-1.100725	-2.135465	-1.529692
H	1.429676	1.024940	-2.504472
H	0.824395	1.975234	-4.708157
H	-1.566669	2.215147	-5.344146
H	-3.332492	1.496154	-3.751351
H	-2.713137	0.548085	-1.556427

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$[B(C_6F_5)Ph_2]^{2-}$

C	1.678568	-1.321867	1.628160
C	2.441449	-2.138803	2.460578
C	3.504668	-2.990470	1.996007
C	3.690071	-2.912776	0.568721
C	2.922270	-2.101550	-0.256489
C	1.901521	-1.286395	0.246089
O	1.218818	-0.492146	-0.653028
B	-0.050219	0.173107	-0.391216
C	0.113215	1.509927	0.555110
C	-1.186472	-0.920413	0.185794
C	-0.592386	0.732739	-1.840945
C	-0.955223	2.341553	0.923416
C	-0.767852	3.533491	1.617337
C	0.518918	3.940361	1.968527
C	1.599979	3.137687	1.614079
C	1.394862	1.947137	0.916235
C	-1.763628	-0.959254	1.450188
C	-2.701285	-1.909390	1.848581
C	-3.091232	-2.896146	0.961350
C	-2.532194	-2.919499	-0.306542
C	-1.601365	-1.950078	-0.659705
C	0.319239	0.953110	-2.883621
C	-0.074570	1.485758	-4.109061
C	-1.409819	1.816445	-4.337164
C	-2.339373	1.599999	-3.322833
C	-1.928766	1.067707	-2.101338
F	-1.438408	-0.062775	2.396194
F	-1.113948	-2.049135	-1.903025
F	-2.907088	-3.876358	-1.173111
F	-3.999880	-3.818059	1.321740
F	-3.235374	-1.882423	3.081869
O	4.205909	-3.729913	2.756346
H	0.903524	-0.691830	2.060926
H	2.242898	-2.145859	3.531585
H	4.477484	-3.533944	0.141919
H	3.096180	-2.078092	-1.332513
H	-1.970307	2.044065	0.660418
H	-1.625121	4.148179	1.886741
H	0.674255	4.869294	2.513367
H	2.610037	3.437627	1.886153
H	2.241897	1.320330	0.648747
H	1.355769	0.677909	-2.708452
H	0.661953	1.640608	-4.895850
H	-1.722242	2.229955	-5.293766
H	-3.388329	1.841158	-3.486579
H	-2.677000	0.890170	-1.328744

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BPh_3-Q

C	1.441493	-1.511654	1.496920
C	2.181198	-2.355153	2.228159
C	3.356643	-3.069295	1.659670
C	3.706342	-2.792256	0.238239
C	2.975931	-1.944768	-0.493134
C	1.794016	-1.280944	0.085277
O	1.153666	-0.536058	-0.673455
B	-0.253999	0.284374	-0.399191
C	0.147960	1.536646	0.539446
C	-1.259749	-0.797419	0.262246
C	-0.661859	0.745386	-1.887657
C	-0.843291	2.510915	0.752725
C	-0.623321	3.617823	1.563504
C	0.615456	3.799031	2.178253
C	1.621948	2.865725	1.965497
C	1.384680	1.753159	1.155898
C	-1.978632	-0.562154	1.441455
C	-2.829925	-1.525296	1.983618
C	-2.979465	-2.758541	1.357186
C	-2.280982	-3.017126	0.179159
C	-1.441514	-2.045353	-0.357174
C	0.258130	1.440237	-2.687554
C	-0.069136	1.882429	-3.964065
C	-1.347879	1.653390	-4.471916
C	-2.283259	0.980791	-3.693829

C	-1.937854	0.529449	-2.419328
H	-1.807328	2.393325	0.261210
H	-1.414683	4.346755	1.710762
H	0.794386	4.665315	2.807258
H	2.597227	3.002560	2.423371
H	2.209924	1.060005	1.000262
H	-1.864461	0.391379	1.951845
H	1.252415	1.642958	-2.292517
H	0.665695	2.413442	-4.562337
H	-1.611168	2.001926	-5.466027
H	-3.283003	0.802370	-4.079033
H	-2.677818	-0.003202	-1.826884
H	-0.920769	-2.252171	-1.291287
H	-2.398339	-3.972664	-0.323673
H	-3.638566	-3.511167	1.778690
H	-3.374665	-1.311848	2.898664
O	4.011669	-3.841081	2.327840
H	0.587636	-0.979100	1.896826
H	1.965194	-2.555931	3.272384
H	4.574126	-3.312592	-0.153619
H	3.187333	-1.712480	-1.531490

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$[BPh_3\text{-}Q]^-$

C	1.559950	-1.466958	1.532462
C	2.341811	-2.272009	2.313625
C	3.488874	-2.993969	1.793543
C	3.759348	-2.802490	0.379373
C	2.978882	-1.997002	-0.396995
C	1.853156	-1.304176	0.144757
O	1.176359	-0.544943	-0.677227
B	-0.135353	0.193365	-0.386115
C	0.149915	1.495727	0.553714
C	-1.223388	-0.863115	0.226458
C	-0.627219	0.717658	-1.852173
C	-0.884981	2.404076	0.834937
C	-0.684503	3.544530	1.606508
C	0.581187	3.826615	2.118517
C	1.631392	2.958359	1.839249
C	1.413185	1.816081	1.068207
C	-2.010537	-0.647020	1.364379
C	-2.939576	-1.588945	1.810751
C	-3.102989	-2.788628	1.126798
C	-2.329186	-3.034771	-0.006976
C	-1.413352	-2.083485	-0.443609
C	0.307615	1.124221	-2.815814
C	-0.080562	1.628291	-4.054030
C	-1.433698	1.748946	-4.367093
C	-2.383850	1.354462	-3.429827
C	-1.979711	0.843204	-2.196556
H	-1.874772	2.212652	0.422371
H	-1.513496	4.219994	1.803465
H	0.746149	4.716101	2.720550
H	2.626901	3.169588	2.221887
H	2.254295	1.159647	0.859147
H	-1.886753	0.276244	1.926220
H	1.365405	1.033013	-2.580351
H	0.672006	1.930139	-4.778870
H	-1.742407	2.142719	-5.331961
H	-3.442923	1.436308	-3.662911
H	-2.735803	0.517562	-1.483855
H	-0.818222	-2.283267	-1.333039
H	-2.442959	-3.970331	-0.548945
H	-3.821542	-3.526637	1.473098
H	-3.531631	-1.385966	2.699937
O	4.200307	-3.728512	2.514019
H	0.713461	-0.933998	1.949384
H	2.129958	-2.398859	3.371039
H	4.614125	-3.332035	-0.030960
H	3.176536	-1.851249	-1.454891

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$[BPh_3\text{-}Q]^{2-}$

C	1.683918	-1.509599	1.511092
C	2.487170	-2.366786	2.260780
C	3.600147	-3.102893	1.721645
C	3.789975	-2.859992	0.314512
C	2.984372	-2.004543	-0.427571
C	1.915311	-1.303158	0.144453
O	1.199606	-0.457529	-0.673039
B	-0.082623	0.197245	-0.358145
C	0.126340	1.533392	0.590687
C	-1.194181	-0.856315	0.245079
C	-0.652422	0.735514	-1.814322
C	-0.871598	2.502927	0.789933
C	-0.667598	3.644352	1.564471
C	0.569233	3.866146	2.165810
C	1.588019	2.935732	1.969475
C	1.367180	1.797890	1.194113
C	-2.216954	-0.540100	1.149079
C	-3.183612	-1.471899	1.537165
C	-3.145178	-2.768382	1.035836
C	-2.125637	-3.119509	0.149412
C	-1.175978	-2.178576	-0.233533
C	0.245335	0.996524	-2.862158
C	-0.175259	1.495121	-4.093023
C	-1.526816	1.751954	-4.323863
C	-2.443351	1.491764	-3.308163
C	-2.006316	0.988256	-2.082299
H	-1.837046	2.371023	0.302280
H	-1.472112	4.367420	1.691094
H	0.738387	4.754110	2.771814

H	2.563379	3.096846	2.424730
H	2.171541	1.081332	1.050457
H	-2.253819	0.460091	1.576746
H	1.295546	0.779836	-2.685126
H	0.552245	1.682984	-4.881471
H	-1.860660	2.140123	-5.284198
H	-3.504390	1.671176	-3.475666
H	-2.742989	0.761745	-1.311726
H	-0.373282	-2.461486	-0.910924
H	-2.068925	-4.135926	-0.235104
H	-3.889900	-3.501278	1.339633
H	-3.962572	-1.184523	2.241931
O	4.336762	-3.881952	2.407500
H	0.857968	-0.986526	1.990498
H	2.278489	-2.505175	3.321118
H	4.614314	-3.385994	-0.167507
H	3.169381	-1.850228	-1.491303

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BEt_3-Q

C	1.640525	-0.647381	1.198954
C	2.784364	-1.160956	1.667357
C	3.560199	-2.176195	0.902658
C	3.018985	-2.599837	-0.417882
C	1.876806	-2.088233	-0.887474
C	1.118610	-1.092350	-0.105867
O	0.061462	-0.676976	-0.590878
O	4.594693	-2.637320	1.337541
B	-1.108487	0.399928	0.003039
C	-1.774200	-0.437995	1.220752
C	-0.354619	1.775591	0.434850
C	-2.037254	0.564755	-1.305945
C	-2.733544	-0.713711	-1.779996
C	0.805683	2.225333	-0.459668
C	-2.995867	0.301203	1.778765
H	1.063870	0.095804	1.734966
H	3.207131	-0.863898	2.621655
H	3.601448	-3.337475	-0.960118
H	1.443699	-2.369041	-1.841709
H	-2.082159	-1.439372	0.890402
H	-1.056213	-0.598667	2.040147
H	-0.030537	1.782343	1.487255
H	-1.134674	2.548544	0.389473
H	-2.798386	1.325820	-1.082127
H	-1.450602	0.986529	-2.135079
H	-3.299131	-0.567600	-2.705841
H	-3.434052	-1.085673	-1.024378
H	-2.005685	-1.512710	-1.962663
H	1.158914	3.230873	-0.211781
H	0.509959	2.228138	-1.513644
H	1.675517	1.560211	-0.375450
H	-3.452522	-0.225219	2.622826
H	-2.726004	1.305648	2.122712
H	-3.765245	0.419473	1.008521

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$[BEt_3\text{-}Q]^{\bullet-}$

C	1.624793	-0.700156	1.192530
C	2.781073	-1.241088	1.683224
C	3.562963	-2.220294	0.951283
C	3.033734	-2.586256	-0.351050
C	1.882018	-2.043685	-0.839362
C	1.125281	-1.082587	-0.092457
O	0.047209	-0.616726	-0.640099
O	4.619560	-2.713284	1.407463
B	-1.030220	0.345222	-0.029908
C	-1.745628	-0.431344	1.221693
C	-0.361588	1.783741	0.406815
C	-2.050185	0.560856	-1.291741
C	-2.729708	-0.721699	-1.778325
C	0.759970	2.271276	-0.516223
C	-2.969691	0.318449	1.757403
H	1.065815	0.033293	1.760071
H	3.164119	-0.949493	2.657190
H	3.601972	-3.316815	-0.920021
H	1.486613	-2.317676	-1.813334
H	-2.052982	-1.442354	0.914301
H	-1.040891	-0.583227	2.052990
H	0.006623	1.789638	1.445608
H	-1.169206	2.532309	0.396832
H	-2.820975	1.300609	-1.026124
H	-1.495903	1.006309	-2.132589
H	-3.331387	-0.582178	-2.686517
H	-3.394912	-1.131002	-1.007989
H	-1.977203	-1.489398	-1.989871
H	1.110672	3.282656	-0.272809
H	0.427845	2.279825	-1.560577
H	1.628477	1.604667	-0.466846
H	-3.435539	-0.172031	2.622098
H	-2.700301	1.336320	2.064897
H	-3.739736	0.415708	0.982820

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$[BEt_3\text{-}Q]^{2-}$

C	1.760275	-0.589105	1.094794
C	2.844891	-1.252811	1.671021
C	3.447219	-2.436152	1.121589
C	2.797366	-2.864359	-0.088797
C	1.710946	-2.201693	-0.652612
C	1.155841	-1.042816	-0.088131
O	0.130932	-0.424257	-0.743520
O	4.443970	-3.040508	1.644099

B	-0.959204	0.392337	-0.109269
C	-1.643678	-0.407785	1.162431
C	-0.430044	1.901064	0.362795
C	-2.050602	0.594867	-1.340468
C	-2.624754	-0.726533	-1.855145
C	0.686639	2.438120	-0.536641
C	-2.889003	0.280321	1.730278
H	1.363008	0.306111	1.569879
H	3.281151	-0.867617	2.593686
H	3.195229	-3.760911	-0.567051
H	1.254855	-2.570112	-1.573021
H	-1.907378	-1.434427	0.861589
H	-0.904224	-0.525879	1.967594
H	-0.072273	1.907015	1.406778
H	-1.274089	2.614165	0.348320
H	-2.875574	1.264199	-1.041574
H	-1.542846	1.104164	-2.176531
H	-3.240930	-0.635411	-2.765159
H	-3.250146	-1.205072	-1.089246
H	-1.798001	-1.413621	-2.065255
H	1.024928	3.454216	-0.275107
H	0.361205	2.459856	-1.584593
H	1.551781	1.768053	-0.493805
H	-3.318018	-0.219548	2.613716
H	-2.661368	1.314220	2.023064
H	-3.685418	0.339497	0.975668

40

$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{2+}$

C	-0.447004	2.022194	1.274101
C	0.825234	1.634219	1.442815
C	1.745508	1.551326	0.288896
C	1.279769	1.915629	-1.057609
C	0.007531	2.303606	-1.226323
C	-0.912744	2.386496	-0.072405
O	-2.067739	2.787081	-0.307429
O	2.900501	1.150733	0.523918
Si	-3.703287	3.025758	0.571572
C	-4.813065	1.847474	-0.250526
C	-5.086655	0.603632	0.349660
C	-5.963524	-0.283300	-0.260335
C	-6.568583	0.061828	-1.469282
C	-6.306628	1.292648	-2.073094
C	-5.432766	2.185931	-1.469142
Si	4.536046	0.912041	-0.355083
C	5.645817	2.090365	0.466969
C	5.919433	3.334164	-0.133294
C	6.796300	4.221126	0.476660
C	7.401330	3.876072	1.685643
C	7.139346	2.645295	2.289533
C	6.265487	1.751982	1.685621
H	-1.141141	2.087155	2.105051
H	1.234450	1.361009	2.410844
H	1.973907	1.850669	-1.888560
H	-0.401684	2.576818	-2.194352
H	-3.337674	2.706013	1.960649
H	-3.827911	4.454410	0.268001
H	-4.635999	0.336259	1.302296
H	-6.186188	-1.235695	0.207590
H	-7.257963	-0.630727	-1.940875
H	-6.793247	1.556090	-3.005491
H	-5.248401	3.150099	-1.936029
H	4.660679	-0.516601	-0.051466
H	4.170427	1.231738	-1.744170
H	5.468801	3.601479	-1.085957
H	7.018986	5.173487	0.008676
H	8.090708	4.568650	2.157206
H	7.625941	2.381910	3.221959
H	6.081102	0.787846	2.152567

40

$[SiPhH_2\text{-}Q\text{-}SiPhH_2]^{\bullet+}$

C	-0.800356	1.499774	0.671573
C	0.283314	0.674041	0.643173
C	1.523684	1.116381	0.080050
C	1.633146	2.438048	-0.455160
C	0.549476	3.263780	-0.426761
C	-0.690894	2.821440	0.136363
O	-1.671774	3.678173	0.133434
O	2.504563	0.259648	0.082979
Si	-3.293624	3.553218	0.773241
C	-4.130309	2.099681	0.001451
C	-4.554849	1.024392	0.797466
C	-5.189227	-0.073963	0.224320
C	-5.403339	-0.109359	-1.151267
C	-4.988908	0.951401	-1.955483
C	-4.359361	2.050705	-1.382790
Si	4.126422	0.384611	-0.556804
C	4.963072	1.838165	0.214992
C	5.387649	2.913438	-0.581024
C	6.021994	4.011808	-0.007868
C	6.236031	4.047235	1.367730
C	5.821562	2.986491	2.171947
C	5.192050	1.887172	1.599244
H	-1.747338	1.158247	1.075776
H	0.243577	-0.336964	1.032874
H	2.580128	2.779575	-0.859364
H	0.589213	4.274786	-0.816461
H	-3.125385	3.363465	2.227609
H	-3.823757	4.870321	0.402839
H	-4.399258	1.046451	1.874243
H	-5.521100	-0.896451	0.848799

H	-5.900701	-0.963528	-1.598731
H	-5.164763	0.923224	-3.025461
H	-4.052465	2.877664	-2.019142
H	4.656562	-0.932483	-0.186381
H	3.958208	0.574348	-2.011177
H	5.232113	2.891356	-1.657808
H	6.353896	4.834285	-0.632346
H	6.733366	4.901416	1.815202
H	5.997359	3.014692	3.241934
H	4.885122	1.060226	2.235597

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$SiPhH_2$-Q-$SiPhH_2$

C	-0.269108	1.262305	2.157031
C	1.039575	1.063781	2.580668
C	2.098495	1.219771	1.689744
C	1.840821	1.585318	0.366942
C	0.530966	1.774712	-0.057635
C	-0.528872	1.611400	0.830966
O	-1.793803	1.823760	0.357465
O	3.364479	1.020744	2.172318
Si	-3.209475	1.264235	1.045477
C	-4.524722	1.585008	-0.229483
C	-4.187832	1.738520	-1.580288
C	-5.174238	1.953031	-2.538910
C	-6.512501	2.014751	-2.159056
C	-6.863791	1.867916	-0.819295
C	-5.874711	1.658439	0.136914
Si	4.711589	0.616592	1.271505
C	5.337666	2.125196	0.366382
C	6.270256	2.017836	-0.673528
C	6.744667	3.150825	-1.327512
C	6.284916	4.411570	-0.953017
C	5.351719	4.536211	0.072767
C	4.882772	3.400291	0.727573
H	-1.085051	1.153450	2.866231
H	1.259662	0.787475	3.605788
H	2.659751	1.738574	-0.329960
H	0.312214	2.057312	-1.081417
H	-3.041006	-0.173819	1.369516
H	-3.531353	1.981436	2.304240
H	-3.143343	1.701008	-1.876888
H	-4.899437	2.074354	-3.581938
H	-7.281993	2.182105	-2.906180
H	-7.905720	1.923074	-0.520429
H	-6.161478	1.559385	1.181926
H	5.689597	0.118297	2.259416
H	4.380707	-0.453027	0.297899
H	6.630122	1.038726	-0.983934
H	7.467313	3.051932	-2.131305
H	6.651127	5.296177	-1.464482
H	4.988188	5.517395	0.361116
H	4.146930	3.500843	1.522178

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[$SiEt_3$-Q-$SiEt_3$]$^{2+}$

C	1.044880	0.915200	-0.379609
C	-0.245250	1.249210	-0.522499
C	-1.312970	0.273940	-0.211339
C	-0.965140	-1.076370	0.262981
C	0.324810	-1.411080	0.404401
C	1.393180	-0.437800	0.087161
O	2.565180	-0.823600	0.225571
O	-2.485370	0.652230	-0.365779
Si	4.308470	-0.105290	0.006391
C	4.469340	-0.058110	-1.849449
C	4.198030	1.562760	0.839401
C	5.281360	-1.390520	0.917861
C	6.791220	-1.251580	0.627621
C	3.400010	1.591960	2.151751
C	5.651510	0.847890	-2.256789
Si	-4.228750	-0.064790	-0.112819
C	-4.149290	-1.770710	-0.872349
C	-5.201620	1.205100	-1.044679
C	-4.354650	0.003720	1.742691
C	-5.147740	2.607650	-0.418529
C	-5.767190	-0.462360	2.157611
C	-5.520170	-2.157360	-1.469449
H	1.849530	1.610190	-0.598739
H	-0.567210	2.228060	-0.864919
H	-1.769170	-1.771380	0.484251
H	0.647000	-2.389150	0.748821
H	4.616060	-1.074830	-2.229469
H	3.542110	0.317070	-2.301299
H	3.855070	2.336350	0.141801
H	5.244870	1.825620	1.050491
H	4.932600	-2.385370	0.619181
H	5.091110	-1.298510	1.993161
H	7.354760	-1.968680	1.226181
H	7.016590	-1.453610	-0.422609
H	7.170960	-0.255550	0.874791
H	3.489360	2.565550	2.636211
H	3.756460	0.839120	2.859701
H	2.329530	1.414360	1.990801
H	5.756790	0.859560	-3.343019
H	5.503870	1.879990	-1.927749
H	6.599120	0.493650	-1.843239
H	-3.862020	-2.506180	-0.110419
H	-3.387130	-1.804210	-1.661189
H	-4.860340	1.220600	-2.086969
H	-6.238950	0.847060	-1.084909
H	-4.173960	1.025750	2.092271

H	-3.595050	-0.637720	2.206031
H	-5.715090	3.316950	-1.022889
H	-5.578880	2.613960	0.585981
H	-4.122120	2.982270	-0.349169
H	-5.877340	-0.413170	3.242251
H	-5.959320	-1.495990	1.855701
H	-6.545530	0.171600	1.722831
H	-5.484390	-3.172530	-1.867729
H	-5.800710	-1.488710	-2.286389
H	-6.315000	-2.129230	-0.718769

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$[SiEt_3\text{-}Q\text{-}SiEt_3]^{\cdot+}$

C	0.938500	-0.310290	-0.890639
C	-0.369570	-0.421280	-1.258169
C	-1.418750	-0.091450	-0.339859
C	-1.085220	0.361780	0.975961
C	0.222440	0.473250	1.343171
C	1.271310	0.140950	0.426031
O	2.490460	0.273430	0.851771
O	-2.636230	-0.226870	-0.767429
Si	4.054310	-0.046600	0.094461
C	4.158300	-1.901630	-0.139209
C	4.090640	0.915130	-1.515119
C	5.228010	0.632500	1.370391
C	6.682660	0.196420	1.127721
C	3.422960	2.295520	-1.427919
C	5.212730	-2.298300	-1.187839
Si	-4.251530	0.014930	-0.099499
C	-4.579050	1.850480	-0.230379
C	-4.274180	-0.644430	1.654501
C	-5.289890	-1.007860	-1.258059
C	-3.596230	-2.012950	1.817101
C	-6.792010	-0.895020	-0.948799
C	-3.558090	2.751350	0.476731
H	1.731820	-0.556630	-1.587879
H	-0.659770	-0.758570	-2.246909
H	-1.880770	0.617200	1.666301
H	0.512600	0.813730	2.330791
H	4.391160	-2.362240	0.827951
H	3.176730	-2.295700	-0.431269
H	3.666360	0.331300	-2.340509
H	5.152960	1.033790	-1.768409
H	4.894420	0.298410	2.359531
H	5.154070	1.726310	1.375901
H	7.353670	0.651210	1.859091
H	6.792040	-0.888570	1.213801
H	7.037770	0.490800	0.134851
H	3.559480	2.858560	-2.353389
H	3.842400	2.893640	-0.613839
H	2.345570	2.211550	-1.251729
H	5.278280	-3.384050	-1.284019
H	4.968670	-1.893780	-2.174309
H	6.208510	-1.933830	-0.920079
H	-5.580450	2.023560	0.185071
H	-4.646880	2.112250	-1.292709
H	-3.868840	0.083080	2.367191
H	-5.337680	-0.729210	1.916171
H	-5.087570	-0.678210	-2.283689
H	-4.967790	-2.054250	-1.205069
H	-3.705910	-2.389910	2.835991
H	-4.034020	-2.754890	1.143371
H	-2.524180	-1.964800	1.599171
H	-7.380610	-1.493250	-1.647079
H	-7.024990	-1.250580	0.059351
H	-7.142990	0.138100	-1.028429
H	-3.832000	3.804450	0.383891
H	-2.557620	2.638730	0.046301
H	-3.494500	2.527620	1.546761

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$SiEt_3\text{-}Q\text{-}SiEt_3$

C	0.633840	0.857140	-1.298990
C	-0.739960	1.073110	-1.274760
C	-1.619279	-0.007881	-1.289500
C	-1.116879	-1.306281	-1.383790
C	0.256111	-1.522980	-1.405450
C	1.139641	-0.444600	-1.338690
O	2.480271	-0.702579	-1.330600
O	-2.968020	0.211119	-1.177960
Si	3.569121	-0.054209	-0.210680
C	4.284850	1.576451	-0.839920
C	2.672780	0.173041	1.428250
C	4.926031	-1.339049	-0.071120
C	6.062731	-0.900998	0.862310
C	2.112971	-1.146070	1.977910
C	4.626820	2.575851	0.274850
Si	-3.667299	0.103789	0.362760
C	-2.546490	0.938249	1.627330
C	-3.923159	-1.707461	0.792830
C	-5.293280	1.015948	0.182330
C	-4.841239	-2.431812	-0.200180
C	-5.100060	2.520848	-0.047770
C	-1.337529	0.115139	2.098700
H	1.318910	1.699540	-1.279570
H	-1.147150	2.078129	-1.226870
H	-1.813279	-2.138391	-1.423920
H	0.666881	-2.525580	-1.460320
H	5.182900	1.345931	-1.427190
H	3.583620	2.032801	-1.547780
H	1.859880	0.899370	1.300660
H	3.366530	0.622341	2.150440

H	5.315531	-1.536099	-1.077110
H	4.488581	-2.282909	0.273750
H	6.841371	-1.664488	0.941710
H	6.541121	0.016142	0.502540
H	5.694651	-0.702959	1.874940
H	1.560671	-0.994100	2.909990
H	2.915571	-1.862189	2.181490
H	1.427531	-1.612220	1.262000
H	5.081480	3.486711	-0.124470
H	3.730720	2.869171	0.830310
H	5.329450	2.149531	0.998560
H	-3.175180	1.200649	2.489640
H	-2.207110	1.894069	1.207860
H	-2.942939	-2.199161	0.832970
H	-4.330919	-1.771411	1.810340
H	-5.838620	0.575068	-0.660820
H	-5.909600	0.838748	1.072780
H	-4.935588	-3.496322	0.031690
H	-5.847929	-2.002662	-0.192860
H	-4.459829	-2.343682	-1.222560
H	-6.052770	3.034298	-0.204020
H	-4.608390	2.992528	0.808960
H	-4.475710	2.700728	-0.928050
H	-0.750990	0.660130	2.845390
H	-0.667639	-0.129460	1.267610
H	-1.652659	-0.828561	2.555280

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$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{2+}$

C	-1.004761	0.047004	-1.512307
C	0.284342	0.301810	-1.790391
C	1.359640	-0.384054	-1.067173
C	1.032655	-1.480800	-0.139025
C	-0.256933	-1.752593	0.121001
C	-1.330719	-0.962643	-0.489056
O	-2.495306	-1.228307	-0.125453
O	2.525909	-0.010468	-1.312490
Si	-4.114621	-0.256615	-0.149926
C	-4.647911	-0.728048	1.586880
C	-3.363481	1.472587	-0.313647
C	-5.134352	-0.925394	-1.578587
C	-6.437409	-0.385101	-1.654498
C	-7.241406	-0.623919	-2.782033
C	-6.773025	-1.453745	-3.810729
C	-5.464007	-1.965724	-3.763742
C	-4.657009	-1.739152	-2.636332
C	-3.740031	2.355422	-1.359015
C	-3.416096	3.721059	-1.274312
C	-2.588999	4.185777	-0.242699
C	-2.129867	3.302611	0.749452
C	-2.522705	1.954293	0.731156
C	-5.020962	0.236054	2.556381
C	-5.226828	-0.160793	3.885931
C	-5.107447	-1.514724	4.250613
C	-4.737164	-2.473941	3.296582
C	-4.550879	-2.092331	1.959439
C	-2.178713	5.638588	-0.213035
C	-4.406999	1.895535	-2.642533
C	-1.254828	3.858148	1.852160
C	-1.989832	1.072164	1.851919
C	-6.996480	0.481015	-0.546283
C	-8.595892	0.037929	-2.899160
C	-7.684589	-1.819355	-4.959256
C	-4.930936	-2.739801	-4.950673
C	-3.307772	-2.423508	-2.581967
C	-4.316922	-3.186663	0.939415
C	-4.555624	-3.917337	3.709820
C	-5.425968	-1.939121	5.664183
C	-5.595757	0.860607	4.937289
C	-5.294369	1.689214	2.220561
C	-3.957502	4.697566	-2.294242
Si	4.123954	-0.146626	-0.316263
C	4.774670	1.569063	-0.704724
C	3.312075	-0.320380	1.387582
C	5.067021	-1.619268	-1.001900
C	6.333688	-1.812140	-0.406246
C	7.054785	-2.996308	-0.633688
C	6.542816	-3.969377	-1.504128
C	5.272385	-3.800252	-2.081869
C	4.550529	-2.613011	-1.871186
C	3.601544	-1.409323	2.251101
C	3.250496	-1.339907	3.610262
C	2.482234	-0.267831	4.085268
C	2.108211	0.773969	3.219382
C	2.527790	0.763119	1.879025
C	5.182376	2.475873	0.305147
C	5.483058	3.803241	-0.035484
C	5.419802	4.225569	-1.376169
C	5.012640	3.334402	-2.379791
C	4.735548	1.998224	-2.054687
C	2.042936	-0.247692	5.529620
C	4.195719	-2.721613	1.772988
C	1.297465	1.919114	3.786729
C	2.086961	1.938130	1.016997
C	6.941458	-0.768827	0.506530
C	8.364433	-3.233901	0.083376
C	7.369868	-5.186937	-1.845929
C	4.685290	-4.918848	-2.915740
C	3.261141	-2.431307	-2.644503
C	4.464540	1.034430	-3.190105
C	4.887551	3.812722	-3.808995
C	5.836820	5.631079	-1.737440

C	5.894265	4.790128	1.033079
C	5.393034	2.070785	1.751050
C	3.698705	-2.419697	4.569515
H	-1.815767	0.555398	-2.018787
H	0.589237	1.035197	-2.529488
H	1.842526	-2.048379	0.302522
H	-0.562711	-2.543962	0.797101
H	-1.226852	5.784326	0.296040
H	-2.926236	6.246387	0.310810
H	-2.077565	6.045001	-1.219927
H	-4.050059	2.502027	-3.476643
H	-5.498537	1.991533	-2.622651
H	-4.186854	0.856472	-2.882858
H	-1.109614	3.160627	2.673405
H	-1.696288	4.765893	2.271947
H	-0.262727	4.134685	1.474595
H	-0.891264	1.077272	1.856630
H	-2.317854	0.037756	1.814720
H	-2.310145	1.441616	2.831528
H	-8.081654	0.398603	-0.488785
H	-6.761650	1.544016	-0.695825
H	-6.625875	0.181667	0.434795
H	-9.376756	-0.534900	-2.385332
H	-8.896850	0.144159	-3.940634
H	-8.586460	1.040426	-2.468290
H	-7.456402	-2.813193	-5.344564
H	-7.595546	-1.111484	-5.791810
H	-8.728118	-1.830681	-4.645546
H	-5.068813	-3.821192	-4.833605
H	-3.867532	-2.554452	-5.107501
H	-5.436733	-2.444041	-5.869001
H	-3.105201	-2.830979	-1.590941
H	-2.478592	-1.750863	-2.852466
H	-3.264965	-3.263316	-3.272384
H	-3.281089	-3.547988	0.939143
H	-4.573710	-2.870682	-0.072024
H	-4.954574	-4.045832	1.157133
H	-3.863636	-4.443749	3.052099
H	-5.504568	-4.466325	3.695388
H	-4.153472	-3.988023	4.721284
H	-4.547501	-1.858628	6.316001
H	-5.772742	-2.971206	5.704692
H	-6.210663	-1.317518	6.096310
H	-5.181297	0.592884	5.910015
H	-6.683252	0.938289	5.056251
H	-5.224602	1.854835	4.690295
H	-5.315684	1.895593	1.153605
H	-6.267076	1.982639	2.626509
H	-4.548456	2.362352	2.658329
H	-3.263649	4.849448	-3.130014
H	-4.137419	5.672301	-1.839784
H	-4.906035	4.359304	-2.710866
H	1.123178	0.318814	5.669429
H	2.809335	0.210772	6.166108
H	1.867804	-1.255624	5.907330
H	3.755673	-3.547072	2.335658
H	5.280661	-2.782865	1.915124
H	4.008725	-2.913606	0.717238
H	0.276398	1.602370	4.032466
H	1.223795	2.766767	3.109588
H	1.746213	2.283589	4.714552
H	0.992292	2.023263	1.017943
H	2.415912	1.896572	-0.016930
H	2.477071	2.883471	1.408156
H	8.029892	-0.779628	0.446763
H	6.675250	-0.934918	1.559639
H	6.641867	0.243092	0.231148
H	9.209855	-2.786002	-0.451976
H	8.570148	-4.298209	0.191484
H	8.350524	-2.809473	1.088534
H	7.155271	-5.541769	-2.853979
H	7.179002	-6.015980	-1.154212
H	8.435643	-4.962858	-1.806365
H	4.923580	-4.807504	-3.980239
H	3.599776	-4.966284	-2.821134
H	5.069932	-5.886692	-2.595336
H	3.126596	-1.400574	-2.970439
H	2.369689	-2.729049	-2.069702
H	3.262981	-3.039465	-3.547539
H	3.432251	1.094226	-3.556851
H	4.674575	0.001748	-2.909424
H	5.118151	1.254029	-4.036453
H	4.164307	3.222317	-4.372028
H	5.844163	3.756741	-4.341771
H	4.553058	4.850187	-3.847366
H	5.000855	6.335024	-1.644759
H	6.205232	5.689781	-2.761093
H	6.635691	5.986047	-1.085688
H	5.546009	5.796139	0.795737
H	6.985194	4.838167	1.135021
H	5.488362	4.529757	2.010094
H	4.663468	2.539428	2.421308
H	6.384773	2.393285	2.082165
H	5.329967	0.998829	1.919400
H	2.945716	-3.208973	4.684284
H	3.887406	-2.004204	5.559875
H	4.623644	-2.892595	4.240101

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$[Si(C_6Me_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{\bullet+}$

C	-0.81572	0.79408	-2.04884
C	0.54417	0.85424	-2.06468

C	1.31237	0.10664	-1.11189	C	2.98840	-2.84338	3.26411
C	0.63813	-0.77460	-0.21039	C	3.06074	-3.25092	1.92055
C	-0.72480	-0.86689	-0.22320	C	3.33312	-2.31402	0.91248
C	-1.49885	-0.02850	-1.09409	C	6.22183	-1.45728	-0.98001
O	-2.79374	0.04551	-1.08520	C	6.94301	-2.18432	-1.93910
O	2.59584	0.28280	-1.13371	C	6.78787	-1.89375	-3.30361
Si	-4.17280	-0.15313	0.00818	C	5.88988	-0.89763	-3.71340
C	-5.21246	-1.40583	-0.94527	C	5.16524	-0.16637	-2.75734
C	-3.31221	-0.65663	1.61309	C	2.65082	-3.87248	4.31875
C	-4.90192	1.58423	-0.04398	C	4.22981	0.73499	3.07200
C	-4.97570	2.27169	-1.27517	C	2.81923	-4.70009	1.56198
C	-5.35635	3.62482	-1.30224	C	3.25885	-2.80619	-0.52148
C	-5.71350	4.27926	-0.11512	C	6.76727	1.98694	-0.32678
C	-5.64894	3.59940	1.11160	C	6.78145	4.84882	-0.59223
C	-5.28440	2.24588	1.14450	C	4.46522	6.40510	0.23297
C	-2.23178	0.12131	2.09229	C	1.96128	5.06941	0.87311
C	-1.35576	-0.41572	3.04925	C	1.85860	2.19718	1.04447
C	-1.52923	-1.73508	3.49741	C	4.33807	1.00849	-3.24366
C	-2.64081	-2.48685	3.08449	C	5.70410	-0.61414	-5.18781
C	-3.56526	-1.92260	2.18722	C	7.62766	-2.62122	-4.32883
C	-6.59504	-1.17760	-1.11688	C	7.88848	-3.28295	-1.50591
C	-7.30941	-1.88967	-2.09303	C	6.55284	-1.69948	0.48034
C	-6.66913	-2.88367	-2.84888	C	3.13324	-1.04898	5.04415
C	-5.30476	-3.14616	-2.65533	H	-1.42443	1.38524	-2.72356
C	-4.58792	-2.43330	-1.68307	H	1.08608	1.49587	-2.75107
C	-0.50898	-2.30698	4.45149	H	1.21804	-1.36297	0.49075
C	-1.95015	1.52261	1.58539	H	-1.22360	-1.54481	0.45650
C	-2.82575	-3.89514	3.60650	H	-0.56983	-1.81571	5.42990
C	-4.84953	-2.67228	1.89246	H	-0.63617	-3.37514	4.61672
C	-4.72923	1.58822	-2.60634	H	0.50425	-2.14128	4.06970
C	-5.38386	4.38174	-2.61193	H	-2.59943	1.83285	0.76842
C	-6.20930	5.70686	-0.16017	H	-2.09152	2.25598	2.38727
C	-5.97304	4.33064	2.39581	H	-0.91217	1.61451	1.24725
C	-5.38514	1.52306	2.47363	H	-1.93186	-4.49727	3.42159
C	-3.16515	-2.85356	-1.38596	H	-3.00360	-3.90396	4.68692
C	-4.61049	-4.19183	-3.49968	H	-3.65617	-4.40974	3.12820
C	-7.46222	-3.70302	-3.84099	H	-5.24828	-3.10556	2.81212
C	-8.77011	-1.58251	-2.33753	H	-5.62158	-2.01497	1.49387
C	-7.36704	-0.23293	-0.21881	H	-4.71603	-3.48603	1.16999
C	-0.16699	0.36825	3.55644	H	-4.71890	0.50207	-2.53841
Si	4.05874	0.23147	-0.14941	H	-5.52092	1.85509	-3.31178
C	5.28385	-0.48399	-1.38733	H	-3.78111	1.90256	-3.05803
C	3.66243	-0.97801	1.25402	H	-4.68311	3.96482	-3.33533
C	4.25956	2.08094	0.18690	H	-6.37907	4.36146	-3.07280
C	5.47073	2.74092	-0.11626	H	-5.11285	5.42879	-2.46802
C	5.51374	4.14435	-0.16222	H	-6.72017	5.92081	-1.09948
C	4.38250	4.89658	0.18668	H	-6.91757	5.90762	0.64419
C	3.18564	4.24979	0.52973	H	-5.38650	6.42551	-0.06172
C	3.13145	2.84896	0.54976	H	-5.68557	5.38120	2.33408
C	3.69252	-0.60678	2.61607	H	-7.04475	4.29679	2.62728
C	3.26626	-1.51189	3.60866	H	-5.44174	3.90259	3.24650

H	-4.52382	1.71641	3.12447
H	-6.28018	1.84623	3.01069
H	-5.45543	0.44076	2.36394
H	-3.07987	-3.94295	-1.39858
H	-2.44077	-2.46318	-2.11131
H	-2.86305	-2.53153	-0.38807
H	-5.00379	-4.19732	-4.51766
H	-3.53865	-4.00570	-3.57277
H	-4.74381	-5.20159	-3.09250
H	-8.49700	-3.82415	-3.51852
H	-7.47938	-3.23147	-4.83109
H	-7.04276	-4.70226	-3.96057
H	-9.01154	-0.55059	-2.08138
H	-9.03044	-1.72148	-3.38783
H	-9.42852	-2.23173	-1.74739
H	-6.84960	-0.04610	0.72329
H	-7.54765	0.74264	-0.68405
H	-8.33612	-0.66807	0.03655
H	-0.26206	1.43787	3.37495
H	-0.02945	0.22897	4.63205
H	0.76204	0.02680	3.07373
H	2.44660	-3.42906	5.29130
H	1.77789	-4.46535	4.03141
H	3.48468	-4.57070	4.45147
H	4.90270	1.17952	2.34132
H	3.43363	1.46568	3.26263
H	4.79478	0.61993	3.99899
H	3.09889	-5.36674	2.37760
H	1.76217	-4.88933	1.33534
H	3.39656	-4.99975	0.68664
H	2.38204	-3.44521	-0.66158
H	3.20408	-2.00813	-1.25910
H	4.14236	-3.40183	-0.78084
H	6.75516	1.01122	0.15760
H	6.99163	1.81803	-1.38621
H	7.59983	2.54443	0.10707
H	7.36453	4.23687	-1.28104
H	6.55611	5.78403	-1.10646
H	7.42630	5.09002	0.26170
H	5.46688	6.73964	0.50498
H	4.22142	6.85260	-0.73828
H	3.77583	6.82098	0.96820
H	1.90278	5.96577	0.25311
H	1.03823	4.51094	0.71583
H	1.97267	5.39739	1.91975
H	1.51471	2.68295	1.96325
H	1.04089	2.28153	0.31737
H	1.99298	1.13963	1.28510
H	4.89190	1.55945	-4.00802
H	3.39110	0.68896	-3.69469
H	4.10802	1.71452	-2.44516
H	5.79127	-1.52815	-5.77743
H	4.72158	-0.19041	-5.39646
H	6.45355	0.09207	-5.56576
H	8.59279	-2.91634	-3.91593
H	7.13051	-3.53103	-4.68681
H	7.82800	-1.99391	-5.19788
H	7.59271	-3.71572	-0.54973
H	7.90783	-4.09539	-2.23397
H	8.91673	-2.91697	-1.39624
H	6.20937	-0.89407	1.13145
H	6.11268	-2.62561	0.86889
H	7.63637	-1.76985	0.60815
H	3.98593	-1.36131	5.65784
H	3.05424	0.03537	5.11307
H	2.23288	-1.45854	5.50795

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$Si(C_6Me_5)_3$-Q-$Si(C_6Me_5)_3$

C	-0.62574	0.48670	-0.29813
C	0.68763	0.23376	-0.15417
C	1.40441	-0.51480	-1.19441
C	0.72569	-0.86776	-2.45105
C	-0.56749	-0.56087	-2.61965
C	-1.32546	0.03561	-1.50797
O	-2.56243	0.11038	-1.65698
O	2.58522	-0.89764	-1.06898
Si	-3.97757	0.04547	-0.40214
C	-4.99675	-1.20097	-1.36674
C	-3.01719	-0.68489	1.05572
C	-4.65355	1.78581	-0.22194
C	-5.80462	1.87196	0.59283
C	-6.30381	3.12467	0.98649
C	-5.69278	4.29724	0.51945
C	-4.52404	4.22274	-0.25931
C	-4.02353	2.97481	-0.66517
C	-3.05383	-0.07344	2.33683
C	-2.76491	-0.83513	3.47996
C	-2.27955	-2.14900	3.35738
C	-2.03733	-2.68963	2.08232
C	-2.45427	-1.98467	0.93717
C	-5.48043	-2.40495	-0.79362
C	-6.06345	-3.37893	-1.61705
C	-6.20857	-3.14940	-2.99863
C	-5.73271	-1.96087	-3.57278
C	-5.16967	-0.96962	-2.75639
C	-2.02843	-2.94331	4.61674
C	-3.31220	1.40685	2.54504
C	-1.41803	-4.06358	1.93672
C	-2.26444	-2.69418	-0.39316
C	-6.51469	0.62869	1.08403
C	-7.47802	3.20742	1.93574

C	-6.30576	5.64289	0.83125	H	-4.34054	1.63165	2.84962
C	-3.80364	5.50033	-0.63466	H	-3.11354	1.99908	1.65252
C	-2.84120	2.95778	-1.61147	H	-0.89670	-4.18147	0.98699
C	-4.82694	0.35964	-3.39455	H	-2.18031	-4.85041	1.98881
C	-5.84254	-1.74853	-5.06595	H	-0.69033	-4.26671	2.72270
C	-6.92052	-4.16857	-3.85437	H	-1.19314	-2.79443	-0.61910
C	-6.55826	-4.67996	-1.02826	H	-2.74892	-2.21243	-1.23858
C	-5.48158	-2.67567	0.69840	H	-2.66823	-3.71015	-0.35786
C	-2.95780	-0.23864	4.85539	H	-7.57859	0.81269	1.23273
Si	3.99906	-0.19485	-0.01927	H	-6.11023	0.27518	2.04287
C	5.41479	-0.69034	-1.13919	H	-6.45564	-0.18898	0.36416
C	3.44761	1.61245	-0.18607	H	-8.43632	3.14464	1.40702
C	3.86515	-0.99844	1.67466	H	-7.47113	4.14240	2.49471
C	4.86148	-0.55864	2.57880	H	-7.45390	2.39954	2.66890
C	4.73979	-0.80619	3.95436	H	-6.11742	6.35830	0.03063
C	3.64650	-1.54156	4.43746	H	-5.90503	6.06881	1.75873
C	2.65232	-1.98176	3.54958	H	-7.38707	5.56687	0.94325
C	2.77855	-1.76257	2.16689	H	-4.11737	5.87757	-1.61517
C	3.20109	2.45598	0.92834	H	-2.72240	5.35887	-0.66286
C	3.08173	3.84569	0.74722	H	-3.99694	6.28664	0.09422
C	3.07520	4.39337	-0.54371	H	-2.95725	2.19813	-2.38468
C	3.27511	3.56529	-1.65966	H	-1.88464	2.78076	-1.09671
C	3.45640	2.18209	-1.49159	H	-2.74282	3.90818	-2.13246
C	6.38525	0.23723	-1.59060	H	-3.87731	0.33167	-3.94305
C	7.30771	-0.15023	-2.57506	H	-4.78232	1.16895	-2.66520
C	7.29368	-1.46046	-3.08657	H	-5.60094	0.64266	-4.11074
C	6.32924	-2.38067	-2.64949	H	-5.08182	-1.06067	-5.43538
C	5.42313	-2.01344	-1.64423	H	-6.82020	-1.33957	-5.34691
C	2.81849	5.87002	-0.73562	H	-5.71465	-2.68781	-5.60554
C	2.96002	1.94313	2.33683	H	-6.22878	-4.93646	-4.22181
C	3.32662	4.17841	-3.04201	H	-7.39068	-3.70650	-4.72179
C	3.64059	1.38392	-2.77280	H	-7.70469	-4.67784	-3.29353
C	6.07312	0.20991	2.09683	H	-6.42826	-5.50438	-1.73047
C	5.76481	-0.24845	4.91566	H	-7.62545	-4.62703	-0.78100
C	3.56486	-1.89697	5.90407	H	-6.02614	-4.94640	-0.11575
C	1.42451	-2.68622	4.08304	H	-5.20382	-1.81480	1.30148
C	1.76517	-2.46488	1.28211	H	-6.48353	-2.98261	1.01298
C	4.50755	-3.08011	-1.08363	H	-4.79806	-3.48835	0.96988
C	6.27731	-3.76508	-3.25581	H	-2.02879	0.20361	5.23604
C	8.34784	-1.88673	-4.07998	H	-3.27018	-0.99613	5.57421
C	8.33349	0.83389	-3.08902	H	-3.71882	0.54127	4.85839
C	6.53519	1.63172	-1.01500	H	2.26513	6.05983	-1.65586
C	2.96340	4.76038	1.94685	H	3.75569	6.43599	-0.79344
H	-1.19516	1.00398	0.46426	H	2.23457	6.28587	0.08492
H	1.23389	0.52979	0.73433	H	2.18556	2.54523	2.81679
H	1.32415	-1.36696	-3.20624	H	3.85020	2.01027	2.97299
H	-1.12507	-0.79988	-3.51945	H	2.63235	0.90572	2.37138
H	-1.55357	-3.90389	4.43207	H	2.34263	4.17302	-3.52719
H	-2.97654	-3.14679	5.12561	H	4.01322	3.64526	-3.69938
H	-1.40320	-2.38608	5.32023	H	3.66503	5.21316	-3.00431
H	-2.65768	1.77771	3.33693	H	2.84660	1.63672	-3.48397

H	3.65415	0.30520	-2.64861
H	4.58870	1.63306	-3.26111
H	6.94588	-0.01166	2.71189
H	5.91827	1.29672	2.13813
H	6.35423	-0.06031	1.07812
H	6.63317	-0.91035	5.01391
H	5.34344	-0.10837	5.91043
H	6.13119	0.72509	4.58570
H	3.03106	-2.83452	6.05869
H	3.05165	-1.12040	6.48350
H	4.55893	-2.02330	6.33291
H	1.54175	-3.77778	4.08966
H	0.54243	-2.44850	3.48242
H	1.20722	-2.37621	5.10551
H	2.13663	-2.63756	0.27493
H	0.79569	-1.94378	1.22348
H	1.54505	-3.45134	1.69668
H	3.61715	-3.24078	-1.70475
H	4.18674	-2.84613	-0.06735
H	5.03036	-4.03615	-1.02000
H	5.27656	-4.19429	-3.20018
H	6.96218	-4.45690	-2.75138
H	6.55593	-3.74087	-4.31004
H	8.04683	-1.65503	-5.10884
H	8.54027	-2.95782	-4.02591
H	9.29440	-1.37828	-3.89458
H	8.55093	0.66115	-4.14378
H	9.28012	0.74728	-2.54203
H	7.99659	1.86556	-2.99400
H	6.28026	2.40756	-1.74601
H	7.57535	1.79915	-0.71979
H	5.91751	1.81315	-0.13945
H	1.91885	4.95955	2.21625
H	3.43762	5.72197	1.74897
H	3.45452	4.33943	2.82392

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$B(C_6F_5)_3$-Q-$B(C_6F_5)_3$

C	-0.998619	-0.129137	-1.049523
C	0.294219	-0.155540	-1.390892
C	1.354918	-0.018839	-0.374975
C	0.998609	0.129296	1.049499
C	-0.294228	0.155697	1.390867
C	-1.354926	0.018964	0.374954
O	-2.518362	0.020819	0.795190
B	-3.903346	-0.122080	-0.048516
C	-3.980929	1.078868	-1.139723
C	-3.815598	-1.640724	-0.611803
C	-5.029140	0.164958	1.072186
C	-5.071663	1.054089	-2.007367
C	-5.357013	2.063569	-2.911914
C	-4.529197	3.179798	-2.962056
C	-3.437313	3.257301	-2.112381
C	-3.193261	2.219394	-1.219420
C	-3.660257	-2.005835	-1.945026
C	-3.597827	-3.325241	-2.377673
C	-3.688493	-4.349085	-1.446855
C	-3.825107	-4.038559	-0.099617
C	-3.877749	-2.707359	0.284819
C	-6.189880	-0.576664	1.262113
C	-7.156998	-0.233716	2.200187
C	-6.981323	0.897514	2.983923
C	-5.844146	1.676925	2.818225
C	-4.907435	1.301757	1.867129
F	-5.893846	-0.001639	-1.975855
F	-6.407366	1.980360	-3.721080
F	-4.780651	4.159623	-3.820528
F	-2.633103	4.316454	-2.150629
F	-2.107321	2.370645	-0.429497
F	-3.509009	-1.069149	-2.899436
F	-6.427929	-1.674115	0.536793
F	-8.247686	-0.980005	2.350759
F	-7.896174	1.235213	3.884850
F	-5.669141	2.769545	3.557847
F	-3.835795	2.099681	1.716742
F	-3.996923	-2.460440	1.594335
F	-3.896540	-5.012202	0.801804
F	-3.627155	-5.614426	-1.837407
F	-3.439290	-3.607623	-3.667465
O	2.518357	-0.020754	-0.795205
B	3.903346	0.122094	0.048509
C	3.980857	-1.078827	1.139752
C	3.815673	1.640760	0.611750
C	5.029136	-0.165033	-1.072176
C	5.071580	-1.054071	2.007411
C	5.356869	-2.063534	2.911995
C	4.529000	-3.179722	2.962163
C	3.437125	-3.257202	2.112473
C	3.193136	-2.219314	1.219473
C	3.877895	2.707365	-0.284903
C	3.825326	4.038580	0.099495
C	3.688715	4.349153	1.446722
C	3.597981	3.325341	2.377570
C	3.660339	2.005919	1.944961
C	4.907378	-1.301840	-1.867099
C	5.844080	-1.677077	-2.818176
C	6.981302	-0.897732	-2.983874
C	7.157028	0.233505	-2.200159
C	6.189919	0.576524	-1.262102
F	5.893814	0.001617	1.975876
F	6.407214	-1.980349	3.721175
F	4.780394	-4.159530	3.820671

F	2.632863	-4.316317	2.150745
F	2.107201	-2.370541	0.429538
F	3.997072	2.460401	-1.594409
F	3.835692	-2.099702	-1.716711
F	5.669026	-2.769702	-3.557779
F	7.896147	-1.235498	-3.884782
F	8.247760	0.979731	-2.350732
F	6.428017	1.673976	-0.536802
F	3.509028	1.069269	2.899398
F	3.439447	3.607770	3.667351
F	3.627448	5.614509	1.837236
F	3.896826	5.012191	-0.801954
H	-1.792852	-0.207989	-1.784071
H	0.631837	-0.264551	-2.415826
H	1.792842	0.208163	1.784045
H	-0.631847	0.264717	2.415800

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$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{\bullet-}$

C	1.002084	-0.055874	1.003765
C	-0.312832	-0.090274	1.360425
C	-1.356310	-0.031857	0.381247
C	-1.002083	0.055891	-1.003766
C	0.312833	0.090291	-1.360427
C	1.356311	0.031873	-0.381249
O	2.568882	0.066211	-0.827027
B	3.839959	-0.123759	-0.008038
C	4.073287	1.083837	1.072951
C	3.735935	-1.629730	0.631989
C	5.054157	0.053106	-1.092113
C	5.177935	0.998726	1.916875
C	5.559924	2.002100	2.791716
C	4.822294	3.178710	2.829625
C	3.725710	3.321283	1.996398
C	3.378590	2.285209	1.132565
C	3.598079	-1.953447	1.975631
C	3.474265	-3.256399	2.446254
C	3.481839	-4.307697	1.544936
C	3.603834	-4.039030	0.188725
C	3.720059	-2.722878	-0.232234
C	6.172708	-0.762091	-1.220314
C	7.194223	-0.514515	-2.131277
C	7.124893	0.599194	-2.952490
C	6.038407	1.454926	-2.846735
C	5.042314	1.172572	-1.921868
F	5.928423	-0.113308	1.896147
F	6.623741	1.859720	3.585349
F	5.170398	4.161583	3.660516
F	3.016558	4.451364	2.021230
F	2.311976	2.509980	0.351473
F	3.533748	-0.992295	2.915142
F	6.328096	-1.852428	-0.457885
F	8.242232	-1.337613	-2.219710
F	8.096886	0.850891	-3.830438
F	5.970926	2.541477	-3.620165
F	4.042600	2.061289	-1.832129
F	3.843417	-2.526345	-1.551424
F	3.610700	-5.044458	-0.688039
F	3.365734	-5.563556	1.973628
F	3.339396	-3.499141	3.751769
O	-2.568881	-0.066198	0.827026
B	-3.839959	0.123764	0.008037
C	-4.073281	-1.083834	-1.072950
C	-3.735944	1.629735	-0.631991
C	-5.054155	-0.053108	1.092113
C	-5.177930	-0.998731	-1.916873
C	-5.559914	-2.002108	-2.791712
C	-4.822278	-3.178714	-2.829621
C	-3.725691	-3.321279	-1.996395
C	-3.378576	-2.285202	-1.132564
C	-3.720074	2.722883	0.232231
C	-3.603857	4.039036	-0.188729
C	-3.481861	4.307703	-1.544940
C	-3.474282	3.256405	-2.446257
C	-3.598088	1.953452	-1.975633
C	-5.042305	-1.172575	1.921867
C	-6.038396	-1.454935	2.846734
C	-7.124888	-0.599209	2.952491
C	-7.194224	0.514500	2.131278
C	-6.172710	0.762082	1.220315
F	-5.928425	0.113298	-1.896145
F	-6.623734	-1.859736	-3.585344
F	-5.170377	-4.161591	-3.660509
F	-3.016532	-4.451356	-2.021225
F	-2.311961	-2.509965	-0.351472
F	-3.843432	2.526351	1.551421
F	-4.042586	-2.061284	1.832128
F	-5.970909	-2.541485	3.620164
F	-8.096879	-0.850913	3.830438
F	-8.242238	1.337592	2.219712
F	-6.328105	1.852419	0.457887
F	-3.533751	0.992299	-2.915143
F	-3.339413	3.499146	-3.751772
F	-3.365763	5.563562	-1.973632
F	-3.610728	5.044465	0.688035
H	1.780382	-0.079722	1.757371
H	-0.619582	-0.152496	2.398449
H	-1.780381	0.079740	-1.757373
H	0.619583	0.152514	-2.398451

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$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_3]^{2-}$

C	-1.002684	-0.082727	0.963422
C	0.336225	-0.025941	1.337843
C	1.359947	0.056561	0.390225
C	1.002680	0.082694	-0.963419
C	-0.336229	0.025906	-1.337840
C	-1.359951	-0.056595	-0.390222
O	-2.631227	-0.124324	-0.853982
B	-3.816930	0.123121	-0.044154
C	-4.191356	-1.086450	1.027005
C	-3.673357	1.608708	0.673345
C	-5.093470	0.057307	-1.104407
C	-5.304845	-0.950337	1.850168
C	-5.777618	-1.946040	2.689635
C	-5.125129	-3.170830	2.710053
C	-4.023002	-3.366087	1.895811
C	-3.581096	-2.334957	1.067190
C	-3.524065	1.878051	2.026605
C	-3.327883	3.154292	2.545273
C	-3.267596	4.235904	1.684861
C	-3.401129	4.022562	0.320996
C	-3.590863	2.730913	-0.147486
C	-6.156213	0.947597	-1.204075
C	-7.201976	0.798006	-2.110174
C	-7.221834	-0.295716	-2.958048
C	-6.199298	-1.228038	-2.880002
C	-5.174767	-1.041548	-1.959732
F	-5.985753	0.209866	1.849236
F	-6.853164	-1.753058	3.467569
F	-5.563063	-4.154338	3.507737
F	-3.400837	-4.551606	1.906701
F	-2.524186	-2.619582	0.304584
F	-3.543545	0.889748	2.939866
F	-6.240918	2.029420	-0.414841
F	-8.194527	1.697906	-2.168820
F	-8.222311	-0.457145	-3.834631
F	-6.224637	-2.303368	-3.679558
F	-4.258868	-2.014860	-1.904235
F	-3.739184	2.601898	-1.473615
F	-3.357169	5.065207	-0.518605
F	-3.088601	5.473485	2.161994
F	-3.195112	3.346776	3.864513
O	2.631223	0.124293	0.853987
B	3.816929	-0.123132	0.044155
C	4.191339	1.086455	-1.026992
C	3.673374	-1.608715	-0.673361
C	5.093468	-0.057316	1.104411
C	5.304827	0.950363	-1.850161
C	5.777585	1.946080	-2.689621
C	5.125081	3.170861	-2.710025
C	4.022954	3.366097	-1.895777
C	3.581063	2.334955	-1.067164
C	3.590894	-2.730930	0.147460
C	3.401180	-4.022577	-0.321036
C	3.267656	-4.235907	-1.684904
C	3.327928	-3.154286	-2.545304
C	3.524090	-1.878047	-2.026624
C	5.174752	1.041532	1.959747
C	6.199278	1.228025	2.880021
C	7.221824	0.295714	2.958061
C	7.201981	-0.798000	2.110175
C	6.156223	-0.947595	1.204072
F	5.985750	-0.209832	-1.849243
F	6.853131	1.753117	-3.467559
F	5.562999	4.154383	-3.507700
F	3.400775	4.551609	-1.906655
F	2.524153	2.619561	-0.304552
F	3.739211	-2.601927	1.473591
F	4.258842	2.014835	1.904256
F	6.224603	2.303348	3.679587
F	8.222298	0.457145	3.834646
F	8.194543	-1.697888	2.168815
F	6.240942	-2.029410	0.414828
F	3.543559	-0.889735	-2.939876
F	3.195164	-3.346759	-3.864547
F	3.088680	-5.473486	-2.162049
F	3.357234	-5.065231	0.518554
H	-1.768443	-0.155047	1.729395
H	0.618064	-0.047209	2.385902
H	1.768440	0.155016	-1.729392
H	-0.618067	0.047174	-2.385899

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$B(C_6F_5)_2Ph$-Q-$B(C_6F_5)_2Ph$

C	0.930400	-0.628480	-0.919340
C	-0.378310	-0.838370	-1.096060
C	-1.373490	-0.248479	-0.183390
C	-0.930400	0.628421	0.919400
C	0.378310	0.838310	1.096120
C	1.373500	0.248430	0.183450
O	2.556470	0.541310	0.394120
B	3.884180	0.170750	-0.494830
C	4.196250	-1.412910	-0.299070
C	3.496400	0.635970	-1.987620
C	5.012200	1.045800	0.261700
C	5.389620	-1.874590	-0.854830
C	5.841419	-3.180611	-0.734710
C	5.085149	-4.093690	-0.010430
C	3.896069	-3.682030	0.570740
C	3.483840	-2.362520	0.421830
C	3.657730	-0.178070	-3.114330
C	3.262610	0.248280	-4.381480
C	2.693910	1.506700	-4.549680

C	2.530200	2.339180	-3.444490
C	2.930300	1.905220	-2.185160
C	5.959810	1.834359	-0.383200
C	6.941710	2.540339	0.305380
C	7.002710	2.458659	1.688460
C	6.089290	1.665859	2.371510
C	5.129790	0.974180	1.647900
F	6.154280	-1.024941	-1.552860
F	6.984469	-3.562591	-1.295500
F	5.494679	-5.349910	0.119150
F	3.159499	-4.544930	1.266860
F	2.314950	-2.048530	1.022680
F	5.974450	1.940139	-1.712750
F	7.824501	3.289389	-0.351790
F	7.933930	3.129729	2.357830
F	6.149320	1.572049	3.699060
F	4.285260	0.194280	2.343510
O	-2.556470	-0.541349	-0.394080
B	-3.884190	-0.170749	0.494840
C	-4.196240	1.412901	0.299060
C	-3.496440	-0.635969	1.987650
C	-5.012210	-1.045799	-0.261690
C	-5.389610	1.874601	0.854790
C	-5.841389	3.180631	0.734640
C	-5.085089	4.093691	0.010380
C	-3.895999	3.682011	-0.570770
C	-3.483790	2.362501	-0.421830
C	-2.930380	-1.905219	2.185210
C	-2.530310	-2.339179	3.444560
C	-2.694020	-1.506679	4.549740
C	-3.262690	-0.248239	4.381500
C	-3.657770	0.178091	3.114350
C	-5.129780	-0.974189	-1.647900
C	-6.089260	-1.665879	-2.371520
C	-7.002710	-2.458648	-1.688470
C	-6.941740	-2.540319	-0.305390
C	-5.959840	-1.834329	0.383200
F	-6.154300	1.024981	1.552820
F	-6.984449	3.562642	1.295400
F	-5.494599	5.349921	-0.119230
F	-3.159399	4.544901	-1.266870
F	-2.314890	2.048491	-1.022640
F	-4.285220	-0.194319	-2.343500
F	-6.149270	-1.572079	-3.699070
F	-7.933930	-3.129708	-2.357850
F	-7.824551	-3.289338	0.351770
F	-5.974510	-1.940099	1.712750
H	1.686080	-1.060310	-1.564240
H	-0.773640	-1.462899	-1.889480
H	-1.686080	1.060251	1.564300
H	0.773650	1.462840	1.889550
H	4.095200	-1.167360	-3.007810
H	3.400730	-0.404570	-5.237780
H	2.384360	1.839810	-5.535000
H	2.097281	3.327140	-3.566700
H	2.812480	2.575360	-1.334540
H	-2.812550	-2.575379	1.334610
H	-2.097411	-3.327139	3.566790
H	-2.384500	-1.839779	5.535060
H	-3.400810	0.404621	5.237800
H	-4.095220	1.167401	3.007810

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$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{\bullet-}$

C	1.20959	-0.16698	0.54547
C	-0.08969	-0.35781	0.91189
C	-1.16452	-0.21227	-0.02570
C	-0.85711	0.14338	-1.37946
C	0.44230	0.34122	-1.74216
C	1.51681	0.18934	-0.80739
O	2.71049	0.38881	-1.25837
B	4.02516	0.13896	-0.51648
C	4.18497	1.15320	0.76689
C	4.05223	-1.46535	-0.15249
C	5.19595	0.55467	-1.55429
C	5.25498	0.98438	1.64305
C	5.55678	1.85893	2.67455
C	4.77311	2.99083	2.85377
C	3.70851	3.21772	1.99855
C	3.44288	2.30988	0.97681
C	3.96935	-2.04611	1.10854
C	4.01041	-3.41734	1.33391
C	4.12967	-4.27901	0.25578
C	4.19147	-3.75548	-1.02690
C	4.14356	-2.37829	-1.20415
C	6.45707	-0.05258	-1.56078
C	7.46755	0.37466	-2.41910
C	7.23880	1.43081	-3.29678
C	5.99335	2.05413	-3.30401
C	4.99140	1.62014	-2.44024
F	6.05885	-0.08259	1.51001
F	6.59133	1.63343	3.48896
F	5.04617	3.85021	3.83735
F	2.95224	4.30736	2.15422
F	2.40500	2.62273	0.18130
F	3.80006	-1.28912	2.20819
F	4.17998	-1.94684	-2.46900
F	4.28925	-4.57903	-2.07323
F	4.17066	-5.59763	0.44808
F	3.92603	-3.90981	2.57224
O	-2.35575	-0.42331	0.42747
B	-3.67266	-0.29025	-0.34725

C	-3.75526	-1.33151	-1.58359
C	-3.80239	1.31004	-0.71739
C	-4.82105	-0.78835	0.71545
C	-4.82768	-1.26416	-2.48539
C	-4.99497	-2.20605	-3.49323
C	-4.08881	-3.25868	-3.62178
C	-3.03023	-3.35994	-2.72663
C	-2.87459	-2.40970	-1.71700
C	-3.99819	2.23306	0.31057
C	-4.09313	3.60291	0.11641
C	-3.97676	4.11552	-1.16792
C	-3.76142	3.24724	-2.22375
C	-3.67556	1.87907	-1.98009
C	-4.60478	-1.90288	1.52280
C	-5.56128	-2.41981	2.38849
C	-6.81309	-1.82829	2.45478
C	-7.08661	-0.73470	1.64884
C	-6.09928	-0.24840	0.80099
F	-4.11766	1.80974	1.57636
F	-3.43726	-2.56038	1.48308
F	-5.29257	-3.48720	3.14647
F	-7.74720	-2.31257	3.27670
F	-8.29430	-0.16330	1.69231
F	-6.45376	0.79869	0.03450
F	-3.42408	1.12429	-3.06367
F	-3.62963	3.72712	-3.46320
F	-4.06225	5.42889	-1.37938
F	-4.29404	4.43111	1.14391
H	2.01022	-0.27123	1.26793
H	-0.36164	-0.62510	1.92709
H	-1.65529	0.22882	-2.10593
H	0.71306	0.60408	-2.75875
H	6.65234	-0.87979	-0.88207
H	8.43484	-0.12017	-2.40500
H	8.02352	1.76503	-3.96931
H	5.80287	2.87976	-3.98436
H	4.02245	2.11409	-2.45323
H	-5.54601	-0.45075	-2.39030
H	-5.83150	-2.12179	-4.18123
H	-4.21333	-3.99550	-4.40979
H	-2.32467	-4.18181	-2.80809
H	-2.05451	-2.52374	-1.01192

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$[B(C_6F_5)_2Ph\text{-}Q\text{-}B(C_6F_5)_2Ph]^{2-}$

C	0.82249	-0.50899	0.94002
C	-0.53963	-0.62803	1.18853
C	-1.48567	-0.54773	0.15926
C	-1.01903	-0.33803	-1.14417
C	0.34734	-0.21756	-1.38973
C	1.29164	-0.30186	-0.36367
O	2.59545	-0.16059	-0.70153
B	3.73317	-0.57080	0.13225
C	4.12491	0.52480	1.32732
C	3.51245	-2.08464	0.70388
C	5.02892	-0.47563	-0.91299
C	5.30441	0.36379	2.05078
C	5.76016	1.25542	3.01230
C	5.02340	2.40127	3.26902
C	3.85559	2.62586	2.55981
C	3.43456	1.70145	1.60527
C	3.75371	-2.52336	2.00909
C	3.51706	-3.84116	2.40105
C	3.02477	-4.76497	1.48585
C	2.76067	-4.35209	0.18071
C	2.99811	-3.03436	-0.19264
C	6.01160	-1.43999	-1.10926
C	7.06006	-1.29130	-2.01453
C	7.16658	-0.12780	-2.75601
C	6.22829	0.87654	-2.57528
C	5.19752	0.68858	-1.66235
F	6.08807	-0.70790	1.82655
F	6.90171	1.03503	3.68284
F	5.44110	3.28236	4.18884
F	3.15146	3.74060	2.79491
F	2.31159	2.02028	0.95964
F	6.01581	-2.58894	-0.42175
F	7.97599	-2.25991	-2.17274
F	8.17158	0.03181	-3.62955
F	6.34135	2.01741	-3.27210
F	4.36514	1.72485	-1.50519
O	-2.78604	-0.70555	0.50357
B	-3.93307	-0.39360	-0.35678
C	-4.15989	-1.43810	-1.58935
C	-3.82818	1.20316	-0.81880
C	-5.28127	-0.63368	0.59566
C	-5.19633	-1.26955	-2.51963
C	-5.46457	-2.21656	-3.50187
C	-4.69618	-3.37863	-3.57671
C	-3.67043	-3.57584	-2.65732
C	-3.41371	-2.61843	-1.67516
C	-3.94859	2.19809	0.14992
C	-3.82407	3.55552	-0.10778
C	-3.54966	3.97783	-1.39987
C	-3.40405	3.03272	-2.39897
C	-3.54019	1.68105	-2.09139
C	-5.33873	-1.70092	1.49208
C	-6.45483	-1.99036	2.27146
C	-7.59428	-1.21095	2.15976
C	-7.59881	-0.15798	1.26114
C	-6.46098	0.09726	0.50456

F	-4.23142	1.87151	1.42056
F	-4.31294	-2.54584	1.63566
F	-6.45010	-3.02805	3.12176
F	-8.68043	-1.47995	2.89964
F	-8.70086	0.59699	1.12873
F	-6.57496	1.12372	-0.36235
F	-3.36015	0.84638	-3.12903
F	-3.13349	3.42892	-3.65082
F	-3.42982	5.28326	-1.67511
F	-3.97405	4.46439	0.86635
H	1.53004	-0.58382	1.76005
H	-0.90610	-0.79150	2.19739
H	-1.71833	-0.28900	-1.97148
H	0.71177	-0.05578	-2.39990
H	4.12439	-1.82086	2.75188
H	3.71253	-4.14395	3.42721
H	2.83503	-5.79191	1.78747
H	2.35726	-5.05771	-0.54128
H	2.76625	-2.71303	-1.20634
H	-5.80742	-0.36823	-2.46605
H	-6.27246	-2.05241	-4.21150
H	-4.89825	-4.12205	-4.34389
H	-3.06614	-4.47860	-2.70340
H	-2.61532	-2.78129	-0.95522

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$B(C_6F_5)Ph_2$-Q-$B(C_6F_5)Ph_2$

C	-1.101080	0.191750	-0.924680
C	0.130920	0.524120	-1.324340
C	1.291330	0.372450	-0.427470
C	1.101080	-0.191860	0.924660
C	-0.130920	-0.524230	1.324310
C	-1.291340	-0.372550	0.427450
O	-2.386120	-0.738310	0.868360
B	-3.850140	-0.894220	0.085160
C	-4.447620	0.614670	-0.069340
C	-3.497530	-1.643470	-1.297740
C	-4.675160	-1.754020	1.158780
C	-5.758970	0.708930	-0.539510
C	-6.442400	1.907050	-0.686070
C	-5.810470	3.095620	-0.342380
C	-4.509040	3.057880	0.130150
C	-3.863040	1.832300	0.256260
C	-3.916410	-1.189650	-2.554840
C	-3.564600	-1.858620	-3.726520
C	-2.778380	-3.005210	-3.667040
C	-2.357169	-3.484820	-2.428500
C	-2.720020	-2.812980	-1.264910
C	-5.376100	-2.911950	0.806460
C	-6.109289	-3.630260	1.749700
C	-6.150589	-3.203490	3.073120
C	-5.462470	-2.050350	3.447210
C	-4.741880	-1.336910	2.495740
F	-6.408940	-0.405870	-0.892590
F	-7.689610	1.930309	-1.148060
F	-6.444590	4.255870	-0.474100
F	-3.884100	4.187690	0.458520
F	-2.594070	1.899400	0.721690
O	2.386120	0.738230	-0.868370
B	3.850110	0.894200	-0.085160
C	4.447660	-0.614660	0.069330
C	3.497460	1.643420	1.297750
C	4.675110	1.754050	-1.158760
C	5.759010	-0.708870	0.539490
C	6.442500	-1.906960	0.686050
C	5.810600	-3.095560	0.342360
C	4.509170	-3.057870	-0.130170
C	3.863120	-1.832310	-0.256260
C	2.719880	2.812890	1.264930
C	2.357000	3.484690	2.428530
C	2.778230	3.005090	3.667060
C	3.564520	1.858550	3.726530
C	3.916370	1.189620	2.554840
C	4.741860	1.336950	-2.495720
C	5.462430	2.050430	-3.447180
C	6.150490	3.203610	-3.073070
C	6.109140	3.630360	-1.749650
C	5.375990	2.912010	-0.806430
F	6.408940	0.405950	0.892570
F	7.689710	-1.930179	1.148030
F	6.444771	-4.255790	0.474060
F	3.884271	-4.187700	-0.458540
F	2.594150	-1.899460	-0.721690
H	-1.974730	0.312350	-1.553530
H	0.339110	0.947220	-2.300860
H	1.974730	-0.312450	1.553500
H	-0.339110	-0.947340	2.300840
H	-4.523850	-0.290840	-2.627430
H	-3.905520	-1.482870	-4.686450
H	-2.500409	-3.525850	-4.577900
H	-1.753169	-4.385130	-2.370240
H	-2.403989	-3.212710	-0.302370
H	-5.352259	-3.254280	-0.224910
H	-6.647699	-4.524340	1.450280
H	-6.717969	-3.763020	3.810450
H	-5.494060	-1.707980	4.477230
H	-4.215650	-0.432140	2.797640
H	2.403830	3.212610	0.302390
H	1.752940	4.384970	2.370270
H	2.500230	3.525700	4.577920
H	3.905460	1.482810	4.686450

H	4.523860	0.290830	2.627420
H	4.215690	0.432150	-2.797640
H	5.494050	1.708060	-4.477200
H	6.717840	3.763160	-3.810390
H	6.647500	4.524470	-1.450220
H	5.352110	3.254340	0.224940

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$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{\bullet-}$

C	1.115180	0.201181	0.850700
C	-0.127660	0.571260	1.269480
C	-1.283720	0.391890	0.442330
C	-1.115180	-0.201230	-0.850680
C	0.127660	-0.571310	-1.269450
C	1.283720	-0.391939	-0.442310
O	2.416340	-0.769399	-0.931820
B	3.773760	-0.865699	-0.199200
C	4.372730	0.643021	0.098060
C	3.550310	-1.771599	1.132800
C	4.747270	-1.569159	-1.292130
C	5.604610	0.758191	0.742840
C	6.248380	1.964591	0.979930
C	5.664530	3.143241	0.539290
C	4.451820	3.085811	-0.126110
C	3.840660	1.852831	-0.337950
C	3.800480	-1.363419	2.448050
C	3.553020	-2.195669	3.539010
C	3.041590	-3.473779	3.338940
C	2.781460	-3.908299	2.040880
C	3.036110	-3.066809	0.962290
C	5.748940	-2.481399	-0.939220
C	6.597950	-3.039809	-1.893500
C	6.463090	-2.696599	-3.235680
C	5.474670	-1.789419	-3.612390
C	4.635520	-1.235989	-2.649510
F	6.239090	-0.341849	1.175520
F	7.423670	2.004571	1.615520
F	6.266200	4.316031	0.752430
F	3.883650	4.212531	-0.565400
F	2.678630	1.901841	-1.010830
O	-2.416330	0.769350	0.931840
B	-3.773750	0.865690	0.199210
C	-4.372750	-0.643020	-0.098070
C	-3.550270	1.771580	-1.132780
C	-4.747250	1.569160	1.292130
C	-5.604630	-0.758160	-0.742840
C	-6.248420	-1.964540	-0.979950
C	-5.664590	-3.143210	-0.539320
C	-4.451890	-3.085810	0.126080
C	-3.840700	-1.852850	0.337930
C	-3.036030	3.066780	-0.962260
C	-2.781350	3.908270	-2.040850
C	-3.041490	3.473770	-3.338910
C	-3.552960	2.195680	-3.538990
C	-3.800450	1.363420	-2.448040
C	-4.635540	1.235960	2.649510
C	-5.474690	1.789400	3.612380
C	-6.463070	2.696620	3.235680
C	-6.597900	3.039860	1.893500
C	-5.748890	2.481440	0.939220
F	-6.239090	0.341890	-1.175510
F	-7.423710	-2.004500	-1.615540
F	-6.266290	-4.315990	-0.752480
F	-3.883730	-4.212550	0.565360
F	-2.678670	-1.901880	1.010810
H	1.984960	0.347111	1.478740
H	-0.288670	1.025330	2.241050
H	-1.984960	-0.347160	-1.478720
H	0.288670	-1.025369	-2.241030
H	4.190510	-0.364309	2.633450
H	3.758200	-1.843369	4.546220
H	2.844560	-4.125029	4.185560
H	2.379260	-4.903169	1.870970
H	2.835520	-3.419459	-0.047700
H	5.860690	-2.761999	0.105220
H	7.364390	-3.747509	-1.588620
H	7.120990	-3.132339	-3.982500
H	5.359440	-1.514479	-4.657600
H	3.864950	-0.530409	-2.953620
H	-2.835430	3.419410	0.047730
H	-2.379110	4.903130	-1.870930
H	-2.844440	4.125020	-4.185520
H	-3.758160	1.843390	-4.546210
H	-4.190520	0.364330	-2.633450
H	-3.865000	0.530350	2.953620
H	-5.359480	1.514440	4.657590
H	-7.120960	3.132370	3.982500
H	-7.364300	3.747590	1.588620
H	-5.860610	2.762070	-0.105210

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$[B(C_6F_5)Ph_2\text{-}Q\text{-}B(C_6F_5)Ph_2]^{2-}$

C	-1.198510	-0.746000	0.818810
C	0.094330	-0.721290	1.336690
C	1.217240	-0.552400	0.520360
C	1.001800	-0.400470	-0.855630
C	-0.288010	-0.422660	-1.375540
C	-1.411520	-0.596130	-0.558220
O	-2.621120	-0.627780	-1.164410
B	-3.925120	-0.575080	-0.472740
C	-4.271440	-1.965880	0.321820
C	-4.003840	0.797290	0.480590

C	-5.061720	-0.449410	-1.647000
C	-5.437240	-2.138650	1.083470
C	-5.780810	-3.361490	1.650140
C	-4.956940	-4.471590	1.465610
C	-3.797940	-4.333580	0.708180
C	-3.469100	-3.100180	0.144840
C	-4.044900	0.865200	1.869220
C	-4.119700	2.055520	2.588600
C	-4.140370	3.260910	1.910380
C	-4.076760	3.255510	0.525650
C	-4.003390	2.043280	-0.149350
C	-6.353150	0.045450	-1.418420
C	-7.324640	0.075510	-2.417030
C	-7.027570	-0.396250	-3.693320
C	-5.750010	-0.890470	-3.949790
C	-4.789450	-0.913590	-2.941110
F	-3.996380	-0.245120	2.625080
F	-3.936720	2.130540	-1.483120
F	-4.091200	4.420910	-0.138380
F	-4.217920	4.418650	2.581980
F	-4.170280	2.049770	3.929620
O	2.428670	-0.524640	1.118980
B	3.724770	-0.691080	0.431700
C	4.180380	0.685200	-0.415440
C	3.718420	-2.035420	-0.504260
C	4.826320	-0.822050	1.641690
C	5.384970	0.729920	-1.115070
C	5.875030	1.855380	-1.764860
C	5.151850	3.035770	-1.710700
C	3.958390	3.058700	-1.009740
C	3.502740	1.903120	-0.377790
C	3.423320	-3.250800	0.134420
C	3.373650	-4.459550	-0.552850
C	3.619460	-4.491930	-1.924650
C	3.904270	-3.303180	-2.588620
C	3.949840	-2.100870	-1.882850
C	4.602860	-0.149100	2.852320
C	5.515450	-0.199030	3.903400
C	6.692980	-0.933750	3.773110
C	6.937550	-1.615680	2.583850
C	6.015210	-1.557120	1.539370
F	6.167370	-0.362810	-1.193840
F	7.040910	1.821960	-2.431130
F	5.606020	4.139670	-2.322990
F	3.261480	4.201660	-0.940440
F	2.353630	2.044890	0.290470
H	-2.040700	-0.903520	1.484080
H	0.260520	-0.840890	2.403440
H	1.848850	-0.265530	-1.520500
H	-0.455210	-0.302980	-2.442100
H	-6.095710	-1.284730	1.240670
H	-6.691720	-3.452270	2.238300
H	-5.216840	-5.430240	1.908300
H	-3.143370	-5.188630	0.555630
H	-2.561470	-3.006460	-0.446150
H	-6.602800	0.434400	-0.431400
H	-8.314330	0.473140	-2.201310
H	-7.779500	-0.373910	-4.478600
H	-5.501370	-1.256390	-4.943980
H	-3.790440	-1.288200	-3.146810
H	3.221740	-3.232760	1.203830
H	3.136590	-5.378540	-0.021770
H	3.579010	-5.431730	-2.469830
H	4.085130	-3.309410	-3.661160
H	4.159670	-1.184110	-2.431180
H	3.677000	0.410640	2.960090
H	5.307880	0.332550	4.829800
H	7.408420	-0.978220	4.591100
H	7.848490	-2.200060	2.471110
H	6.215050	-2.102600	0.620070

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BPh_3-Q-BPh_3

C	0.997864	-0.003511	1.054655
C	-0.296685	-0.033463	1.395860
C	-1.361561	-0.019758	0.377070
C	-0.997865	0.003503	-1.054655
C	0.296684	0.033454	-1.395860
C	1.361560	0.019751	-0.377070
O	2.528301	0.031427	-0.790704
B	3.955247	-0.047313	0.061450
C	4.119023	1.417250	0.725830
C	3.759773	-1.271179	1.099942
C	5.019876	-0.316456	-1.113262
C	5.363268	1.698715	1.317738
C	5.613620	2.905374	1.959541
C	4.625548	3.888748	2.011103
C	3.396455	3.648988	1.410860
C	3.154134	2.428332	0.777306
C	4.036253	-1.165263	2.469401
C	3.837986	-2.237540	3.339625
C	3.349419	-3.448077	2.857931
C	3.073780	-3.583390	1.498493
C	3.284257	-2.510085	0.637662
C	5.918179	-1.388596	-1.088403
C	6.857752	-1.575016	-2.103332
C	6.909785	-0.691268	-3.175239
C	6.025709	0.386622	-3.221955
C	5.104015	0.569778	-2.198077
H	6.150036	0.948605	1.265552
H	6.583402	3.085311	2.413659
H	4.819450	4.835863	2.504307

H	2.624667	4.412716	1.424985
H	2.185360	2.299699	0.296448
H	4.404891	-0.222084	2.865727
H	5.885117	-2.092239	-0.260266
H	7.546297	-2.413563	-2.056457
H	7.636655	-0.835691	-3.968770
H	6.064921	1.085799	-4.052101
H	4.433482	1.427051	-2.232524
H	3.087567	-2.638242	-0.426085
H	2.703241	-4.527624	1.110438
H	3.189590	-4.282290	3.533831
H	4.062360	-2.124835	4.396187
O	-2.528302	-0.031432	0.790703
B	-3.955249	0.047313	-0.061451
C	-4.119028	-1.417249	-0.725834
C	-3.759770	1.271180	-1.099940
C	-5.019877	0.316455	1.113261
C	-5.363273	-1.698710	-1.317741
C	-5.613628	-2.905368	-1.959546
C	-4.625558	-3.888744	-2.011109
C	-3.396465	-3.648988	-1.410866
C	-3.154142	-2.428334	-0.777310
C	-3.284250	2.510084	-0.637658
C	-3.073768	3.583389	-1.498487
C	-3.349407	3.448080	-2.857925
C	-3.837979	2.237545	-3.339622
C	-4.036250	1.165268	-2.469399
C	-5.104023	-0.569785	2.198071
C	-6.025715	-0.386627	3.221951
C	-6.909781	0.691271	3.175242
C	-6.857741	1.575025	2.103341
C	-5.918171	1.388603	1.088409
H	-6.150040	-0.948599	-1.265556
H	-6.583410	-3.085302	-2.413665
H	-4.819464	-4.835859	-2.504314
H	-2.624680	-4.412718	-1.424991
H	-2.185367	-2.299704	-0.296452
H	-3.087559	2.638239	0.426090
H	-4.433497	-1.427064	2.232512
H	-6.064932	-1.085809	4.052092
H	-7.636650	0.835695	3.968774
H	-7.546279	2.413578	2.056470
H	-5.885105	2.092250	0.260276
H	-4.404891	0.222090	-2.865727
H	-4.062352	2.124842	-4.396184
H	-3.189575	4.282292	-3.533824
H	-2.703227	4.527621	-1.110430
H	1.797368	0.007985	1.784973
H	-0.629360	-0.045194	2.428061
H	-1.797369	-0.007993	-1.784974
H	0.629359	0.045184	-2.428061

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$[BPh_3\text{-}Q\text{-}BPh_3]^{\bullet-}$

C	-1.004182	0.023700	-1.001888
C	0.310437	-0.013186	-1.362072
C	1.361449	-0.035702	-0.387154
C	1.004183	-0.023656	1.001881
C	-0.310436	0.013232	1.362066
C	-1.361448	0.035745	0.387148
O	-2.572193	0.079433	0.832048
B	-3.888331	-0.016542	0.004934
C	-4.123085	1.382582	-0.790285
C	-3.797228	-1.340669	-0.943981
C	-5.042604	-0.186571	1.138456
C	-5.318005	1.571091	-1.505969
C	-5.592862	2.749269	-2.191877
C	-4.675194	3.798910	-2.171354
C	-3.494107	3.651001	-1.452880
C	-3.229318	2.460472	-0.774318
C	-4.056829	-1.360584	-2.320071
C	-3.972778	-2.535346	-3.069371
C	-3.617771	-3.731902	-2.455959
C	-3.351790	-3.742571	-1.087306
C	-3.447077	-2.565730	-0.351857
C	-6.178078	-0.982273	0.940342
C	-7.192956	-1.067598	1.893424
C	-7.090878	-0.358845	3.086401
C	-5.968876	0.437479	3.311374
C	-4.968787	0.521085	2.347301
H	-6.055232	0.769458	-1.512521
H	-6.526971	2.854481	-2.737597
H	-4.884334	4.722974	-2.702757
H	-2.774222	4.464330	-1.416299
H	-2.301745	2.382494	-0.211942
H	-4.320831	-0.432852	-2.823157
H	-6.263322	-1.559065	0.021178
H	-8.060667	-1.695511	1.707230
H	-7.875299	-0.426651	3.835235
H	-5.877132	0.995126	4.240090
H	-4.099830	1.149094	2.531542
H	-3.247467	-2.588618	0.718184
H	-3.072044	-4.670541	-0.595644
H	-3.546411	-4.647520	-3.036206
H	-4.179732	-2.512562	-4.136220
O	2.572194	-0.079396	-0.832054
B	3.888331	0.016551	-0.004935
C	4.123046	-1.382576	0.790292
C	3.797256	1.340686	0.943972
C	5.042614	0.186545	-1.138451
C	5.317937	-1.571095	1.506021
C	5.592761	-2.749278	2.191933

C	4.675089	-3.798914	2.171370
C	3.494031	-3.650994	1.452849
C	3.229274	-2.460461	0.774284
C	3.447181	2.565759	0.351826
C	3.351918	3.742610	1.087265
C	3.617845	3.731937	2.455928
C	3.972776	2.535369	3.069361
C	4.056804	1.360599	2.320071
C	4.968766	-0.521076	-2.347314
C	5.968865	-0.437499	-3.311379
C	7.090909	0.358759	-3.086379
C	7.193018	1.067476	-1.893384
C	6.178129	0.982182	-0.940311
H	6.055167	-0.769465	1.512609
H	6.526849	-2.854498	2.737690
H	4.884202	-4.722982	2.702777
H	2.774143	-4.464321	1.416237
H	2.301724	-2.382475	0.211872
H	3.247615	2.588649	-0.718222
H	4.099778	-1.149034	-2.531577
H	5.877097	-0.995118	-4.240110
H	7.875337	0.426542	-3.835208
H	8.060761	1.695338	-1.707169
H	6.263398	1.558947	-0.021133
H	4.320747	0.432859	2.823175
H	4.179688	2.512583	4.136218
H	3.546503	4.647562	3.036166
H	3.072232	4.670589	0.595586
H	-1.790660	0.052849	-1.745171
H	0.611700	-0.016863	-2.404048
H	1.790660	-0.052806	1.745165
H	-0.611699	0.016909	2.404042

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$[BPh_3\text{-}Q\text{-}BPh_3]^{2-}$

C	1.005315	0.108282	0.959022
C	-0.334775	0.068828	1.333751
C	-1.368476	-0.040755	0.394192
C	-1.005317	-0.108335	-0.959023
C	0.334773	-0.068881	-1.333752
C	1.368474	0.040701	-0.394193
O	2.634310	0.092818	-0.862531
B	3.880722	0.006048	-0.044641
C	4.204592	1.428823	0.711207
C	3.836448	-1.285841	0.970174
C	5.082360	-0.243218	-1.140112
C	5.425167	1.666668	1.366308
C	5.722388	2.882362	1.978196
C	4.797873	3.924517	1.943172
C	3.587674	3.728965	1.282767
C	3.304175	2.504442	0.677980
C	4.314881	-1.314048	2.286375
C	4.297878	-2.478512	3.058272
C	3.785873	-3.659316	2.532046
C	3.288409	-3.659176	1.228299
C	3.319582	-2.493846	0.470526
C	6.285917	-0.892357	-0.828393
C	7.314057	-1.039972	-1.759481
C	7.161993	-0.545248	-3.052186
C	5.970479	0.092809	-3.395261
C	4.955491	0.237822	-2.452438
H	6.174821	0.876156	1.380524
H	6.680276	3.021244	2.476015
H	5.021418	4.877334	2.417583
H	2.858204	4.534641	1.237317
H	2.356098	2.373791	0.163207
H	4.697936	-0.397257	2.729685
H	6.411427	-1.311357	0.169549
H	8.232458	-1.552429	-1.478827
H	7.957239	-0.661741	-3.785178
H	5.833741	0.476440	-4.404667
H	4.023306	0.725564	-2.725438
H	2.922087	-2.498520	-0.542624
H	2.870238	-4.570948	0.807603
H	3.763367	-4.566863	3.130768
H	4.677407	-2.458208	4.078147
O	-2.634312	-0.092873	0.862529
B	-3.880723	-0.006061	0.044641
C	-4.204623	-1.428815	-0.711234
C	-3.836421	1.285845	-0.970150
C	-5.082356	0.243208	1.140116
C	-5.425205	-1.666623	-1.366337
C	-5.722450	-2.882298	-1.978249
C	-4.797956	-3.924471	-1.943250
C	-3.587751	-3.728956	-1.282844
C	-3.304227	-2.504451	-0.678032
C	-3.319522	2.493829	-0.470483
C	-3.288326	3.659172	-1.228234
C	-3.785796	3.659349	-2.531978
C	-4.297834	2.478567	-3.058224
C	-4.314860	1.314089	-2.286348
C	-4.955502	-0.237872	2.452429
C	-5.970487	-0.092858	3.395255
C	-7.161984	0.545241	3.052197
C	-7.314032	1.040005	1.759505
C	-6.285896	0.892389	0.828414
H	-6.174843	-0.876096	-1.380533
H	-6.680343	-3.021152	-2.476069
H	-5.021520	-4.877275	-2.417680
H	-2.858297	-4.534648	-1.237413
H	-2.356146	-2.373829	-0.163260
H	-2.922022	2.498474	0.542665

H	-4.023330	-0.725646	2.725416
H	-5.833761	-0.476521	4.404651
H	-7.957227	0.661735	3.785191
H	-8.232420	1.552495	1.478865
H	-6.411393	1.311419	-0.169516
H	-4.697941	0.397315	-2.729673
H	-4.677368	2.458291	-4.078096
H	-3.763272	4.566906	-3.130683
H	-2.870129	4.570925	-0.807523
H	1.778275	0.195383	1.715605
H	-0.612986	0.121791	2.382763
H	-1.778278	-0.195432	-1.715607
H	0.612983	-0.121843	-2.382765

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BEt_3-Q-BEt_3

C	-0.939089	-0.825620	0.503500
C	0.341921	-1.164269	0.692990
C	1.446291	-0.304219	0.215070
C	1.119361	0.955031	-0.484360
C	-0.161589	1.291340	-0.677310
C	-1.262849	0.428090	-0.204730
O	-2.415399	0.800740	-0.434180
O	2.598751	-0.676949	0.424510
B	-3.928289	0.083910	-0.075740
C	-3.951499	-1.202990	-1.073020
C	-3.929599	-0.252440	1.515200
C	-4.895859	1.305640	-0.493160
C	-6.369459	0.902550	-0.622880
C	-3.257499	0.778530	2.427400
C	-4.975599	-2.265540	-0.652150
B	4.185701	-0.002259	-0.092680
C	4.193581	1.554321	0.392040
C	4.113001	-0.266349	-1.685410
C	5.125561	-0.988109	0.754830
C	4.018941	-1.728039	-2.130730
C	4.981661	-0.883209	2.276750
C	4.315260	2.621631	-0.704580
H	-1.765879	-1.433520	0.848450
H	0.639261	-2.073189	1.205160
H	1.944161	1.570271	-0.820850
H	-0.460300	2.201630	-1.186100
H	-4.165399	-0.880180	-2.101130
H	-2.962469	-1.686920	-1.118760
H	-3.553229	-1.256150	1.762860
H	-4.996729	-0.298780	1.778540
H	-4.565459	1.721440	-1.455210
H	-4.817700	2.129950	0.230640
H	-7.014579	1.762809	-0.826540
H	-6.512239	0.188560	-1.440670
H	-6.742539	0.427569	0.291920
H	-3.456549	0.589890	3.486380
H	-3.601789	1.792120	2.199250
H	-2.164629	0.781050	2.314190
H	-5.007269	-3.102840	-1.356560
H	-4.738949	-2.675590	0.334940
H	-5.985459	-1.850480	-0.591100
H	5.051461	1.685071	1.064210
H	3.325831	1.778551	1.031580
H	3.293431	0.306821	-2.146870
H	5.026291	0.176351	-2.109680
H	4.967001	-2.032429	0.456160
H	6.164601	-0.757999	0.473130
H	3.937401	-1.825769	-3.217610
H	4.900671	-2.292629	-1.815590
H	3.147981	-2.227319	-1.689770
H	5.657881	-1.560569	2.807210
H	5.188531	0.130131	2.635510
H	3.960901	-1.132799	2.587850
H	4.319650	3.635341	-0.292500
H	3.511370	2.579761	-1.450320
H	5.245670	2.493171	-1.265880

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$[BEt_3$-Q-$BEt_3]^{\bullet-}$

C	-0.967380	-0.330950	0.815730
C	0.344220	-0.480619	1.161200
C	1.411350	-0.218779	0.237440
C	1.057270	0.207051	-1.086110
C	-0.253970	0.355461	-1.432290
C	-1.321740	0.099380	-0.507180
O	-2.523060	0.274850	-0.926100
O	2.613590	-0.391519	0.654600
B	-3.883000	0.058550	-0.136500
C	-4.015100	-1.551150	0.170790
C	-3.893480	1.013010	1.199310
C	-4.973550	0.564220	-1.241540
C	-6.429500	0.230540	-0.905080
C	-3.280180	2.402260	0.995950
C	-4.899150	-1.900880	1.374370
B	3.986440	-0.096379	-0.085030
C	4.069920	1.522221	-0.294690
C	4.079170	-0.940239	-1.489780
C	5.075730	-0.652959	0.994570
C	3.452400	-2.337869	-1.449120
C	5.063910	0.074601	2.341530
C	5.444300	1.970462	-0.801840
H	-1.759790	-0.530960	1.524880
H	0.633720	-0.802719	2.156170
H	1.850960	0.398701	-1.796000
H	-0.543720	0.674091	-2.428210
H	-4.412990	-2.059140	-0.721330

H	-3.025840	-2.004280	0.334070
H	-3.422640	0.552660	2.080860
H	-4.948630	1.133930	1.490880
H	-4.725710	0.102600	-2.209260
H	-4.887210	1.649570	-1.404530
H	-7.139200	0.619539	-1.646070
H	-6.581070	-0.853900	-0.850650
H	-6.722170	0.642870	0.068580
H	-3.423731	3.062200	1.860060
H	-3.715160	2.901050	0.123100
H	-2.200520	2.336490	0.817310
H	-5.020080	-2.982690	1.512110
H	-4.476540	-1.500190	2.302710
H	-5.901440	-1.469490	1.276510
H	3.851110	2.041341	0.650050
H	3.305790	1.874051	-1.004210
H	3.669930	-0.390099	-2.352360
H	5.150210	-1.049008	-1.718250
H	4.900750	-1.725559	1.170230
H	6.084670	-0.591338	0.559630
H	3.644190	-2.919739	-2.358870
H	3.839520	-2.913539	-0.601170
H	2.364520	-2.284649	-1.324320
H	5.737390	-0.373358	3.083160
H	5.360230	1.124002	2.224900
H	4.053770	0.074171	2.765980
H	5.505439	3.051212	-0.979680
H	5.697320	1.468532	-1.743370
H	6.230160	1.711572	-0.082820

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[BEt_3-Q-BEt_3]$^{2-}$

C	-0.960970	-0.284280	0.790800
C	0.378560	-0.441160	1.143780
C	1.427810	-0.296260	0.222130
C	1.056370	0.023690	-1.096090
C	-0.281490	0.184110	-1.448920
C	-1.333010	0.036250	-0.527780
O	-2.585070	0.216580	-0.970880
O	2.682370	-0.504130	0.649650
B	-3.861800	0.048830	-0.165410
C	-4.033190	-1.531790	0.313590
C	-3.925750	1.119820	1.098810
C	-5.025780	0.432400	-1.274370
C	-6.468010	0.121199	-0.866020
C	-3.343160	2.491450	0.745290
C	-4.874520	-1.763960	1.575050
B	3.966250	-0.090070	-0.049550
C	3.975630	1.535760	-0.321130
C	4.224330	-0.938270	-1.452990
C	5.131690	-0.517450	1.039410
C	3.682360	-2.369670	-1.399940
C	5.011370	0.210580	2.379970
C	5.323140	2.064380	-0.823630
H	-1.732700	-0.413940	1.541470
H	0.648300	-0.689230	2.167890
H	1.830540	0.142170	-1.846530
H	-0.552050	0.431030	-2.472940
H	-4.472090	-2.116030	-0.513570
H	-3.042480	-1.978030	0.479720
H	-3.413450	0.759100	2.004160
H	-4.977650	1.245800	1.410720
H	-4.796530	-0.121400	-2.198350
H	-4.957280	1.497700	-1.548790
H	-7.215590	0.417329	-1.618370
H	-6.600110	-0.953781	-0.688740
H	-6.737140	0.629549	0.069550
H	-3.453100	3.236360	1.547890
H	-3.822200	2.902040	-0.151840
H	-2.275770	2.400190	0.518340
H	-5.003380	-2.827380	1.828920
H	-4.412760	-1.279590	2.443860
H	-5.878220	-1.330521	1.478500
H	3.704860	2.070750	0.602770
H	3.199140	1.811040	-1.049850
H	3.799630	-0.434590	-2.337970
H	5.309790	-0.978350	-1.649090
H	5.061350	-1.602000	1.222920
H	6.139080	-0.352660	0.622170
H	3.917730	-2.966590	-2.294430
H	4.087100	-2.903850	-0.531670
H	2.593740	-2.359320	-1.280390
H	5.701300	-0.155200	3.156580
H	5.201040	1.285450	2.259780
H	3.988000	0.108410	2.756460
H	5.322030	3.140540	-1.054470
H	5.631740	1.537440	-1.736140
H	6.114230	1.893380	-0.081710

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[B(C_6F_5)$_3$-Q-$SiPhH_2$]$^+$

C	-2.934375	-0.083789	-2.228885
C	-1.596658	-0.085784	-2.310732
C	-0.763915	0.074339	-1.092655
C	-1.420550	0.270415	0.222852
C	-2.759639	0.294762	0.284276
C	-3.562098	0.103108	-0.921750
O	-4.813214	0.107523	-0.773270
O	0.451916	0.038611	-1.254916
H	-3.561540	-0.218789	-3.103971
H	-1.056637	-0.223026	-3.242504
H	-0.797343	0.384907	1.105572

H	-3.303075	0.433177	1.212720
Si	-6.199494	-0.115341	-1.932267
C	-7.710028	-0.102678	-0.916979
C	-8.224535	-1.304265	-0.400575
C	-9.373710	-1.292786	0.380150
C	-10.018931	-0.086159	0.646067
C	-9.523357	1.111711	0.133248
C	-8.374565	1.106099	-0.647893
H	-5.991614	1.042054	-2.819020
H	-5.837851	-1.404279	-2.546565
H	-7.734254	-2.250977	-0.612728
H	-9.770214	-2.221402	0.775365
H	-10.918886	-0.079947	1.252032
H	-10.036050	2.045121	0.337256
H	-8.001570	2.043175	-1.053390
B	1.686199	0.084503	-0.099400
C	1.368237	-1.074093	0.989184
C	1.586087	1.625746	0.371270
C	2.962676	-0.353274	-0.963495
C	2.217390	-1.101935	2.095519
C	2.184811	-2.091363	3.065315
C	1.268860	-3.130906	2.940329
C	0.407241	-3.152623	1.854143
C	0.483131	-2.140546	0.904931
C	1.974863	2.645432	-0.499037
C	1.943095	3.991844	-0.164359
C	1.484637	4.367842	1.092336
C	1.058010	3.393672	1.984630
C	1.114768	2.057416	1.607985
C	2.886705	-1.494488	-1.757320
C	3.956236	-1.996441	-2.481117
C	5.182528	-1.346709	-2.401856
C	5.312237	-0.215282	-1.607494
C	4.210938	0.258279	-0.903972
F	3.112757	-0.119564	2.237017
F	3.012750	-2.058363	4.099068
F	1.212643	-4.085395	3.855291
F	-0.484878	-4.129829	1.723009
F	-0.405759	-2.232298	-0.117574
F	2.393721	2.339449	-1.730143
F	1.719200	-2.162008	-1.836311
F	3.821494	-3.082801	-3.234467
F	6.221791	-1.806634	-3.080894
F	6.482478	0.404670	-1.525262
F	4.399000	1.345144	-0.151199
F	0.635487	1.173536	2.504633
F	0.590405	3.739355	3.177903
F	1.431864	5.646055	1.427386
F	2.326026	4.916228	-1.034594

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$[B(C_6F_5)_3\text{-}Q\text{-}SiPhH_2]^{\bullet}$

C	-3.005191	-0.160842	-2.093932
C	-1.645288	-0.136901	-2.208226
C	-0.806826	-0.115677	-1.041466
C	-1.420206	-0.138588	0.260007
C	-2.779428	-0.161847	0.361123
C	-3.597804	-0.169441	-0.802815
O	-4.906222	-0.188998	-0.612514
O	0.454072	-0.080889	-1.247614
H	-3.630619	-0.173864	-2.980739
H	-1.147065	-0.130149	-3.170911
H	-0.796077	-0.150910	1.146032
H	-3.277496	-0.182600	1.323782
Si	-6.155580	-0.205000	-1.785886
C	-7.757765	-0.220867	-0.872739
C	-8.364179	-1.433678	-0.514675
C	-9.567163	-1.445565	0.183232
C	-10.181014	-0.243332	0.526972
C	-9.595744	0.970000	0.172733
C	-8.392753	0.980351	-0.525190
H	-5.983422	1.018057	-2.598808
H	-5.955484	-1.424613	-2.597132
H	-7.896049	-2.377213	-0.784192
H	-10.027492	-2.389372	0.455738
H	-11.121049	-0.252114	1.069201
H	-10.078214	1.905034	0.437100
H	-7.947072	1.932298	-0.803074
B	1.570130	0.060200	-0.173468
C	1.589959	-1.225329	0.831022
C	1.279777	1.511528	0.520364
C	2.950968	-0.022416	-1.029252
C	2.500509	-1.198058	1.885181
C	2.715801	-2.262965	2.744405
C	2.005013	-3.441351	2.548552
C	1.099431	-3.524397	1.503832
C	0.917489	-2.428657	0.665053
C	1.398728	2.662887	-0.256458
C	1.154452	3.942524	0.218755
C	0.755308	4.110231	1.538147
C	0.603240	2.996799	2.348461
C	0.864328	1.733950	1.827524
C	3.113521	-1.073806	-1.928131
C	4.265363	-1.274303	-2.675165
C	5.332487	-0.401377	-2.515925
C	5.226845	0.647266	-1.615166
C	4.052164	0.814269	-0.889824
F	3.214111	-0.083432	2.094333
F	3.592245	-2.175133	3.742851
F	2.192158	-4.478928	3.359381
F	0.412680	-4.649783	1.304843
F	0.024601	-2.593456	-0.327782

F	1.775525	2.560087	-1.537158
F	2.125882	-1.969268	-2.089362
F	4.360673	-2.294747	-3.528068
F	6.449305	-0.573648	-3.218224
F	6.250430	1.484554	-1.451145
F	4.031445	1.843826	-0.034679
F	0.637984	0.704193	2.663755
F	0.195440	3.140037	3.609049
F	0.505288	5.326417	2.013331
F	1.291411	5.004956	-0.572750

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$[B(C_6F_5)_3\text{-Q-SiPhH}_2]^-$

C	-3.003047	-0.351191	-2.184080
C	-1.625896	-0.217952	-2.282647
C	-0.803371	-0.321168	-1.149766
C	-1.407100	-0.570473	0.092676
C	-2.789567	-0.701037	0.189368
C	-3.587511	-0.592945	-0.943149
O	-4.967299	-0.747539	-0.844183
O	0.512756	-0.186029	-1.342836
H	-3.637611	-0.276385	-3.062178
H	-1.146659	-0.029872	-3.237252
H	-0.798297	-0.672298	0.983800
H	-3.258486	-0.901856	1.148096
Si	-5.889333	0.591327	-0.515353
C	-7.652817	-0.031361	-0.484946
C	-8.724517	0.825895	-0.203079
C	-10.034079	0.356054	-0.185646
C	-10.292265	-0.987306	-0.450945
C	-9.239722	-1.853750	-0.731787
C	-7.930026	-1.378482	-0.748542
H	-5.528897	1.195087	0.791352
H	-5.720519	1.629205	-1.563542
H	-8.538444	1.877609	0.007994
H	-10.852734	1.034391	0.035042
H	-11.313194	-1.357091	-0.437428
H	-9.438430	-2.901222	-0.937475
H	-7.107176	-2.053769	-0.966023
B	1.495680	0.026187	-0.264844
C	1.758392	-1.303300	0.678699
C	1.027484	1.366239	0.582437
C	2.942924	0.231124	-1.032597
C	2.653977	-1.212240	1.740246
C	3.042058	-2.287994	2.522328
C	2.532291	-3.546717	2.232726
C	1.652111	-3.695316	1.174801
C	1.289664	-2.584544	0.414966
C	0.969393	2.583171	-0.093497
C	0.518094	3.765027	0.474823
C	0.081928	3.760497	1.791878
C	0.107175	2.575975	2.506609
C	0.572692	1.417132	1.892664
C	3.315971	-0.709267	-1.991886
C	4.515802	-0.662377	-2.690354
C	5.419076	0.354572	-2.421389
C	5.106403	1.297550	-1.456945
C	3.892270	1.214750	-0.782200
F	3.188417	-0.017633	2.044556
F	3.900673	-2.137012	3.537633
F	2.891424	-4.603930	2.968318
F	1.164744	-4.907951	0.887422
F	0.446321	-2.824674	-0.594926
F	1.390111	2.661804	-1.363406
F	2.517798	-1.749296	-2.265494
F	4.818218	-1.591555	-3.605068
F	6.581727	0.417557	-3.078684
F	5.976862	2.276299	-1.181734
F	3.686973	2.163107	0.143679
F	0.522357	0.308550	2.654513
F	-0.324552	2.554428	3.773097
F	-0.360993	4.885859	2.360575
F	0.500177	4.905763	-0.223999

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$[B(C_6F_5)_3\text{-Q-SiEt}_3]^+$

C	-2.900600	0.190591	-2.566000
C	-1.565430	0.267261	-2.473270
C	-0.902950	0.198840	-1.155280
C	-1.727130	0.097131	0.068160
C	-3.065040	0.041191	-0.037580
C	-3.700980	0.059451	-1.351350
O	-4.947960	-0.040239	-1.499230
O	0.328530	0.229740	-1.170480
B	1.609930	0.110080	-0.175270
C	2.020990	1.670710	-0.184790
C	2.562240	-0.932430	-0.953920
C	1.201620	-0.519390	1.251750
C	3.188471	2.220640	-0.710700
C	3.463561	3.582780	-0.646270
C	2.543021	4.450700	-0.069300
C	3.831440	-1.124040	-0.413840
C	4.742140	-2.041970	-0.909250
C	4.374930	-2.833370	-1.993010
C	1.707960	-0.072340	2.469030
C	1.468890	-0.737230	3.669040
C	0.696350	-1.890730	3.673700
C	3.112610	-2.691810	-2.549730
C	2.229560	-1.756590	-2.020670
C	0.168260	-2.372790	2.479750
C	0.449420	-1.689140	1.309150
C	1.351041	3.949890	0.441280

C	1.124821	2.587670	0.365080
F	-0.054069	2.134880	0.850120
F	0.449631	4.766450	0.975810
F	2.794721	5.746560	-0.015750
F	4.593841	4.062720	-1.141780
F	4.105530	1.462020	-1.305190
F	-0.097650	-2.159130	0.164800
F	-0.591800	-3.463600	2.473380
F	0.448290	-2.523470	4.809150
F	1.967310	-0.273870	4.806080
F	2.457180	1.027280	2.531090
F	4.193830	-0.379430	0.639610
F	5.943600	-2.176460	-0.363990
F	5.224040	-3.721910	-2.485800
F	2.746490	-3.453740	-3.575580
F	1.012680	-1.701200	-2.599130
H	-3.433330	0.203771	-3.510380
H	-0.908990	0.336490	-3.334680
H	-1.220800	0.103420	1.024930
H	-3.697890	-0.016179	0.841730
Si	-6.350670	-0.288859	-0.348130
C	-6.050860	-1.977859	0.382890
C	-6.229570	1.134951	0.863320
C	-7.765490	-0.193559	-1.545530
C	-7.980630	1.193681	-2.170270
C	-5.605579	2.431321	0.320270
C	-7.163820	-2.317199	1.394440
H	-5.073220	-2.022109	0.877430
H	-6.030030	-2.723229	-0.419840
H	-7.263050	1.334601	1.177450
H	-5.712330	0.809511	1.774460
H	-8.670720	-0.509589	-1.011450
H	-7.601790	-0.948899	-2.323510
H	-7.087960	1.539761	-2.700130
H	-8.234099	1.938231	-1.410510
H	-8.800290	1.169591	-2.890550
H	-4.543529	2.307661	0.082880
H	-6.108619	2.776971	-0.586000
H	-5.672779	3.229461	1.061640
H	-8.147750	-2.338169	0.917910
H	-7.200890	-1.593969	2.214570
H	-6.994920	-3.301819	1.833830

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$[B(C_6F_5)_3\text{-Q-SiEt}_3]^{\cdot}$

C	-2.796530	0.041840	-2.759900
C	-1.437310	0.083870	-2.696120
C	-0.760020	-0.010290	-1.432290
C	-1.540760	-0.161920	-0.234150
C	-2.903910	-0.204930	-0.310850
C	-3.563400	-0.105340	-1.568820
O	-4.872750	-0.141239	-1.698500
O	0.517570	0.045880	-1.456760
B	1.469510	0.087649	-0.230320
C	1.066580	1.469939	0.545850
C	2.958540	0.082139	-0.885770
C	1.367720	-1.283391	0.650090
C	1.280891	2.687879	-0.097860
C	0.949941	3.918529	0.449130
C	0.357821	3.964730	1.704260
C	4.017890	0.906449	-0.524850
C	5.284010	0.803899	-1.090650
C	5.528710	-0.165011	-2.051670
C	2.119600	-1.349641	1.821250
C	2.226490	-2.487031	2.604680
C	1.567209	-3.644121	2.206550
C	4.506530	-1.023971	-2.430220
C	3.259390	-0.889421	-1.837340
C	0.819689	-3.634401	1.040720
C	0.742990	-2.468401	0.284460
C	0.105601	2.781730	2.379600
C	0.460920	1.572280	1.792100
F	0.130270	0.470280	2.491390
F	-0.487219	2.808470	3.573410
F	0.021291	5.131960	2.244830
F	1.185911	5.048849	-0.214500
F	1.843661	2.703769	-1.312190
F	0.001480	-2.545710	-0.835180
F	0.182379	-4.738280	0.648510
F	1.651449	-4.749761	2.941330
F	2.950970	-2.487751	3.721890
F	2.779880	-0.257281	2.228890
F	3.864501	1.860199	0.401950
F	6.263200	1.626648	-0.716300
F	6.734860	-0.274602	-2.602470
F	4.733690	-1.969271	-3.342680
F	2.316500	-1.770291	-2.208430
H	-3.331850	0.112750	-3.699750
H	-0.818740	0.190140	-3.579900
H	-1.039220	-0.254230	0.722080
H	-3.493820	-0.313770	0.593430
Si	-6.116580	-0.453649	-0.529410
C	-5.872170	-2.189969	0.128870
C	-6.005140	0.858431	0.813090
C	-7.662590	-0.302759	-1.564680
C	-7.939710	1.117871	-2.075490
C	-5.424059	2.204531	0.351900
C	-6.892310	-2.519859	1.231120
H	-4.853110	-2.311859	0.514110
H	-5.969570	-2.898349	-0.701900
H	-7.025760	1.005481	1.191340
H	-5.433210	0.473631	1.666850

H	-8.511930	-0.661399	-0.969600
H	-7.568070	-0.998959	-2.406670
H	-7.094570	1.502491	-2.654150
H	-8.119199	1.808771	-1.246180
H	-8.821660	1.143581	-2.720090
H	-4.379509	2.105031	0.042490
H	-5.977239	2.613301	-0.497740
H	-5.457059	2.942591	1.156600
H	-7.919810	-2.450439	0.860980
H	-6.799760	-1.835799	2.080400
H	-6.751001	-3.534259	1.610870

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$[B(C_6F_5)_3\text{-Q-SiEt}_3]^-$

C	2.876570	0.529671	-2.533970
C	1.549031	0.122700	-2.492950
C	0.696660	0.539440	-1.460980
C	1.206150	1.413530	-0.486950
C	2.537860	1.814130	-0.527270
C	3.382470	1.359491	-1.535070
O	4.722530	1.709121	-1.518250
O	-0.559179	0.074540	-1.473230
Si	5.802930	0.606741	-0.853080
C	7.392430	1.596992	-0.610780
C	5.167791	-0.088399	0.779660
C	6.105041	-0.814879	-2.051850
C	7.190551	-1.775658	-1.548210
C	4.090131	-1.179069	0.668210
C	8.249970	1.171132	0.588190
B	-1.386389	-0.052090	-0.257450
C	-0.455309	-0.796410	0.886450
C	-2.693549	-0.948781	-0.711350
C	-2.052250	1.370599	0.248240
C	0.035741	-2.068890	0.600740
C	0.945361	-2.745240	1.399640
C	1.407291	-2.138680	2.558400
C	-3.225549	-2.046861	-0.046970
C	-4.352179	-2.735121	-0.486290
C	-5.005579	-2.316361	-1.633130
C	-2.848470	1.379939	1.389320
C	-3.548480	2.488889	1.836140
C	-3.476350	3.667179	1.104630
C	-4.526699	-1.210901	-2.319820
C	-3.399659	-0.551831	-1.845560
C	-2.708170	3.706769	-0.046270
C	-2.020240	2.566519	-0.457800
C	0.959521	-0.872060	2.886100
C	0.043611	-0.235780	2.053350
F	-0.298990	1.010000	2.428720
F	1.423701	-0.266660	3.985420
F	2.319861	-2.751070	3.321410
F	1.390771	-3.962120	1.068040
F	-0.374469	-2.708770	-0.502800
F	-1.306270	2.692700	-1.581750
F	-2.639891	4.839949	-0.754850
F	-4.143410	4.752639	1.510640
F	-4.292270	2.442679	2.947800
F	-2.954849	0.257859	2.120730
F	-2.668719	-2.517291	1.078750
F	-4.813409	-3.795401	0.188000
F	-6.090279	-2.965201	-2.069390
F	-5.163739	-0.786801	-3.417930
F	-3.020770	0.535609	-2.529560
H	3.536581	0.199541	-3.331160
H	1.140741	-0.541060	-3.247510
H	0.564630	1.764080	0.314480
H	2.940550	2.473161	0.236260
H	7.103600	2.649172	-0.508250
H	7.981260	1.535342	-1.534980
H	6.038471	-0.491779	1.315880
H	4.798650	0.740841	1.397000
H	5.164881	-1.355969	-2.210200
H	6.388531	-0.397319	-3.026030
H	7.345641	-2.616348	-2.231240
H	6.927571	-2.193789	-0.570060
H	8.152501	-1.263138	-1.436610
H	3.153801	-0.783069	0.261020
H	4.414521	-1.994389	0.012100
H	3.871341	-1.619839	1.645460
H	8.529901	0.113602	0.533180
H	7.707700	1.310592	1.528090
H	9.175640	1.751702	0.652630

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$[B(C_6F_5)_3\text{-Q-Si}(C_6Me_5)_3]^+$

C	-0.78036	0.24290	0.02108
C	0.54842	0.35023	0.17752
C	1.43589	0.25958	-1.00109
C	0.85037	0.18912	-2.35049
C	-0.47261	0.07551	-2.50684
C	-1.35920	0.07896	-1.32569
O	-2.56756	-0.03919	-1.54511
O	2.68225	0.22793	-0.95440
B	-3.80932	-0.01209	-0.46984
C	-5.09630	0.00680	-1.43600
C	-3.56355	-1.37249	0.37907
C	-3.75923	1.39669	0.33596
C	-4.71120	1.55610	1.34230
C	-4.89444	2.73393	2.04867
C	-4.10449	3.83638	1.74033
C	-3.15134	3.73260	0.73927
C	-3.00832	2.53045	0.05606

C	-3.26363	-1.45093	1.73565	C	1.95163	0.75077	5.02840
C	-3.15159	-2.65313	2.42093	C	4.23421	0.97615	3.24488
C	-3.28571	-3.84986	1.73440	C	2.62331	2.82374	0.50003
C	-3.55415	-3.82768	0.37177	C	3.80210	5.27254	-0.48709
C	-3.68109	-2.60294	-0.26814	C	6.68612	5.44001	-0.85530
C	-6.22909	-0.78634	-1.29165	C	8.33578	3.06027	-0.60969
C	-7.33897	-0.66968	-2.12060	C	7.19251	0.59348	0.34691
C	-7.33894	0.27613	-3.13644	C	6.53264	-4.79117	-0.40402
C	-6.23256	1.09868	-3.31000	H	-1.45541	0.30665	0.86927
C	-5.15018	0.95253	-2.45676	H	0.98040	0.50017	1.15786
F	-3.11947	-5.00006	2.36994	H	1.54921	0.19131	-3.17962
F	-3.01079	-0.33979	2.45247	H	-0.95738	-0.01197	-3.47347
F	-3.66999	-4.96465	-0.30278	H	7.70993	-4.85801	-2.64702
F	-3.93798	-2.62988	-1.57969	H	6.28001	-5.02366	-3.66615
F	-5.49188	0.51587	1.65587	H	7.52349	-3.83767	-4.06327
F	-5.80952	2.82100	3.00496	H	5.41172	-1.77236	1.84626
F	-4.25539	4.97324	2.40394	H	4.67712	-3.34567	1.59285
F	-2.38032	4.77388	0.43595	H	6.43281	-3.17325	1.60427
F	-2.05246	2.51377	-0.90315	H	5.84298	-2.83585	-5.01589
F	-4.10636	1.78272	-2.63847	H	5.21135	-1.20452	-4.88643
F	-6.22296	2.01228	-4.27590	H	6.94418	-1.48639	-4.74586
F	-8.38842	0.39595	-3.93658	H	5.68423	0.55660	-3.52081
F	-8.39565	-1.45540	-1.94779	H	3.98838	0.10410	-3.54970
F	-6.29562	-1.71330	-0.33015	H	4.64395	1.03886	-2.19923
F	-2.82625	-2.66948	3.71466	H	2.88643	-2.33239	-0.50799
Si	4.11538	-0.04896	0.22906	H	2.25966	-3.62136	0.49463
C	4.87296	1.66497	0.21104	H	1.13825	-2.52197	-0.27492
C	5.05114	-1.28792	-0.81613	H	-0.50016	-2.71762	1.26194
C	3.10414	-0.68163	1.67350	H	0.56461	-3.94992	1.92507
C	2.14557	-1.70043	1.46286	H	-0.58614	-3.12473	2.97422
C	1.13855	-1.92158	2.41806	H	-0.10271	-2.37163	4.87322
C	1.06012	-1.11112	3.56521	H	0.04264	-0.71972	5.44489
C	2.03743	-0.12474	3.79765	H	-1.03574	-1.09918	4.10081
C	3.09474	0.04408	2.88476	H	0.93727	1.12989	5.16715
C	5.52885	-2.47922	-0.22190	H	2.21969	0.19690	5.93467
C	6.09854	-3.47999	-1.02005	H	2.60807	1.61633	4.96225
C	6.26945	-3.26494	-2.39817	H	4.50229	0.84760	4.29563
C	5.81029	-2.08023	-2.99237	H	5.13231	0.76676	2.66267
C	5.22202	-1.07694	-2.20322	H	3.98864	2.03368	3.09235
C	6.27183	1.75630	0.03823	H	2.38847	3.71108	1.09265
C	6.84886	2.97368	-0.35266	H	1.93261	2.83181	-0.35527
C	6.04651	4.11695	-0.50668	H	2.39929	1.96429	1.13329
C	4.66120	4.04321	-0.29478	H	4.15307	5.86522	-1.33349
C	4.08038	2.82876	0.09956	H	2.76137	5.01694	-0.68669
C	6.98292	-4.29952	-3.23677	H	3.81942	5.92234	0.39597
C	5.50479	-2.69881	1.27788	H	7.69203	5.51575	-0.44129
C	5.95804	-1.88951	-4.48558	H	6.76650	5.57125	-1.94110
C	4.85569	0.22459	-2.88946	H	6.11101	6.27920	-0.46436
C	2.11586	-2.57033	0.22274	H	8.75298	2.09528	-0.89718
C	0.10210	-2.98315	2.14379	H	8.55306	3.75920	-1.41869
C	-0.06459	-1.32794	4.55033	H	8.88046	3.40593	0.27717

H	6.71618	-0.15679	0.98192
H	7.54294	0.07817	-0.55402
H	8.06884	0.94887	0.89399
H	5.95265	-5.02935	0.48775
H	6.39696	-5.61683	-1.10375
H	7.59056	-4.77575	-0.11552

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$[B(C_6F_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^{\bullet}$

C	-0.80448	0.29053	-0.05713
C	0.54947	0.40289	0.08513
C	1.41589	0.19743	-1.03592
C	0.84517	-0.07774	-2.31534
C	-0.50405	-0.17344	-2.46687
C	-1.37800	0.00420	-1.34145
O	-2.63594	-0.08689	-1.57023
O	2.72387	0.26243	-0.98592
B	-3.77278	-0.01050	-0.53104
C	-5.13456	-0.08192	-1.42486
C	-3.54699	-1.31077	0.43887
C	-3.82069	1.44108	0.21678
C	-4.76953	1.61564	1.22198
C	-5.00540	2.82287	1.85909
C	-4.27883	3.94224	1.47150
C	-3.33887	3.82637	0.46093
C	-3.13691	2.59281	-0.15134
C	-3.25526	-1.30541	1.79785
C	-3.13306	-2.46299	2.55627
C	-3.24514	-3.70027	1.94503
C	-3.50397	-3.76252	0.58344
C	-3.64327	-2.58012	-0.12972
C	-6.25181	-0.86695	-1.16466
C	-7.40173	-0.83277	-1.94611
C	-7.46623	0.02529	-3.03287
C	-6.38321	0.84420	-3.31962
C	-5.25693	0.78085	-2.51171
F	-3.06823	-4.81197	2.65356
F	-3.02895	-0.15344	2.45648
F	-3.60799	-4.94464	-0.02110
F	-3.90924	-2.69930	-1.43590
F	-5.50607	0.56390	1.60776
F	-5.91787	2.92556	2.82415
F	-4.48497	5.11418	2.06698
F	-2.63884	4.89497	0.07726
F	-2.21645	2.57152	-1.13050
F	-4.25621	1.62507	-2.80752
F	-6.43974	1.68577	-4.35259
F	-8.55938	0.06890	-3.79070
F	-8.44130	-1.61580	-1.65785
F	-6.27494	-1.71395	-0.12701
F	-2.82000	-2.39942	3.85498
Si	4.03925	-0.02844	0.12327
C	4.94685	1.63289	0.15017
C	5.04223	-1.31233	-0.83837
C	3.10982	-0.61317	1.65549
C	2.14203	-1.63079	1.50628
C	1.15243	-1.81402	2.48629
C	1.09847	-0.96230	3.60160
C	2.08712	0.02241	3.77944
C	3.12675	0.15177	2.84217
C	5.51696	-2.49355	-0.22621
C	6.12861	-3.49352	-0.99628
C	6.33965	-3.29192	-2.36890
C	5.87805	-2.12138	-2.98527
C	5.25312	-1.11962	-2.22132
C	6.35551	1.66047	0.06615
C	7.01923	2.85023	-0.27078
C	6.29011	4.03437	-0.45623
C	4.89345	4.02666	-0.33078
C	4.22893	2.83840	0.00869
C	7.09653	-4.32340	-3.17563
C	5.44073	-2.71248	1.27187
C	6.04877	-1.94129	-4.47806
C	4.88132	0.16637	-2.93432
C	2.08177	-2.53542	0.29371
C	0.09978	-2.87132	2.25936
C	-0.02077	-1.12205	4.60495
C	2.02195	0.95124	4.97333
C	4.27908	1.08672	3.15338
C	2.74678	2.89947	0.30285
C	4.10500	5.29563	-0.56929
C	7.01484	5.32964	-0.74485
C	8.52222	2.85638	-0.44445
C	7.19880	0.45048	0.41325
C	6.55607	-4.79397	-0.35120
H	-1.45666	0.44736	0.79512
H	0.96632	0.63559	1.05633
H	1.52691	-0.21745	-3.14656
H	-0.96717	-0.38372	-3.42411
H	7.81731	-4.86049	-2.55802
H	6.42352	-5.06738	-3.61934
H	7.65384	-3.85896	-3.99010
H	5.29404	-1.78857	1.82983
H	4.61586	-3.37906	1.55197
H	6.36597	-3.16578	1.63660
H	6.01126	-2.89894	-4.99925
H	5.26153	-1.31580	-4.89961
H	7.00758	-1.46887	-4.72585
H	5.70115	0.48167	-3.58562
H	3.99716	0.03585	-3.56892
H	4.67747	0.99343	-2.25784
H	2.83760	-2.31562	-0.45848

H	2.22425	-3.58036	0.59101
H	1.09862	-2.48191	-0.18891
H	-0.51149	-2.61775	1.38163
H	0.54812	-3.84880	2.05767
H	-0.57709	-2.98310	3.10419
H	-0.09473	-2.15683	4.94936
H	0.11989	-0.50013	5.48623
H	-0.98821	-0.86645	4.16117
H	1.00926	1.33580	5.11130
H	2.30720	0.44282	5.90143
H	2.67460	1.81445	4.85386
H	4.54613	1.01240	4.20998
H	5.16993	0.83096	2.58004
H	4.05065	2.13792	2.94066
H	2.50136	3.81771	0.84171
H	2.12566	2.87450	-0.60013
H	2.44654	2.07239	0.94748
H	4.56093	5.89896	-1.35627
H	3.08313	5.08067	-0.88285
H	4.04903	5.91959	0.33131
H	8.00340	5.34346	-0.28391
H	7.15174	5.48558	-1.82200
H	6.46593	6.18839	-0.35687
H	8.89484	1.87640	-0.74412
H	8.82592	3.56505	-1.21673
H	9.04074	3.13727	0.48081
H	6.64976	-0.27025	1.02094
H	7.55880	-0.08551	-0.47215
H	8.06884	0.75683	0.99968
H	5.92645	-5.04159	0.50408
H	6.48297	-5.62565	-1.05345
H	7.59293	-4.75465	0.00560

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$[B(C_6F_5)_3\text{-}Q\text{-}Si(C_6Me_5)_3]^-$

C	0.81866	0.59161	-0.02501
C	-0.54881	0.85057	0.06177
C	-1.42705	0.34324	-0.88992
C	-0.92873	-0.41986	-1.94595
C	0.43275	-0.66085	-2.04736
C	1.33350	-0.15475	-1.09668
O	2.62825	-0.43936	-1.28430
O	-2.77660	0.59301	-0.80474
B	3.73349	0.13431	-0.50270
C	3.79702	-0.42066	1.05347
C	5.11050	-0.49348	-1.16759
C	3.66141	1.78026	-0.63609
C	3.36718	2.69548	0.36491
C	3.24246	4.06460	0.15172
C	3.41439	4.57160	-1.12446
C	3.70182	3.70022	-2.16493
C	3.81175	2.34280	-1.90169
C	6.27467	0.19521	-1.48870
C	7.40603	-0.41650	-2.01977
C	7.40790	-1.78439	-2.23403
C	6.28025	-2.52094	-1.90563
C	5.17283	-1.87082	-1.37582
C	4.77597	0.07031	1.91313
C	5.01577	-0.42865	3.18364
C	4.26333	-1.50406	3.63632
C	3.29969	-2.05193	2.80731
C	3.08152	-1.50629	1.54389
F	8.48679	-2.38897	-2.74173
F	6.37610	1.51961	-1.30293
F	6.27964	-3.84693	-2.08727
F	4.14373	-2.65584	-1.03120
F	3.13957	2.29169	1.62908
F	2.94863	4.89147	1.16199
F	3.30027	5.88320	-1.35357
F	3.87236	4.18036	-3.40188
F	4.10851	1.56089	-2.94879
F	2.12942	-2.10720	0.81380
F	2.58760	-3.10410	3.23205
F	4.47890	-2.01405	4.85302
F	5.96312	0.09527	3.96950
F	5.55914	1.08167	1.50459
F	8.49393	0.30192	-2.32200
Si	-4.00133	-0.17184	0.04460
C	-5.33779	1.18620	-0.06101
C	-3.33262	-0.52852	1.79306
C	-4.47628	-1.68277	-1.01705
C	-4.69146	-2.96581	-0.47169
C	-4.79968	-4.08816	-1.30672
C	-4.76630	-3.93064	-2.69992
C	-4.58047	-2.65820	-3.25577
C	-4.47007	-1.53109	-2.42159
C	-2.11020	-1.22669	1.93977
C	-1.40843	-1.17898	3.15790
C	-1.94051	-0.47869	4.24862
C	-3.17679	0.17107	4.13193
C	-3.89343	0.10345	2.92742
C	-6.66842	0.90134	-0.42758
C	-7.53938	1.93346	-0.81205
C	-7.10935	3.26672	-0.76511
C	-5.79923	3.56588	-0.36576
C	-4.92750	2.53436	0.02051
C	-1.19802	-0.46227	5.56625
C	-1.55304	-2.12031	0.84987
C	-3.72791	0.95892	5.30166
C	-5.30628	0.65492	2.92261
C	-4.86119	-3.17431	1.01978
C	-4.93040	-5.47120	-0.70536

C	-4.96843	-5.12924	-3.60141
C	-4.48155	-2.49784	-4.75770
C	-4.42174	-0.16882	-3.08972
C	-3.57834	2.91618	0.59603
C	-5.31713	5.00078	-0.36966
C	-8.07117	4.38554	-1.10246
C	-8.93577	1.60559	-1.29682
C	-7.22543	-0.50639	-0.35453
C	-0.07053	-1.86572	3.29756
H	1.47897	0.96453	0.74939
H	-0.94367	1.41884	0.89857
H	-1.62356	-0.84669	-2.66335
H	0.83973	-1.25218	-2.86061
H	-0.58596	-1.35636	5.68849
H	-0.52757	0.40309	5.64008
H	-1.88554	-0.41863	6.41306
H	-2.19258	-2.16294	-0.03138
H	-0.55825	-1.80875	0.51783
H	-1.46174	-3.14396	1.23378
H	-2.92201	1.40250	5.88911
H	-4.36673	1.77715	4.96580
H	-4.32320	0.33464	5.98098
H	-5.78034	0.47501	3.89088
H	-5.34869	1.73297	2.72545
H	-5.92582	0.17097	2.16801
H	-5.13202	-2.25517	1.53859
H	-5.65000	-3.90584	1.21604
H	-3.94244	-3.53969	1.49460
H	-4.44625	-5.52643	0.27049
H	-5.97895	-5.76637	-0.56842
H	-4.45826	-6.22419	-1.33882
H	-5.60529	-5.87908	-3.12920
H	-5.44815	-4.84454	-4.53920
H	-4.01792	-5.61625	-3.85303
H	-4.03073	-3.37718	-5.22115
H	-5.46431	-2.34657	-5.22306
H	-3.86170	-1.64099	-5.02417
H	-5.14524	-0.13523	-3.91013
H	-4.66335	0.64355	-2.40829
H	-3.43492	0.05522	-3.50927
H	-3.67017	3.81801	1.20769
H	-3.18126	2.12993	1.23971
H	-2.83134	3.10193	-0.18266
H	-5.79387	5.57573	-1.16592
H	-5.53013	5.51192	0.57812
H	-4.24056	5.05530	-0.53428
H	-9.10056	4.11090	-0.86613
H	-7.84194	5.28981	-0.53637
H	-8.03713	4.64836	-2.16742
H	-8.97465	0.61635	-1.75513
H	-9.67175	1.61816	-0.48228
H	-9.27083	2.32068	-2.05056
H	-6.64366	-1.13777	0.31740
H	-8.24991	-0.49001	0.02756
H	-7.23602	-1.00883	-1.32911
H	0.38062	-2.09106	2.33404
H	0.63728	-1.23476	3.84267
H	-0.14871	-2.81066	3.84969

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$B(C_6F_5)_3$-Q-$B(C_6F_5)_2Ph$

C	-0.699266	-0.347938	0.848052
C	0.602770	-0.461724	1.130761
C	1.631629	-0.236222	0.096029
C	1.226988	0.181504	-1.261412
C	-0.075206	0.298377	-1.543063
C	-1.099638	0.050339	-0.515821
O	-2.277374	0.218654	-0.860922
B	-3.622837	0.069825	0.029964
C	-3.719804	-1.446541	0.604675
C	-3.467177	1.268698	1.113151
C	-4.797376	0.245073	-1.064766
C	-4.789259	-1.716148	1.456893
C	-5.088764	-2.980214	1.937350
C	-4.299033	-4.055826	1.546297
C	-3.230414	-3.841629	0.690458
C	-2.970621	-2.554256	0.232376
C	-3.266106	1.109907	2.480194
C	-3.144929	2.173184	3.367248
C	-3.221058	3.470878	2.884885
C	-3.402636	3.685004	1.524307
C	-3.514055	2.592758	0.677538
C	-5.937746	1.024872	-0.908776
C	-6.950152	1.076774	-1.860114
C	-6.843143	0.318574	-3.016947
C	-5.729138	-0.488167	-3.207614
C	-4.745369	-0.514497	-2.230634
F	-5.574906	-0.703141	1.842115
F	-6.117030	-3.175797	2.755989
F	-4.564757	-5.276946	1.993147
F	-2.463501	-4.860495	0.309761
F	-1.911228	-2.428631	-0.595578
F	-3.125824	-0.116972	3.014913
F	-6.111689	1.773458	0.185252
F	-8.019449	1.844925	-1.669329
F	-7.801906	0.360283	-3.934802
F	-5.621088	-1.228854	-4.308538
F	-3.699802	-1.333675	-2.437626
F	-3.677420	2.851968	-0.624971
F	-3.461538	4.925079	1.049772
F	-3.103610	4.499776	3.712976
F	-2.944621	1.953564	4.663632

O	2.803481	-0.423709	0.438248
B	4.167879	-0.387446	-0.485518
C	4.474389	1.164686	-0.857718
C	3.820003	-1.357127	-1.723195
C	5.261373	-0.925557	0.572750
C	5.687073	1.408851	-1.502592
C	6.136865	2.675856	-1.843820
C	5.357962	3.779946	-1.520287
C	4.148437	3.591655	-0.869910
C	3.739526	2.302095	-0.549399
C	3.247407	-2.614047	-1.472056
C	2.878418	-3.468580	-2.505447
C	3.081887	-3.084593	-3.829272
C	3.659090	-1.848918	-4.103735
C	4.022187	-0.998219	-3.060641
C	5.336816	-0.353084	1.840487
C	6.267335	-0.730387	2.796605
C	7.193508	-1.715802	2.478838
C	7.173389	-2.297458	1.219903
C	6.219739	-1.893767	0.290313
F	6.472628	0.373044	-1.824625
F	7.298934	2.843460	-2.466470
F	5.765506	5.002855	-1.836450
F	3.389702	4.638212	-0.554455
F	2.548912	2.211931	0.084960
F	4.477005	0.623638	2.176025
F	6.287988	-0.158341	3.999214
F	8.097446	-2.094072	3.375788
F	8.067921	-3.233125	0.910163
F	6.272237	-2.477894	-0.907587
H	-1.470789	-0.541204	1.585495
H	0.970657	-0.745843	2.110750
H	2.004309	0.364575	-1.993317
H	-0.443855	0.593608	-2.519071
H	3.099942	-2.937666	-0.442440
H	2.439090	-4.435388	-2.280458
H	2.796860	-3.747311	-4.639899
H	3.828310	-1.544524	-5.131924
H	4.466822	-0.035948	-3.300780

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$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_2Ph]^{\bullet-}$

C	0.602938	-0.070172	-1.146490
C	-0.677035	-0.057591	-1.614124
C	-1.800522	-0.011122	-0.725574
C	-1.562609	0.018976	0.686997
C	-0.281810	0.008560	1.153884
C	0.839892	-0.026657	0.265060
O	2.012367	-0.020351	0.811626
B	3.344690	0.095260	0.084507
C	3.661516	-1.210192	-0.851876
C	3.299689	1.533166	-0.703475
C	4.468878	0.030913	1.273381
C	4.831656	-1.203256	-1.607057
C	5.280242	-2.286196	-2.344762
C	4.543864	-3.464020	-2.326721
C	3.382608	-3.529094	-1.575522
C	2.969558	-2.414641	-0.849190
C	3.272351	1.728683	-2.078191
C	3.187911	2.981016	-2.677489
C	3.123217	4.112293	-1.881556
C	3.135184	3.972736	-0.500701
C	3.215974	2.702651	0.049878
C	5.577839	0.858511	1.405133
C	6.522513	0.709996	2.415075
C	6.382692	-0.313257	3.338636
C	5.304390	-1.179504	3.235151
C	4.386319	-0.997837	2.209553
F	5.583060	-0.091807	-1.632379
F	6.406246	-2.218462	-3.058873
F	4.955309	-4.522477	-3.025676
F	2.674261	-4.659709	-1.546913
F	1.842863	-2.566819	-0.138615
F	3.284594	0.683500	-2.925571
F	5.798463	1.864815	0.548786
F	7.564221	1.541474	2.501460
F	7.280686	-0.469521	4.312611
F	5.170817	-2.181051	4.108494
F	3.393729	-1.895419	2.131546
F	3.233411	2.632087	1.387348
F	3.072146	5.055907	0.275621
F	3.042466	5.321653	-2.434788
F	3.158733	3.099372	-4.006877
O	-2.969261	0.005847	-1.271416
B	-4.321559	-0.064815	-0.553221
C	-4.556245	1.259115	0.392178
C	-4.351416	-1.509376	0.232247
C	-5.439887	0.024762	-1.719611
C	-5.664861	1.311007	1.234623
C	-6.028754	2.429055	1.967986
C	-5.271365	3.587422	1.857961
C	-4.170418	3.597202	1.018910
C	-3.843046	2.449198	0.302524
C	-4.386586	-2.675628	-0.533688
C	-4.438472	-3.953137	0.009985
C	-4.438449	-4.106486	1.388319
C	-4.374847	-2.981852	2.194890
C	-4.327666	-1.723401	1.606220
C	-5.199971	0.807951	-2.855770
C	-6.161713	0.965477	-3.850150
C	-7.401442	0.343111	-3.726379
C	-7.665437	-0.433170	-2.601280

C	-6.695105	-0.585696	-1.613722
F	-6.447291	0.228475	1.368579
F	-7.098270	2.410034	2.767830
F	-5.604134	4.677967	2.550702
F	-3.438687	4.707303	0.896043
F	-2.773646	2.558974	-0.505586
F	-4.362334	-2.605225	-1.868474
F	-4.214293	-0.692479	2.463992
F	-4.350499	-3.116616	3.523064
F	-4.485964	-5.322955	1.931102
F	-4.482568	-5.031417	-0.775600
H	1.440923	-0.125858	-1.831145
H	-0.895205	-0.093354	-2.675677
H	-2.401197	0.063961	1.371232
H	-0.063169	0.037409	2.215473
H	-4.235610	1.299747	-2.961527
H	-5.944247	1.574592	-4.723328
H	-8.154640	0.462039	-4.499883
H	-8.628723	-0.924248	-2.493871
H	-6.917970	-1.196003	-0.741431

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$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)_2Ph]^{2-}$

C	0.594073	-0.195663	-1.100629
C	-0.708979	-0.165645	-1.586522
C	-1.810187	-0.038882	-0.733233
C	-1.564750	0.060344	0.641967
C	-0.260124	0.033028	1.127475
C	0.838510	-0.093857	0.274489
O	2.069157	-0.129477	0.843776
B	3.314302	0.083115	0.119863
C	3.778156	-1.179972	-0.850491
C	3.224447	1.527227	-0.686213
C	4.504755	0.085454	1.278548
C	4.952900	-1.080429	-1.589423
C	5.494777	-2.117184	-2.331970
C	4.850620	-3.346531	-2.335617
C	3.687739	-3.505252	-1.601938
C	3.177143	-2.433524	-0.869969
C	3.181874	1.723707	-2.059251
C	3.020700	2.969146	-2.658613
C	2.887320	4.093904	-1.864214
C	2.914384	3.953758	-0.484629
C	3.072874	2.690252	0.064927
C	5.554515	0.987365	1.408324
C	6.529002	0.896025	2.397846
C	6.487529	-0.148308	3.304948
C	5.476299	-1.090523	3.202430
C	4.523934	-0.963085	2.198254
F	5.627575	0.083405	-1.598785
F	6.628012	-1.958731	-3.032223
F	5.354670	-4.369492	-3.039408
F	3.072790	-4.694745	-1.596260
F	2.063230	-2.683971	-0.180420
F	3.279918	0.688925	-2.914262
F	5.696372	2.024061	0.568288
F	7.511875	1.804809	2.480567
F	7.419464	-0.253961	4.262134
F	5.444194	-2.119563	4.060676
F	3.617957	-1.944698	2.128821
F	3.118950	2.632304	1.403472
F	2.800036	5.038611	0.292517
F	2.740581	5.303202	-2.419001
F	2.991211	3.090967	-3.992789
O	-3.034688	-0.007317	-1.304087
B	-4.307886	-0.114397	-0.588842
C	-4.643304	1.214815	0.361194
C	-4.347731	-1.548751	0.254646
C	-5.484246	-0.087871	-1.723823
C	-5.731392	1.237748	1.229388
C	-6.140445	2.354881	1.941855
C	-5.451074	3.547316	1.782318
C	-4.372453	3.588966	0.916386
C	-3.996077	2.440027	0.223033
C	-4.390903	-2.734298	-0.479321
C	-4.415719	-4.000163	0.094060
C	-4.377988	-4.123781	1.473682
C	-4.309692	-2.979919	2.250068
C	-4.289942	-1.734359	1.631234
C	-5.242154	0.553867	-2.945853
C	-6.225501	0.658403	-3.927105
C	-7.491559	0.118128	-3.711482
C	-7.756539	-0.525694	-2.505295
C	-6.765258	-0.621956	-1.530534
F	-6.465078	0.124628	1.422757
F	-7.195215	2.304103	2.770217
F	-5.830826	4.644478	2.452748
F	-3.710808	4.741204	0.745492
F	-2.961219	2.593249	-0.610374
F	-4.417948	-2.705692	-1.817037
F	-4.193999	-0.688261	2.472280
F	-4.261901	-3.087578	3.585233
F	-4.405281	-5.333617	2.047785
F	-4.477670	-5.102791	-0.665769
H	1.420346	-0.305186	-1.796218
H	-0.902528	-0.245980	-2.651840
H	-2.390140	0.167200	1.337183
H	-0.066464	0.111458	2.192823
H	-4.251340	0.965368	-3.118858
H	-6.003091	1.160062	-4.866328
H	-8.261377	0.195040	-4.475467
H	-8.738446	-0.957572	-2.324443

H	-6.990014	-1.129516	-0.595080

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$B(C_6F_5)_3$-Q-$B(C_6F_5)Ph_2$

C	0.244892	-0.284728	-1.029642
C	-1.028406	-0.424495	-1.413627
C	-2.134371	-0.392697	-0.432642
C	-1.835238	-0.141100	0.993159
C	-0.561894	0.009232	1.374417
C	0.535783	-0.053294	0.397951
O	1.679891	0.121195	0.843346
B	3.080613	0.157757	0.039338
C	3.303367	-1.258626	-0.725117
C	2.929845	1.484957	-0.884018
C	4.173991	0.236209	1.227017
C	4.438037	-1.355777	-1.528564
C	4.841290	-2.525884	-2.150432
C	4.093360	-3.682806	-1.961788
C	2.962657	-3.641013	-1.161897
C	2.598840	-2.442806	-0.556286
C	2.822772	1.505356	-2.270478
C	2.695873	2.673080	-3.013900
C	2.668483	3.894720	-2.358838
C	2.754396	3.929133	-0.972781
C	2.875012	2.737725	-0.273674
C	5.276122	1.083163	1.259385
C	6.221929	1.049676	2.277814
C	6.085234	0.133446	3.310342
C	5.008543	-0.743240	3.310841
C	4.091298	-0.679456	2.272820
F	5.185455	-0.261681	-1.720233
F	5.928921	-2.556397	-2.913793
F	4.457665	-4.817129	-2.547186
F	2.235541	-4.739896	-0.974109
F	1.484698	-2.484561	0.204892
F	2.786364	0.358303	-2.972981
F	5.476085	1.985035	0.292716
F	7.256072	1.886921	2.268709
F	6.980530	0.091673	4.290520
F	4.873286	-1.634155	4.291030
F	3.082835	-1.567754	2.294036
F	2.943562	2.824010	1.059818
F	2.714360	5.094242	-0.334149
F	2.543361	5.020734	-3.048562
F	2.587774	2.623418	-4.338953
O	-3.269658	-0.578637	-0.875784
B	-4.729751	-0.815632	-0.062710
C	-5.237525	0.672323	0.359712
C	-4.363254	-1.791922	1.162926
C	-5.607471	-1.450881	-1.242638
C	-6.547142	0.756417	0.836321
C	-7.158489	1.945495	1.205915
C	-6.449324	3.135428	1.098848
C	-5.143798	3.106529	0.636462
C	-4.571772	1.889122	0.282226
C	-3.615437	-2.956949	0.922980
C	-3.238068	-3.810415	1.955622
C	-3.616423	-3.524064	3.265754
C	-4.376328	-2.387953	3.527545
C	-4.741718	-1.535068	2.486685
C	-5.738660	-0.775604	-2.464682
C	-6.502110	-1.292714	-3.505123
C	-7.168661	-2.505659	-3.337821
C	-7.063129	-3.188235	-2.130277
C	-6.287143	-2.664673	-1.097265
F	-7.264723	-0.363632	0.975069
F	-8.408310	1.958716	1.659718
F	-7.013421	4.286483	1.446658
F	-4.444546	4.235504	0.536315
F	-3.289176	1.961791	-0.146423
H	1.070318	-0.340225	-1.731006
H	-1.316184	-0.598694	-2.444868
H	-2.665274	-0.089194	1.687122
H	-0.272253	0.198463	2.401964
H	-3.334625	-3.206982	-0.099380
H	-2.656449	-4.701245	1.739407
H	-3.326183	-4.186355	4.075010
H	-4.684462	-2.162994	4.543980
H	-5.325980	-0.647511	2.716310
H	-5.230539	0.177991	-2.602847
H	-6.584350	-0.751592	-4.442896
H	-7.769703	-2.912927	-4.144912
H	-7.584946	-4.130126	-1.991331
H	-6.214733	-3.206046	-0.157558

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$[B(C_6F_5)_3$-Q-$B(C_6F_5)Ph_2]^{\bullet-}$

C	-0.239121	-0.475321	0.976127
C	1.050455	-0.643313	1.385542
C	2.150317	-0.530251	0.472669
C	1.872583	-0.228057	-0.901109
C	0.584107	-0.057541	-1.309261
C	-0.510797	-0.166475	-0.394313
O	-1.696165	0.023507	-0.882447
B	-2.989952	0.110144	-0.092210
C	-3.390655	-1.311101	0.618214
C	-2.809358	1.379468	0.932126
C	-4.149770	0.340149	-1.227070
C	-4.534655	-1.347415	1.411558
C	-5.050892	-2.505154	1.969615
C	-4.415573	-3.714490	1.717797
C	-3.284952	-3.735419	0.919039

C	-2.800981	-2.546058	0.378897
C	-2.729948	1.326130	2.317662
C	-2.527644	2.442398	3.122468
C	-2.391128	3.688345	2.534270
C	-2.450542	3.796756	1.151926
C	-2.649449	2.654052	0.391831
C	-5.187734	1.263186	-1.174391
C	-6.167013	1.364848	-2.156978
C	-6.138323	0.506633	-3.244133
C	-5.134956	-0.447085	-3.330218
C	-4.178931	-0.516729	-2.325738
F	-5.190603	-0.203676	1.661280
F	-6.147318	-2.477246	2.731528
F	-4.893806	-4.844894	2.240099
F	-2.674081	-4.895149	0.666423
F	-1.711612	-2.657887	-0.393167
F	-2.806050	0.151900	2.970272
F	-5.301136	2.123381	-0.153628
F	-7.136498	2.279051	-2.061090
F	-7.070901	0.590917	-4.194675
F	-5.109195	-1.292325	-4.364401
F	-3.264845	-1.490344	-2.440055
F	-2.708155	2.823525	-0.935623
F	-2.319833	4.992857	0.574903
F	-2.197978	4.771401	3.286428
F	-2.455053	2.321336	4.450217
O	3.329816	-0.696437	0.960066
B	4.668604	-0.818745	0.184441
C	5.096144	0.643675	-0.444374
C	4.479737	-1.996194	-0.919514
C	5.742845	-1.187242	1.342937
C	6.285440	0.733346	-1.168500
C	6.795395	1.918000	-1.680725
C	6.112468	3.104414	-1.455103
C	4.937219	3.076594	-0.723821
C	4.461855	1.863776	-0.232473
C	4.104304	-3.268737	-0.460571
C	3.885926	-4.332289	-1.330849
C	4.043564	-4.151677	-2.703426
C	4.417753	-2.902324	-3.187332
C	4.630490	-1.845681	-2.302956
C	5.653937	-0.576989	2.602120
C	6.577430	-0.837459	3.610269
C	7.629923	-1.720804	3.378122
C	7.743698	-2.334917	2.134282
C	6.810028	-2.068734	1.133919
F	7.008966	-0.371198	-1.404155
F	7.935861	1.932174	-2.376808
F	6.584624	4.256820	-1.935021
F	4.274838	4.212678	-0.490606
F	3.325759	1.944149	0.482580
H	-1.059698	-0.586147	1.675098
H	1.293207	-0.880682	2.415448
H	2.698116	-0.137482	-1.595723
H	0.338793	0.176341	-2.339121
H	3.985870	-3.423421	0.610316
H	3.592061	-5.302602	-0.940495
H	3.873664	-4.977156	-3.388421
H	4.542527	-2.747824	-4.255533
H	4.912748	-0.875882	-2.708599
H	4.834862	0.113555	2.793524
H	6.478495	-0.352152	4.577634
H	8.353962	-1.928493	4.160995
H	8.560198	-3.026088	1.942869
H	6.906678	-2.558656	0.168188

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$[B(C_6F_5)_3\text{-}Q\text{-}B(C_6F_5)Ph_2]^{2-}$

C	-0.243870	-0.599331	0.904888
C	1.071543	-0.754869	1.333533
C	2.157398	-0.548553	0.475781
C	1.879453	-0.170656	-0.844845
C	0.565885	-0.012741	-1.273629
C	-0.516261	-0.222664	-0.414794
O	-1.762357	-0.064550	-0.932619
B	-2.968230	0.091288	-0.135548
C	-3.502127	-1.297823	0.600122
C	-2.754506	1.348267	0.922155
C	-4.184219	0.390856	-1.228509
C	-4.646169	-1.260381	1.390937
C	-5.244779	-2.379792	1.946672
C	-4.695102	-3.628671	1.693259
C	-3.567697	-3.724369	0.896093
C	-2.997484	-2.570793	0.358151
C	-2.660285	1.277362	2.304830
C	-2.391341	2.372675	3.119926
C	-2.196646	3.616100	2.545788
C	-2.271431	3.742565	1.166725
C	-2.537454	2.619835	0.396929
C	-5.166309	1.371684	-1.153502
C	-6.167687	1.531931	-2.106896
C	-6.225493	0.672103	-3.189788
C	-5.285418	-0.340578	-3.297417
C	-4.303040	-0.466463	-2.322366
F	-5.232182	-0.076347	1.645877
F	-6.344540	-2.280033	2.708806
F	-5.255799	-4.730134	2.212140
F	-3.045302	-4.931116	0.641342
F	-1.927060	-2.762007	-0.413200
F	-2.811735	0.108654	2.954807
F	-5.210485	2.243344	-0.134067
F	-7.081961	2.506153	-1.986862

F	-7.184667	0.809573	-4.115900
F	-5.350318	-1.193516	-4.329588
F	-3.471839	-1.504341	-2.466155
F	-2.623517	2.820791	-0.925820
F	-2.098642	4.945393	0.602767
F	-1.945852	4.685442	3.311401
F	-2.317111	2.237308	4.451231
O	3.394970	-0.704912	0.988680
B	4.638925	-0.846842	0.201100
C	5.158217	0.615903	-0.435890
C	4.473830	-2.010755	-0.938532
C	5.783403	-1.259439	1.302438
C	6.332228	0.691908	-1.183447
C	6.878233	1.872197	-1.670962
C	6.249199	3.074409	-1.390693
C	5.091421	3.063895	-0.632101
C	4.576911	1.854474	-0.168479
C	4.091581	-3.285559	-0.490371
C	3.906869	-4.355277	-1.360475
C	4.100271	-4.180993	-2.729964
C	4.469578	-2.927517	-3.206689
C	4.649937	-1.866437	-2.319287
C	5.685118	-0.772719	2.614605
C	6.640581	-1.067454	3.584257
C	7.736108	-1.868439	3.265763
C	7.855933	-2.368691	1.971747
C	6.891763	-2.065841	1.010701
F	7.024343	-0.424249	-1.477763
F	8.008823	1.868365	-2.395705
F	6.758693	4.229735	-1.843185
F	4.486110	4.224623	-0.344646
F	3.470446	1.963458	0.574688
H	-1.057121	-0.779705	1.601291
H	1.286331	-1.047275	2.357110
H	2.697053	-0.001194	-1.537655
H	0.349281	0.278927	-2.296810
H	3.930129	-3.427536	0.576580
H	3.604433	-5.325650	-0.973964
H	3.953801	-5.010631	-3.417050
H	4.611170	-2.771779	-4.273784
H	4.923047	-0.892823	-2.722385
H	4.822603	-0.161177	2.868218
H	6.530459	-0.675871	4.593379
H	8.484276	-2.104025	4.019134
H	8.701443	-3.002017	1.711196
H	6.993229	-2.471816	0.006976

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$B(C_6F_5)_3$-Q-BPh_3

C	-2.336659	-0.107380	-1.198422
C	-1.036816	-0.130378	-1.521489
C	0.006380	-0.033902	-0.493039
C	-0.365693	0.084003	0.927702
C	-1.662720	0.123831	1.253742
C	-2.719750	0.011546	0.225358
O	-3.885879	0.030229	0.630401
O	1.181392	-0.037107	-0.895635
H	-3.126577	-0.166524	-1.937575
H	-0.688101	-0.210325	-2.545032
H	0.419093	0.131923	1.674559
H	-2.008030	0.210657	2.278500
B	-5.331586	-0.112520	-0.209834
C	-5.523424	1.342928	-0.887944
C	-5.104935	-1.333215	-1.240007
C	-6.364422	-0.395566	0.986569
C	-6.806840	1.626362	-1.387828
C	-7.084165	2.809869	-2.061296
C	-6.084761	3.767133	-2.235806
C	-4.814812	3.524975	-1.728483
C	-4.546035	2.327190	-1.063194
C	-5.400579	-1.235319	-2.605982
C	-5.163586	-2.296338	-3.480578
C	-4.615330	-3.484267	-3.006460
C	-4.321612	-3.611508	-1.649916
C	-4.572279	-2.550996	-0.783813
C	-7.193105	-1.522416	1.016098
C	-8.105726	-1.727162	2.051770
C	-8.199788	-0.806481	3.089137
C	-7.385846	0.326288	3.080962
C	-6.490533	0.526485	2.037112
H	-7.599812	0.896206	-1.240616
H	-8.083696	2.991949	-2.444279
H	-6.300195	4.697010	-2.752135
H	-4.032346	4.269556	-1.839112
H	-3.542337	2.198438	-0.659178
H	-5.813980	-0.307699	-2.994681
H	-5.403378	-2.192140	-4.534529
H	-4.423417	-4.308366	-3.686247
H	-3.904923	-4.538777	-1.268364
H	-4.359612	-2.673446	0.277615
H	-7.127673	-2.253759	0.214511
H	-8.740528	-2.608190	2.047653
H	-8.905904	-0.964817	3.898496
H	-7.459552	1.054036	3.883617
H	-5.875792	1.425147	2.027942
B	2.536162	0.094006	-0.036142
C	2.622586	-1.127560	1.032607
C	2.441400	1.600563	0.565889
C	3.691126	-0.156727	-1.139894
C	3.708365	-1.113149	1.906288
C	3.995347	-2.138349	2.792262
C	3.174741	-3.260703	2.814713

C	2.089013	-3.328693	1.956679
C	1.842235	-2.274613	1.083134
C	2.500936	2.687620	-0.305675
C	2.434530	4.009477	0.107791
C	2.287940	4.289032	1.460566
C	2.201736	3.243979	2.367390
C	2.277433	1.934814	1.905755
C	3.596516	-1.275806	-1.963181
C	4.557289	-1.621022	-2.901903
C	5.691110	-0.829302	-3.025116
C	5.840188	0.284310	-2.211512
C	4.849951	0.597159	-1.287087
F	4.524336	-0.051499	1.900466
F	5.040830	-2.064987	3.609948
F	3.428209	-4.256703	3.655127
F	1.293301	-4.395629	1.968474
F	0.765505	-2.417024	0.282288
F	2.632601	2.471818	-1.619716
F	2.531767	-2.088236	-1.853657
F	4.408596	-2.698496	-3.669877
F	6.628672	-1.138967	-3.913763
F	6.928264	1.042710	-2.320611
F	5.064936	1.678953	-0.530692
F	2.129476	0.977266	2.839184
F	2.033977	3.496688	3.662833
F	2.212742	5.545875	1.878733
F	2.502716	5.004505	-0.771711

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$[B(C_6F_5)_3\text{-}Q\text{-}BPh_3]^{\bullet-}$

C	-2.352901	-0.113906	-1.130925
C	-1.034473	-0.143039	-1.475409
C	-0.000536	-0.109301	-0.488351
C	-0.365241	-0.058506	0.893650
C	-1.683653	-0.026825	1.241796
C	-2.725375	-0.052673	0.254631
O	-3.936725	-0.003586	0.685018
O	1.221343	-0.129002	-0.924771
H	-3.132182	-0.125564	-1.882077
H	-0.719620	-0.182455	-2.512151
H	0.406927	-0.058262	1.654080
H	-1.995775	0.007950	2.279906
B	-5.252663	-0.132490	-0.153971
C	-5.474609	1.241072	-0.994050
C	-5.138234	-1.483365	-1.058653
C	-6.412171	-0.268155	0.976032
C	-6.664542	1.403042	-1.724541
C	-6.932443	2.554398	-2.456700
C	-6.013636	3.603278	-2.469149
C	-4.838426	3.482382	-1.736607
C	-4.580167	2.317949	-1.011555
C	-5.378905	-1.544226	-2.436975
C	-5.273096	-2.738927	-3.150984
C	-4.914571	-3.913705	-2.498667
C	-4.668000	-3.883440	-1.126846
C	-4.785337	-2.687343	-0.426366
C	-7.526456	-1.099946	0.810541
C	-8.548806	-1.157103	1.757822
C	-8.475070	-0.382617	2.911113
C	-7.374574	0.451667	3.102694
C	-6.367325	0.506729	2.144372
H	-7.402120	0.602045	-1.706114
H	-7.862073	2.639579	-3.013188
H	-6.217589	4.506403	-3.037019
H	-4.118443	4.296201	-1.725045
H	-3.656979	2.262733	-0.439126
H	-5.645187	-0.633879	-2.969646
H	-5.465517	-2.748785	-4.220614
H	-4.825344	-4.844404	-3.051554
H	-4.385439	-4.793922	-0.605424
H	-4.601729	-2.679070	0.646755
H	-7.589435	-1.726437	-0.077110
H	-9.400079	-1.813899	1.598062
H	-9.265374	-0.427990	3.655281
H	-7.305895	1.061451	3.999931
H	-5.516722	1.166780	2.301376
B	2.473239	0.064582	-0.093122
C	2.728703	-1.161884	0.963786
C	2.342548	1.553981	0.585818
C	3.705110	-0.060913	-1.168131
C	3.828144	-1.076214	1.814132
C	4.224542	-2.091350	2.668783
C	3.507559	-3.281031	2.677814
C	2.416974	-3.424297	1.837034
C	2.054369	-2.376040	0.994139
C	2.306839	2.667258	-0.251643
C	2.160201	3.970187	0.200107
C	2.027480	4.203975	1.561599
C	2.039984	3.131494	2.437185
C	2.193499	1.843016	1.936053
C	3.725067	-1.160768	-2.023916
C	4.734046	-1.398360	-2.947643
C	5.801318	-0.516141	-3.025730
C	5.839422	0.578862	-2.178132
C	4.806185	0.781405	-1.269201
F	4.559228	0.049337	1.821964
F	5.282955	-1.947950	3.470577
F	3.869693	-4.276152	3.489083
F	1.728106	-4.567839	1.835214
F	0.995829	-2.602630	0.204777
F	2.441054	2.506904	-1.574688
F	2.747091	-2.074882	-1.962978

F	4.697526	-2.468265	-3.746896
F	6.785213	-0.725037	-3.902626
F	6.869512	1.427624	-2.239528
F	4.933111	1.857273	-0.480784
F	2.147187	0.859859	2.853209
F	1.895248	3.340461	3.748102
F	1.882162	5.447274	2.019847
F	2.148094	4.997137	-0.652650

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$[B(C_6F_5)_3\text{-Q-}BPh_3]^{2-}$

C	-2.336659	-0.107380	-1.198422
C	-1.036816	-0.130378	-1.521489
C	0.006380	-0.033902	-0.493039
C	-0.365693	0.084003	0.927702
C	-1.662720	0.123831	1.253742
C	-2.719750	0.011546	0.225358
O	-3.885879	0.030229	0.630401
O	1.181392	-0.037107	-0.895635
H	-3.126577	-0.166524	-1.937575
H	-0.688101	-0.210325	-2.545032
H	0.419093	0.131923	1.674559
H	-2.008030	0.210657	2.278500
B	-5.331586	-0.112520	-0.209834
C	-5.523424	1.342928	-0.887944
C	-5.104935	-1.333215	-1.240007
C	-6.364422	-0.395566	0.986569
C	-6.806840	1.626362	-1.387828
C	-7.084165	2.809869	-2.061296
C	-6.084761	3.767133	-2.235806
C	-4.814812	3.524975	-1.728483
C	-4.546035	2.327190	-1.063194
C	-5.400579	-1.235319	-2.605982
C	-5.163586	-2.296338	-3.480578
C	-4.615330	-3.484267	-3.006460
C	-4.321612	-3.611508	-1.649916
C	-4.572279	-2.550996	-0.783813
C	-7.193105	-1.522416	1.016098
C	-8.105726	-1.727162	2.051770
C	-8.199788	-0.806481	3.089137
C	-7.385846	0.326288	3.080962
C	-6.490533	0.526485	2.037112
H	-7.599812	0.896206	-1.240616
H	-8.083696	2.991949	-2.444279
H	-6.300195	4.697010	-2.752135
H	-4.032346	4.269556	-1.839112
H	-3.542337	2.198438	-0.659178
H	-5.813980	-0.307699	-2.994681
H	-5.403378	-2.192140	-4.534529
H	-4.423417	-4.308366	-3.686247
H	-3.904923	-4.538777	-1.268364
H	-4.359612	-2.673446	0.277615
H	-7.127673	-2.253759	0.214511
H	-8.740528	-2.608190	2.047653
H	-8.905904	-0.964817	3.898496
H	-7.459552	1.054036	3.883617
H	-5.875792	1.425147	2.027942
B	2.536162	0.094006	-0.036142
C	2.622586	-1.127560	1.032607
C	2.441400	1.600563	0.565889
C	3.691126	-0.156727	-1.139894
C	3.708365	-1.113149	1.906288
C	3.995347	-2.138349	2.792262
C	3.174741	-3.260703	2.814713
C	2.089013	-3.328693	1.956679
C	1.842235	-2.274613	1.083134
C	2.500936	2.687620	-0.305675
C	2.434530	4.009477	0.107791
C	2.287940	4.289032	1.460566
C	2.201736	3.243979	2.367390
C	2.277433	1.934814	1.905755
C	3.596516	-1.275806	-1.963181
C	4.557289	-1.621022	-2.901903
C	5.691110	-0.829302	-3.025116
C	5.840188	0.284310	-2.211512
C	4.849951	0.597159	-1.287087
F	4.524336	-0.051499	1.900466
F	5.040830	-2.064987	3.609948
F	3.428209	-4.256703	3.655127
F	1.293301	-4.395629	1.968474
F	0.765505	-2.417024	0.282288
F	2.632601	2.471818	-1.619716
F	2.531767	-2.088236	-1.853657
F	4.408596	-2.698496	-3.669877
F	6.628672	-1.138967	-3.913763
F	6.928264	1.042710	-2.320611
F	5.064936	1.678953	-0.530692
F	2.129476	0.977266	2.839184
F	2.033977	3.496688	3.662833
F	2.212742	5.545875	1.878733
F	2.502716	5.004505	-0.771711

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$B(C_6F_5)_3\text{-Q-}BEt_3$

C	-3.498820	0.567849	-0.966514
C	-2.222469	0.367361	-1.311055
C	-1.146594	0.504419	-0.316751
C	-1.461823	0.889296	1.066118
C	-2.738276	1.108102	1.405128
C	-3.849770	0.954779	0.425717
O	-5.000967	1.145995	0.762429
O	0.000344	0.292602	-0.744586

B	-7.151507	0.227594	-0.366913
C	-6.984084	0.925930	-1.782307
C	-6.670638	-1.270318	-0.177127
C	-8.037611	0.918346	0.745231
C	-9.371450	0.166582	0.920680
C	-7.525694	-2.192734	-1.069937
C	-8.361574	1.160114	-2.431740
B	1.476192	0.089436	-0.194616
C	2.173899	1.490495	-0.617181
C	1.992764	-1.241193	-0.964237
C	1.476533	-0.266034	1.391212
C	3.104768	1.670431	-1.635487
C	3.649351	2.912660	-1.949707
C	3.251530	4.037772	-1.245115
C	3.332035	-1.583033	-0.795540
C	3.903699	-2.732403	-1.313567
C	3.103529	-3.614849	-2.030271
C	2.373767	0.243524	2.324137
C	2.418029	-0.195909	3.644422
C	1.545279	-1.186607	4.068980
C	1.760135	-3.327646	-2.208328
C	1.226645	-2.159533	-1.670434
C	0.635587	-1.731252	3.170289
C	0.635375	-1.271033	1.863475
C	2.312131	3.910502	-0.229819
C	1.801242	2.654604	0.048875
F	0.887169	2.581515	1.037948
F	1.911707	4.982270	0.450988
F	3.757574	5.228760	-1.541306
F	4.539380	3.028455	-2.931623
F	3.526605	0.647520	-2.383511
F	-0.267280	-1.812943	1.021412
F	-0.212157	-2.677110	3.567564
F	1.572353	-1.608772	5.327338
F	3.291120	0.325459	4.501070
F	3.250142	1.192250	1.987519
F	4.123215	-0.752364	-0.100157
F	5.193766	-3.002595	-1.130925
F	3.623943	-4.727791	-2.536900
F	0.983678	-4.173359	-2.884198
F	-0.090633	-1.976896	-1.870762
H	-4.324945	0.461222	-1.662638
H	-1.906114	0.067680	-2.304104
H	-0.642515	1.019793	1.759179
H	-3.028824	1.410905	2.405827
H	-6.362434	0.341819	-2.476237
H	-6.494538	1.900734	-1.646859
H	-6.732338	-1.604753	0.865348
H	-5.621158	-1.381585	-0.485807
H	-7.495099	0.888978	1.698477
H	-8.237326	1.974240	0.525574
H	-9.998047	0.632069	1.686329
H	-9.201433	-0.872491	1.220746
H	-9.950810	0.148453	-0.008939
H	-7.430450	-1.918119	-2.125664
H	-8.587637	-2.129559	-0.811196
H	-7.226584	-3.239732	-0.972099
H	-8.993570	1.784845	-1.793455
H	-8.890613	0.214716	-2.592322
H	-8.274228	1.655934	-3.402253

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$[B(C_6F_5)_3\text{-Q-}BEt_3]^{\bullet-}$

C	-2.930026	-0.033764	-2.838511
C	-1.573111	0.006352	-2.744130
C	-0.927020	-0.075863	-1.472675
C	-1.729407	-0.218805	-0.300768
C	-3.093730	-0.260890	-0.391778
C	-3.752354	-0.164396	-1.665448
O	-5.019351	-0.185901	-1.835753
O	0.373142	-0.020983	-1.477948
B	-6.179409	-0.325417	-0.742772
C	-6.049202	-1.838127	-0.117929
C	-6.028008	0.885102	0.351733
C	-7.504820	-0.144370	-1.673876
C	-8.821862	-0.511875	-0.984539
C	-5.627940	2.242310	-0.235910
C	-6.654388	-1.998043	1.282207
B	1.267972	0.068455	-0.264423
C	0.846004	1.450654	0.515861
C	2.790851	0.102062	-0.877192
C	1.234136	-1.289924	0.653828
C	1.025509	2.665564	-0.142375
C	0.667658	3.894311	0.390958
C	0.083394	3.942171	1.648813
C	3.817922	0.960618	-0.502750
C	5.100293	0.894303	-1.037911
C	5.399796	-0.074562	-1.981492
C	1.987755	-1.312783	1.824630
C	2.141335	-2.434148	2.622919
C	1.532134	-3.621731	2.238495
C	4.414419	-0.969245	-2.371256
C	3.148457	-0.870003	-1.809665
C	0.787964	-3.657491	1.071734
C	0.660009	-2.504669	0.300179
C	-0.132118	2.762408	2.340640
C	0.247469	1.554204	1.764669
F	-0.039403	0.456452	2.486704
F	-0.707246	2.793096	3.545102
F	-0.270775	5.111863	2.181791
F	0.880042	5.026399	-0.285015
F	1.596706	2.686156	-1.354649

F	-0.063024	-2.632562	-0.820517
F	0.208599	-4.798790	0.691173
F	1.667782	-4.718317	2.986517
F	2.870091	-2.393763	3.741862
F	2.612911	-0.192445	2.219468
F	3.623312	1.920506	0.411538
F	6.047067	1.753613	-0.648847
F	6.625683	-0.152018	-2.504137
F	4.697782	-1.920401	-3.266442
F	2.256242	-1.794309	-2.191631
H	-3.443310	0.032817	-3.791522
H	-0.935855	0.105960	-3.615775
H	-1.247834	-0.307724	0.666331
H	-3.703757	-0.373081	0.494695
H	-4.997271	-2.157633	-0.070792
H	-6.531648	-2.555207	-0.799340
H	-7.013709	0.987951	0.831144
H	-5.348180	0.651607	1.184396
H	-7.578013	0.887317	-2.050597
H	-7.392809	-0.775792	-2.567995
H	-9.697662	-0.335749	-1.620878
H	-8.969945	0.066823	-0.064541
H	-8.834726	-1.570738	-0.701727
H	-4.602246	2.223302	-0.623656
H	-6.278171	2.516886	-1.073445
H	-5.675193	3.052899	0.500181
H	-7.704599	-1.688227	1.305387
H	-6.127523	-1.374745	2.012999
H	-6.609333	-3.032314	1.643723

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$[B(C_6F_5)_3\text{-Q-}BEt_3]^{2-}$

C	-3.005889	0.191886	-2.768645
C	-1.622569	0.204226	-2.687356
C	-0.966330	-0.070683	-1.482593
C	-1.751344	-0.354810	-0.364369
C	-3.147503	-0.362806	-0.443301
C	-3.817759	-0.092212	-1.650014
O	-5.135118	-0.073206	-1.829043
O	0.398052	-0.061914	-1.503003
B	-6.206213	-0.378583	-0.781137
C	-6.093489	-1.962703	-0.308635
C	-6.124224	0.688056	0.480364
C	-7.596433	-0.134026	-1.635082
C	-8.886485	-0.597658	-0.953749
C	-5.793221	2.117497	0.040494
C	-6.638496	-2.281073	1.089423
B	1.231164	0.055891	-0.323307
C	0.757978	1.383569	0.547238
C	2.787345	0.206417	-0.897581
C	1.339458	-1.323297	0.596820
C	0.852283	2.633551	-0.058891
C	0.423261	3.814576	0.527751
C	-0.151424	3.774693	1.789276
C	3.753368	1.122403	-0.497864
C	5.042173	1.161236	-1.022751
C	5.417791	0.239034	-1.983787
C	2.118341	-1.323899	1.749472
C	2.376207	-2.450309	2.514261
C	1.849810	-3.668842	2.109637
C	4.500075	-0.713355	-2.397952
C	3.224026	-0.717807	-1.846888
C	1.083335	-3.727889	0.958772
C	0.847302	-2.568258	0.220640
C	-0.281422	2.556830	2.432382
C	0.166814	1.399517	1.802647
F	-0.022545	0.263690	2.497497
F	-0.835593	2.506037	3.651036
F	-0.566704	4.902859	2.379574
F	0.566575	4.992511	-0.096948
F	1.426293	2.751072	-1.265808
F	0.117619	-2.726671	-0.883690
F	0.588744	-4.907966	0.561227
F	2.089047	-4.777805	2.824442
F	3.131145	-2.387688	3.622412
F	2.674035	-0.172403	2.169504
F	3.497950	2.047665	0.439867
F	5.927888	2.078951	-0.605470
F	6.655635	0.259437	-2.499340
F	4.864377	-1.626365	-3.310702
F	2.419776	-1.704876	-2.257181
H	-3.510575	0.405185	-3.706933
H	-1.011594	0.426313	-3.558180
H	-1.277555	-0.578143	0.587967
H	-3.728087	-0.590485	0.442470
H	-5.045767	-2.293869	-0.346768
H	-6.616636	-2.598316	-1.043354
H	-7.096031	0.691173	1.003506
H	-5.399257	0.396574	1.255716
H	-7.699864	0.929767	-1.903607
H	-7.496223	-0.667541	-2.593436
H	-9.794223	-0.389444	-1.540225
H	-9.018479	-0.114484	0.023316
H	-8.864070	-1.679159	-0.769844
H	-4.790234	2.157928	-0.397732
H	-6.489695	2.461699	-0.733455
H	-5.826110	2.846787	0.862616
H	-7.684025	-1.966219	1.197604
H	-6.073297	-1.742279	1.859074
H	-6.592586	-3.350308	1.343751

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$[H\text{-}Q\text{-}SiPhH_2]^{2+}$

C	-2.092070	-0.826480	0.812330
C	-3.334020	-0.401300	1.099120
C	-3.997570	0.544440	0.202640
C	-3.356650	1.058930	-0.995990
C	-2.112240	0.639480	-1.286070
C	-1.432620	-0.347660	-0.414720
O	-0.320310	-0.755510	-0.793230
O	-5.172180	0.882110	0.557410
Si	1.144590	-1.764020	-0.175460
C	2.390520	-0.455760	0.030110
C	3.146820	-0.015690	-1.078950
C	4.137350	0.937620	-0.904040
C	4.373310	1.467800	0.368540
C	3.626220	1.044720	1.473550
C	2.631660	0.093600	1.307550
H	-1.569720	-1.531740	1.450990
H	-3.886940	-0.727450	1.975720
H	-3.885830	1.767690	-1.628230
H	-1.567500	0.979110	-2.162770
H	-5.645000	1.514750	-0.022160
H	0.599780	-2.344730	1.060620
H	1.219330	-2.656600	-1.333800
H	2.978780	-0.436560	-2.066880
H	4.734350	1.263630	-1.748340
H	5.150000	2.213930	0.502090
H	3.833880	1.450300	2.457430
H	2.070240	-0.247020	2.173960

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$[H\text{-}Q\text{-}SiPhH_2]^{\bullet+}$

C	-2.333990	-1.087880	0.000000
C	-3.695710	-1.034800	0.000000
C	-4.358320	0.229050	-0.000010
C	-3.617100	1.443980	0.000000
C	-2.255350	1.392810	0.000000
C	-1.576420	0.128130	0.000010
O	-0.281030	0.160670	0.000010
O	-5.671640	0.191660	-0.000010
Si	0.888330	-1.158510	0.000020
C	2.551270	-0.394020	0.000000
C	3.197990	-0.099420	-1.210810
C	4.457300	0.489070	-1.209530
C	5.083620	0.783280	-0.000020
C	4.457300	0.489090	1.209510
C	3.198000	-0.099390	1.210810
H	-1.821240	-2.043910	0.000010
H	-4.308180	-1.929610	-0.000010
H	-4.139120	2.396210	-0.000010
H	-1.645280	2.289170	0.000010
H	-6.077360	1.072520	-0.000020
H	0.552900	-1.907530	1.226590
H	0.552890	-1.907540	-1.226550
H	2.721870	-0.335460	-2.159200
H	4.953040	0.712260	-2.147910
H	6.068690	1.238150	-0.000020
H	4.953050	0.712310	2.147890
H	2.721880	-0.335410	2.159210

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$H\text{-}Q\text{-}SiPhH_2$

C	-2.291950	-1.092920	0.073220
C	-3.676700	-1.066620	-0.039970
C	-4.355520	0.149720	-0.043080
C	-3.637520	1.339810	0.069430
C	-2.252240	1.313060	0.178570
C	-1.572070	0.098300	0.177680
O	-0.209100	0.130980	0.298640
O	-5.714350	0.112970	-0.155990
Si	0.842200	-1.088590	-0.144000
C	2.536140	-0.325300	-0.063340
C	2.705100	1.060060	-0.182390
C	3.976220	1.626570	-0.149100
C	5.096970	0.813830	0.001690
C	4.945840	-0.565130	0.125630
C	3.673180	-1.127390	0.096890
H	-1.775410	-2.048690	0.092420
H	-4.248940	-1.983760	-0.122610
H	-4.161190	2.292620	0.070540
H	-1.680290	2.230180	0.265810
H	-6.058920	1.012360	-0.141810
H	0.766010	-2.247960	0.779490
H	0.472710	-1.560110	-1.501510
H	1.831170	1.696670	-0.289250
H	4.093270	2.701970	-0.238410
H	6.088330	1.255260	0.027790
H	5.817640	-1.199280	0.251260
H	3.567660	-2.204510	0.209650

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$[H\text{-}Q\text{-}SiEt_3]^{2+}$

C	1.578710	-0.886520	-0.375100
C	2.900300	-1.061220	-0.531890
C	3.808690	0.056510	-0.275480
C	3.336690	1.369660	0.140440
C	2.015310	1.554440	0.292440
C	1.064590	0.436030	0.046020
O	-0.136810	0.675060	0.198600
O	5.040010	-0.208040	-0.445600
Si	-1.846700	-0.213630	0.076490
C	-2.113630	-0.129850	-1.763880
C	-1.503300	-1.898470	0.801850

C	-2.832620	0.961580	1.111750
C	-2.993730	2.354840	0.482120
C	-0.664090	-1.907870	2.088960
C	-3.527840	-0.683150	-2.052320
H	0.865430	-1.685620	-0.554450
H	3.345850	-2.002130	-0.842810
H	4.053990	2.167820	0.316170
H	1.585000	2.504740	0.597390
H	5.677520	0.518360	-0.282970
H	-2.031200	0.905230	-2.110820
H	-1.356710	-0.720720	-2.292510
H	-1.102130	-2.583340	0.044960
H	-2.503770	-2.295590	1.028180
H	-3.815580	0.493730	1.261000
H	-2.388790	1.025140	2.112270
H	-3.569970	3.004190	1.142730
H	-3.522850	2.305440	-0.472910
H	-2.026900	2.837160	0.309820
H	-0.590990	-2.919300	2.491960
H	-1.105350	-1.276320	2.863860
H	0.363800	-1.558320	1.924790
H	-3.724240	-0.649120	-3.125760
H	-3.635700	-1.723710	-1.733580
H	-4.303810	-0.088820	-1.561660

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$[H\text{-}Q\text{-}SiEt_3]^{\bullet+}$

C	1.479270	-0.798280	-0.372490
C	2.808760	-1.021290	-0.572570
C	3.751420	0.014900	-0.306700
C	3.325020	1.285440	0.169370
C	1.995710	1.510580	0.370800
C	1.033330	0.478360	0.105070
O	-0.207910	0.765210	0.317970
O	5.014080	-0.281160	-0.526490
Si	-1.715020	-0.159680	0.100570
C	-1.907770	-0.385170	-1.743460
C	-1.510890	-1.753890	1.064240
C	-2.955130	1.012680	0.839250
C	-3.093500	2.322920	0.049630
C	-0.744720	-1.596240	2.386650
C	-3.286020	-0.995260	-2.059150
H	0.751640	-1.578540	-0.566560
H	3.186660	-1.972190	-0.931320
H	4.057650	2.062230	0.367370
H	1.622760	2.462340	0.732200
H	5.614850	0.454200	-0.331030
H	-1.801780	0.586510	-2.239200
H	-1.112780	-1.026620	-2.141920
H	-1.057980	-2.535290	0.442310
H	-2.529290	-2.107870	1.271440
H	-3.921400	0.495940	0.893930
H	-2.667710	1.216980	1.877500
H	-3.803380	2.998020	0.531430
H	-3.452590	2.139110	-0.967250
H	-2.136110	2.846970	-0.023690
H	-0.740540	-2.530690	2.950980
H	-1.195800	-0.829470	3.022680
H	0.299350	-1.312080	2.218750
H	-3.414270	-1.136620	-3.133990
H	-3.414350	-1.971950	-1.582480
H	-4.097040	-0.346420	-1.714890

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$H\text{-}Q\text{-}SiEt_3$

C	-1.638840	1.241710	-0.609470
C	-2.970820	1.346580	-0.233970
C	-3.702680	0.197870	0.069070
C	-3.092150	-1.051880	-0.009100
C	-1.755390	-1.154080	-0.385890
C	-1.021820	-0.008810	-0.685270
O	0.288040	-0.105710	-1.080600
O	-5.007010	0.362310	0.432230
Si	1.537880	-0.118840	0.056340
C	1.374580	1.377720	1.181780
C	1.452590	-1.718710	1.039820
C	3.099110	-0.020300	-0.974690
C	3.258830	1.334190	-1.677610
C	1.710910	-2.962210	0.178490
C	2.580970	1.540180	2.117490
H	-1.059620	2.125800	-0.856140
H	-3.464830	2.309840	-0.171960
H	-3.660240	-1.949820	0.221500
H	-1.273100	-2.123750	-0.459860
H	-5.400130	-0.500230	0.603630
H	1.261460	2.272270	0.556370
H	0.447970	1.296970	1.762690
H	0.463660	-1.779310	1.512070
H	2.176700	-1.672620	1.863000
H	3.968000	-0.228000	-0.336940
H	3.066100	-0.827230	-1.716520
H	4.145830	1.358900	-2.316640
H	3.353100	2.149010	-0.952140
H	2.388990	1.550620	-2.304710
H	1.581420	-3.887620	0.746720
H	2.730130	-2.959960	-0.219840
H	1.031110	-2.999030	-0.679210
H	2.482490	2.420540	2.758370
H	2.698730	0.671400	2.772920
H	3.511930	1.649570	1.550870

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$[H\text{-}Q\text{-}Si(C_6Me_5)_3]^{2+}$

C	1.00292	-1.17675	3.38414
C	0.77088	-2.06422	4.38359
C	-0.24092	-3.06443	4.21232
C	-0.98936	-3.15974	2.99985
C	-0.76094	-2.27445	1.99009
C	0.22821	-1.22596	2.16031
O	0.46755	-0.32096	1.29344
O	-0.41566	-3.87234	5.21896
Si	0.11181	0.23383	-0.39013
C	1.85702	-0.16522	-0.97302
C	-1.35487	-0.74939	-1.00221
C	-0.26057	2.03198	-0.01269
C	0.36464	2.69564	1.08066
C	-0.16101	3.91733	1.55899
C	-1.25682	4.50359	0.91842
C	-1.85719	3.86337	-0.19120
C	-1.33199	2.64953	-0.68187
C	-2.56284	-0.74008	-0.25877
C	-3.66889	-1.47257	-0.72020
C	-3.56842	-2.22268	-1.90710
C	-2.36344	-2.26065	-2.62805
C	-1.28033	-1.46831	-2.21840
C	2.66683	0.82180	-1.54782
C	4.05912	0.61287	-1.63417
C	4.63973	-0.61768	-1.20361
C	3.84128	-1.61026	-0.63610
C	2.44283	-1.41543	-0.57104
C	-4.76932	-2.97463	-2.42698
C	-2.72224	0.05954	1.02170
C	-2.24888	-3.13849	-3.85317
C	-0.08242	-1.36213	-3.14088
C	1.65103	2.20215	1.69760
C	0.45645	4.59441	2.75998
C	-1.77991	5.84120	1.37793
C	-3.04927	4.49698	-0.85736
C	-1.88623	2.11541	-1.98593
C	1.58350	-2.57213	-0.17377
C	4.45878	-2.89439	-0.13672
C	6.11430	-0.84338	-1.40405
C	4.94648	1.68883	-2.18771
C	2.08708	2.08873	-2.13642
C	-4.98402	-1.46287	0.02648
H	1.76654	-0.41046	3.46175
H	1.32681	-2.05591	5.31474
H	-1.73821	-3.93908	2.89303
H	-1.32428	-2.31886	1.06307
H	-1.10245	-4.54476	5.07654
H	-5.70437	-2.51683	-2.10728
H	-4.77698	-3.00478	-3.51684
H	-4.77212	-4.01202	-2.07093
H	-1.82234	0.58804	1.33345
H	-3.49588	0.82588	0.90306
H	-3.03937	-0.57677	1.85522
H	-2.85370	-4.03952	-3.74686
H	-2.58966	-2.62071	-4.75755
H	-1.22137	-3.46056	-4.02390
H	-0.39285	-1.45904	-4.18181
H	0.41987	-0.39631	-3.06011
H	0.67021	-2.13869	-2.95406
H	2.14070	1.43306	1.10038
H	2.35038	3.03571	1.80377
H	1.49062	1.80002	2.70638
H	0.99650	3.89475	3.39663
H	1.16140	5.37846	2.45877
H	-0.30918	5.06567	3.37758
H	-0.99793	6.43909	1.84464
H	-2.17834	6.42095	0.54515
H	-2.58705	5.72113	2.11077
H	-3.69325	4.98404	-0.12326
H	-2.74186	5.26698	-1.57671
H	-3.65381	3.76753	-1.39507
H	-2.85038	1.60907	-1.86251
H	-2.03062	2.93708	-2.69147
H	-1.21229	1.40498	-2.46847
H	1.95021	-3.50241	-0.61537
H	1.60762	-2.73825	0.92336
H	0.54179	-2.44546	-0.47412
H	5.42776	-2.70437	0.32662
H	3.83626	-3.38377	0.61220
H	4.61958	-3.60791	-0.95313
H	6.46429	-0.37880	-2.32679
H	6.69449	-0.40985	-0.57972
H	6.35745	-1.90337	-1.45807
H	4.51789	2.68084	-2.04955
H	5.93039	1.67665	-1.71740
H	5.10309	1.54621	-3.26611
H	1.01870	1.99719	-2.33479
H	2.22415	2.95414	-1.47864
H	2.56814	2.31627	-3.09011
H	-4.90423	-1.04172	1.02635
H	-5.73292	-0.87232	-0.51245
H	-5.38709	-2.47361	0.12513

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$[H\text{-}Q\text{-}Si(C_6Me_5)_3]^{\cdot+}$

C	-0.68648	-1.09957	3.54506
C	-1.58922	-1.59118	4.43785
C	-2.91078	-1.88601	4.00338
C	-3.29399	-1.67965	2.65252
C	-2.39354	-1.18970	1.74920

C	-1.05467	-0.87490	2.17324
O	-0.13864	-0.40956	1.40183
O	-3.73876	-2.35743	4.91771
Si	0.27490	0.06704	-0.27462
C	1.41499	-1.36801	-0.71242
C	-1.40343	0.24980	-1.11437
C	1.14751	1.69655	0.07712
C	1.97582	1.82925	1.21289
C	2.43258	3.09951	1.60367
C	2.11175	4.22856	0.83655
C	1.30930	4.09923	-0.30841
C	0.86381	2.83287	-0.71351
C	-2.39573	1.06370	-0.51542
C	-3.67849	1.13941	-1.08386
C	-3.97555	0.41195	-2.24850
C	-3.00466	-0.41436	-2.83321
C	-1.70307	-0.44688	-2.30617
C	2.70979	-1.11005	-1.21381
C	3.66763	-2.13583	-1.24135
C	3.31717	-3.43918	-0.85419
C	2.02049	-3.71348	-0.39485
C	1.06559	-2.68710	-0.34947
C	-5.33540	0.54906	-2.89375
C	-2.12792	1.89658	0.72527
C	-3.35996	-1.26126	-4.03508
C	-0.63679	-1.18645	-3.08898
C	2.47432	0.63184	1.99799
C	3.27373	3.25726	2.85106
C	2.66904	5.58121	1.21639
C	0.92853	5.32880	-1.10288
C	0.15526	2.72968	-2.05032
C	-0.35842	-3.05191	0.00774
C	1.66030	-5.11364	0.04970
C	4.32718	-4.55663	-0.97464
C	5.08188	-1.83904	-1.68699
C	3.08874	0.23170	-1.80617
C	-4.75354	2.00328	-0.46156
H	0.33320	-0.86711	3.82987
H	-1.33825	-1.77087	5.47700
H	-4.30727	-1.91708	2.34124
H	-2.67486	-1.02448	0.71567
H	-4.61996	-2.53896	4.55955
H	-5.75991	1.53830	-2.72103
H	-5.27998	0.40530	-3.97296
H	-6.04678	-0.18720	-2.49996
H	-1.09498	1.86590	1.06524
H	-2.35573	2.94925	0.52992
H	-2.76570	1.58735	1.56218
H	-4.40512	-1.57156	-4.00206
H	-3.20731	-0.72057	-4.97691
H	-2.75654	-2.16865	-4.07604
H	-0.84229	-1.12863	-4.15891
H	0.35567	-0.76209	-2.93486
H	-0.57346	-2.24826	-2.82109
H	2.31424	-0.31405	1.48212
H	3.55043	0.72395	2.16862
H	2.00145	0.56580	2.98499
H	3.09627	2.45420	3.56620
H	4.34597	3.25890	2.62014
H	3.04925	4.19603	3.35994
H	3.63588	5.48900	1.71192
H	2.81528	6.21242	0.33953
H	1.99837	6.11632	1.89964
H	0.80258	6.19395	-0.45029
H	1.69196	5.58756	-1.84671
H	-0.01283	5.18879	-1.63484
H	-0.90232	3.01339	-1.99491
H	0.63662	3.38703	-2.77828
H	0.18845	1.72206	-2.46781
H	-0.65680	-3.96698	-0.51100
H	-0.49360	-3.24063	1.08104
H	-1.06457	-2.27836	-0.30187
H	2.49810	-5.58946	0.56225
H	0.81852	-5.11768	0.74245
H	1.39136	-5.75360	-0.79937
H	5.01263	-4.38410	-1.80502
H	4.93105	-4.65284	-0.06417
H	3.84265	-5.51722	-1.15047
H	5.35495	-0.80219	-1.48940
H	5.80010	-2.46677	-1.15786
H	5.21766	-2.01769	-2.76063
H	2.21646	0.79913	-2.13259
H	3.63880	0.86618	-1.10189
H	3.71761	0.08681	-2.68718
H	-4.55453	2.22695	0.58537
H	-4.84553	2.96207	-0.98542
H	-5.72922	1.51544	-0.51148

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H-Q-Si(C_6Me_5)$_3$

C	2.03547	1.60431	1.77488
C	2.76491	2.67769	2.26822
C	2.21691	3.50553	3.24680
C	0.93438	3.24983	3.72723
C	0.20353	2.17558	3.22910
C	0.74669	1.34809	2.24960
O	-0.00190	0.28999	1.82035
O	2.98184	4.54389	3.69517
Si	-0.12195	-0.32387	0.24604
C	-1.96332	-0.84359	0.17890
C	0.25970	1.18603	-0.85733
C	1.05389	-1.81806	0.01676

C	1.03647	-2.46050	-1.24513
C	2.00977	-3.40692	-1.59319
C	2.97365	-3.79507	-0.65115
C	3.00382	-3.17778	0.60494
C	2.03701	-2.21413	0.95592
C	1.30947	1.25938	-1.80098
C	1.36203	2.31884	-2.72601
C	0.44610	3.37442	-2.64423
C	-0.56306	3.34637	-1.67116
C	-0.64872	2.27180	-0.77184
C	-2.88307	-0.46757	-0.82874
C	-4.25678	-0.72452	-0.66711
C	-4.72637	-1.38797	0.47419
C	-3.82719	-1.76026	1.48144
C	-2.45182	-1.53235	1.31390
C	0.57874	4.57006	-3.56232
C	2.47949	0.29350	-1.81708
C	-1.57126	4.47239	-1.59916
C	-1.73384	2.36310	0.28610
C	-0.02687	-2.12514	-2.26708
C	2.04901	-3.97549	-2.99626
C	3.95163	-4.90373	-0.97540
C	4.09420	-3.54263	1.58987
C	2.10049	-1.69625	2.38036
C	-1.51750	-2.09125	2.36811
C	-4.33963	-2.39681	2.75589
C	-6.19323	-1.73978	0.59569
C	-5.23856	-0.28011	-1.73009
C	-2.47232	0.16349	-2.14600
C	2.41836	2.32165	-3.81082
H	2.46685	0.95850	1.01547
H	3.76472	2.88910	1.90594
H	0.50235	3.89018	4.49257
H	-0.79705	1.96484	3.59195
H	2.49065	5.03057	4.36567
H	1.60491	4.69893	-3.90689
H	-0.05927	4.47788	-4.44999
H	0.29585	5.49158	-3.05104
H	2.59356	-0.24351	-0.87901
H	2.40524	-0.46362	-2.60764
H	3.40617	0.84710	-1.99046
H	-1.70226	4.95642	-2.56749
H	-2.55191	4.11207	-1.28480
H	-1.26664	5.24428	-0.88118
H	-2.73551	2.27442	-0.15111
H	-1.65820	1.60535	1.06022
H	-1.67865	3.33818	0.78081
H	-0.98213	-1.92411	-1.78446
H	0.24205	-1.24755	-2.87058
H	-0.19904	-2.95419	-2.95404
H	1.77212	-3.21932	-3.73375
H	3.04955	-4.32032	-3.25794
H	1.36276	-4.82189	-3.12288
H	3.52395	-5.61524	-1.68267
H	4.88065	-4.51884	-1.41392
H	4.22065	-5.46673	-0.08076
H	4.99975	-3.86888	1.07713
H	4.36850	-2.69254	2.21522
H	3.78483	-4.35299	2.26221
H	2.27479	-2.52851	3.06819
H	2.92618	-0.98877	2.52121
H	1.18822	-1.19839	2.68816
H	-1.89137	-3.04720	2.74113
H	-0.52413	-2.28470	1.96430
H	-1.40236	-1.41302	3.22029
H	-5.34286	-2.04293	2.99822
H	-4.38382	-3.49093	2.68412
H	-3.70080	-2.15196	3.60538
H	-6.62796	-1.96142	-0.38033
H	-6.34156	-2.62203	1.21905
H	-6.77655	-0.92180	1.03652
H	-4.90782	0.63259	-2.22704
H	-5.36918	-1.04221	-2.50913
H	-6.22169	-0.07510	-1.30454
H	-1.39913	0.18422	-2.30074
H	-2.91909	-0.39220	-2.97767
H	-2.81959	1.20028	-2.22913
H	2.72057	1.30814	-4.07661
H	2.04531	2.79328	-4.72139
H	3.32308	2.86321	-3.50641

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$[H\text{-}Q\text{-}B(C_6F_5)_3]^+$

C	-2.812900	0.498610	-0.773710
C	-4.124580	0.464670	-1.083930
C	-4.534580	0.128260	-2.424780
C	-3.589280	-0.136480	-3.482640
C	-2.273690	-0.084690	-3.198200
C	-1.822490	0.181000	-1.820210
O	-0.604000	0.100960	-1.620520
B	0.214400	0.093090	-0.204390
C	-0.535850	-0.946860	0.795790
C	0.198260	1.666500	0.161570
C	1.630110	-0.556750	-0.584350
C	-0.082880	-0.937590	2.118030
C	-0.504990	-1.837940	3.082540
C	-1.409660	-2.833650	2.725990
C	-1.874140	-2.899200	1.418860
C	-1.421880	-1.975210	0.486060
C	-0.583260	2.254350	1.149420
C	-0.566390	3.615220	1.431480
C	0.264610	4.453800	0.693910

C	1.051600	3.919520	-0.316490
C	0.990890	2.553610	-0.571260
C	1.677480	-1.721970	-1.350190
C	2.852440	-2.386420	-1.654410
C	4.056160	-1.885880	-1.160330
C	4.059380	-0.738310	-0.375770
C	2.858240	-0.099840	-0.099490
F	0.805410	-0.008960	2.480910
F	-0.053080	-1.766780	4.324290
F	-1.834690	-3.701860	3.625650
F	-2.749650	-3.833050	1.066470
F	-1.933000	-2.114090	-0.762350
F	-1.432510	1.509950	1.884090
F	0.532150	-2.248400	-1.818350
F	2.845150	-3.485120	-2.396840
F	5.188630	-2.504790	-1.435650
F	5.202100	-0.266200	0.099710
F	2.915560	0.991180	0.663740
F	1.738560	2.095370	-1.575950
F	1.827230	4.707630	-1.044400
F	0.288790	5.749270	0.946710
F	-1.328780	4.113900	2.392210
O	-5.808630	0.096240	-2.623780
H	-2.465670	0.749150	0.224350
H	-4.904190	0.682830	-0.362110
H	-3.951310	-0.373470	-4.478930
H	-1.499730	-0.285290	-3.932280
H	-6.072500	-0.127370	-3.534110

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$[H\text{-}Q\text{-}B(C_6F_5)_3]^{\cdot}$

C	-2.589960	-1.171780	-0.765650
C	-3.817050	-1.675140	-1.083170
C	-4.223280	-1.768880	-2.439410
C	-3.367820	-1.348840	-3.487040
C	-2.137990	-0.841790	-3.182200
C	-1.708970	-0.728570	-1.814830
O	-0.546850	-0.235490	-1.623410
B	0.117170	0.088900	-0.249790
C	0.337150	-1.267430	0.628950
C	-0.858680	1.224000	0.405010
C	1.603970	0.611280	-0.648810
C	0.855270	-1.118280	1.913660
C	1.208550	-2.180710	2.729170
C	1.061790	-3.477010	2.249170
C	0.565760	-3.677860	0.971570
C	0.225530	-2.579270	0.187930
C	-1.659500	1.074510	1.530760
C	-2.492710	2.074000	2.021530
C	-2.548100	3.293920	1.366860
C	-1.779430	3.490540	0.227210
C	-0.966950	2.462290	-0.226190
C	2.370610	-0.164470	-1.514970
C	3.668050	0.155310	-1.888080
C	4.258170	1.296650	-1.363280
C	3.542680	2.088860	-0.478490
C	2.242930	1.733580	-0.134610
F	1.024060	0.117510	2.402740
F	1.689060	-1.977700	3.953830
F	1.393610	-4.514550	3.011560
F	0.421680	-4.915970	0.498980
F	-0.243090	-2.860420	-1.042040
F	-1.708920	-0.097390	2.190550
F	1.858710	-1.298670	-2.020340
F	4.350600	-0.621520	-2.729450
F	5.501610	1.624470	-1.703400
F	4.105140	3.181930	0.035120
F	1.621930	2.543500	0.731160
F	-0.252990	2.704590	-1.332570
F	-1.835010	4.654210	-0.417850
F	-3.342380	4.260860	1.814600
F	-3.244610	1.861350	3.100630
O	-5.433200	-2.270340	-2.663480
H	-2.263920	-1.114890	0.266410
H	-4.505400	-2.021960	-0.321010
H	-3.695390	-1.434390	-4.519140
H	-1.444530	-0.507750	-3.945290
H	-5.630650	-2.308100	-3.609250

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$[H\text{-}Q\text{-}B(C_6F_5)_3]^{-}$

C	-2.495990	-1.411520	-0.808820
C	-3.756200	-1.934300	-1.080460
C	-4.294320	-1.854350	-2.360250
C	-3.557800	-1.245010	-3.372900
C	-2.300690	-0.718080	-3.102630
C	-1.746640	-0.788830	-1.818970
O	-0.523270	-0.263890	-1.651790
B	0.073950	0.043150	-0.343560
C	0.537450	-1.288930	0.517670
C	-0.972590	1.030320	0.471980
C	1.511500	0.782050	-0.686420
C	1.104780	-1.117440	1.776880
C	1.636950	-2.147640	2.535260
C	1.630510	-3.435410	2.016010
C	1.093690	-3.657600	0.759600
C	0.569100	-2.590520	0.032290
C	-1.693710	0.727380	1.618400
C	-2.631350	1.580920	2.191970
C	-2.882310	2.808110	1.604220
C	-2.194320	3.159150	0.451690
C	-1.272260	2.272230	-0.083680

C	2.368130	0.159200	-1.593060
C	3.611510	0.665230	-1.950350
C	4.057530	1.843220	-1.370990
C	3.254540	2.485460	-0.443690
C	2.014730	1.945120	-0.115940
F	1.149800	0.114420	2.311930
F	2.161590	-1.922740	3.745990
F	2.140050	-4.449410	2.723710
F	1.092090	-4.896500	0.253040
F	0.083030	-2.897050	-1.175220
F	-1.547070	-0.457840	2.239450
F	2.028440	-1.009330	-2.152230
F	4.389850	0.025040	-2.831620
F	5.252390	2.347590	-1.697130
F	3.681640	3.617200	0.129650
F	1.317570	2.630080	0.802650
F	-0.632260	2.681410	-1.187940
F	-2.427640	4.345320	-0.122440
F	-3.778890	3.644350	2.136900
F	-3.298470	1.223680	3.295910
O	-5.544990	-2.388210	-2.573170
H	-2.092060	-1.494400	0.194140
H	-4.336320	-2.415060	-0.299580
H	-3.969170	-1.178190	-4.378870
H	-1.716650	-0.237500	-3.880090
H	-5.771820	-2.252470	-3.498800

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[H-Q-B(C_6F_5)$_2$Ph]$^+$

C	1.13301	-2.49734	-2.01314
C	2.46268	-2.53374	-1.82463
C	3.19809	-1.28907	-1.85034
C	2.61196	-0.03530	-2.27733
C	1.28998	0.01219	-2.50921
C	0.44380	-1.20848	-2.32152
O	-0.76104	-1.14060	-2.41342
O	4.42652	-1.35575	-1.48139
H	0.50435	-3.37793	-1.93168
H	3.00930	-3.43364	-1.56566
H	3.25431	0.83600	-2.37222
H	0.77187	0.91656	-2.80960
H	4.84929	-0.48217	-1.37781
B	-0.42703	-0.35846	0.94930
C	0.73714	0.70242	1.09916
C	-0.19240	-1.86385	1.22448
C	-1.79558	0.12736	0.35900
C	0.49630	2.05519	1.37343
C	1.47889	3.03562	1.30947
C	2.76738	2.68902	0.91109
C	3.04857	1.36041	0.62919
C	2.05901	0.40375	0.77655
C	0.74687	-2.31036	2.17225
C	0.94108	-3.66431	2.41224
C	0.21462	-4.60840	1.68546
C	-0.71843	-4.19587	0.73510
C	-0.92913	-2.83771	0.52060
C	-1.87530	1.05965	-0.67717
C	-3.06712	1.47234	-1.24381
C	-4.26035	0.96169	-0.74125
C	-4.23888	0.04301	0.30162
C	-3.01834	-0.36321	0.82622
F	-0.72689	2.45623	1.69485
F	1.19522	4.29759	1.58112
F	3.70192	3.61111	0.78536
F	4.25763	0.99930	0.15653
F	2.43645	-0.85389	0.47784
F	-0.74348	1.57374	-1.19806
F	-3.08125	2.33886	-2.24812
F	-5.41083	1.34836	-1.25871
F	-5.37524	-0.43616	0.78370
F	-3.04857	-1.23467	1.83170
H	1.31838	-1.58228	2.74240
H	1.65195	-3.98830	3.16479
H	0.36756	-5.66697	1.86999
H	-1.29543	-4.93140	0.18370
H	-1.66796	-2.52111	-0.21252

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[H-Q-B(C_6F_5)$_2$Ph]$^\bullet$

C	3.054140	-0.485670	-0.008890
C	4.405520	-0.615360	-0.135200
C	4.955910	-1.288780	-1.254890
C	4.121410	-1.832710	-2.260910
C	2.766600	-1.710960	-2.144140
C	2.184030	-1.042690	-1.012330
O	0.911100	-0.976180	-0.981970
O	6.282840	-1.374130	-1.306420
H	2.614540	0.025220	0.838480
H	5.089300	-0.209100	0.601070
H	4.564320	-2.338030	-3.114480
H	2.084620	-2.105470	-2.888510
H	6.573240	-1.840880	-2.101510
B	0.006210	-0.433390	0.185700
C	0.134380	1.192510	0.290850
C	0.468690	-1.252190	1.503460
C	-1.491830	-0.774360	-0.351690
C	-0.690910	1.833430	1.214970
C	-0.748310	3.210380	1.374380
C	0.036730	4.018150	0.561980
C	0.858120	3.431500	-0.387100
C	0.883310	2.045990	-0.509950
C	0.838240	-0.656660	2.713770

C	1.277770	-1.415870	3.797780
C	1.357050	-2.800380	3.694040
C	0.992560	-3.418900	2.499490
C	0.556890	-2.650460	1.425690
C	-1.850690	-0.415680	-1.649270
C	-3.109920	-0.638080	-2.187030
C	-4.084920	-1.229030	-1.394840
C	-3.784120	-1.577460	-0.087370
C	-2.506690	-1.340710	0.412890
F	-1.486640	1.098400	2.003810
F	-1.548830	3.762740	2.283880
F	0.000220	5.341140	0.694200
F	1.612410	4.195190	-1.178080
F	1.699700	1.564170	-1.466390
F	-0.955730	0.195830	-2.442440
F	-3.395250	-0.283690	-3.441240
F	-5.301760	-1.451670	-1.886210
F	-4.722110	-2.132410	0.680590
F	-2.302240	-1.682730	1.687100
H	0.789540	0.424500	2.819570
H	1.555090	-0.923280	4.725000
H	1.695950	-3.394500	4.536990
H	1.043000	-4.500020	2.409550
H	0.265930	-3.147730	0.501430

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$[H\text{-}Q\text{-}B(C_6F_5)_2Ph]^-$

C	-0.648640	2.448670	-0.061010
C	-1.121600	3.720570	-0.370030
C	-1.639160	4.544720	0.622690
C	-1.679810	4.085060	1.936860
C	-1.210710	2.815000	2.247740
C	-0.687560	1.971250	1.258610
O	-0.250250	0.768930	1.652020
O	-2.094100	5.793540	0.261010
H	-0.240980	1.827890	-0.850060
H	-1.091370	4.089000	-1.390370
H	-2.082860	4.722150	2.722850
H	-1.239470	2.442230	3.266140
H	-2.414010	6.232890	1.055500
B	0.113190	-0.340070	0.746160
C	1.494080	-0.029680	-0.124220
C	-1.202910	-0.700520	-0.200680
C	0.508630	-1.602370	1.697730
C	1.920930	-0.899020	-1.124800
C	3.124480	-0.778730	-1.802520
C	3.988040	0.254040	-1.467740
C	3.623410	1.137360	-0.466760
C	2.402800	0.977540	0.185540
C	-1.358440	-0.489230	-1.565860
C	-2.514410	-0.798310	-2.274840
C	-3.596980	-1.342200	-1.604900
C	-3.505920	-1.556530	-0.238480
C	-2.331010	-1.228910	0.427680
C	1.054980	-1.359760	2.965040
C	1.464970	-2.398250	3.797590
C	1.339490	-3.721250	3.379660
C	0.800660	-3.987930	2.123680
C	0.395320	-2.940330	1.299200
F	1.141670	-1.932260	-1.491410
F	3.468360	-1.644690	-2.764650
F	5.158440	0.390690	-2.102310
F	4.454020	2.132590	-0.129460
F	2.154010	1.870180	1.154760
F	-0.378940	0.073060	-2.298800
F	-2.332310	-1.448530	1.747460
F	-4.551940	-2.071540	0.419910
F	-4.719350	-1.647670	-2.265080
F	-2.596290	-0.568110	-3.591380
H	1.146950	-0.328770	3.297090
H	1.882080	-2.176550	4.777100
H	1.656360	-4.535260	4.026230
H	0.693160	-5.015870	1.786140
H	-0.023980	-3.167700	0.321670

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$[H\text{-}Q\text{-}B(C_6F_5)Ph_2]^+$

C	-3.20304	0.08668	-0.20690
C	-4.45376	0.59428	-0.19136
C	-4.85771	1.49155	-1.23401
C	-3.99078	1.88542	-2.32644
C	-2.74596	1.38348	-2.37324
C	-2.26394	0.43374	-1.32160
O	-1.15273	-0.03509	-1.39765
O	-6.06496	1.94139	-1.14832
H	-2.84597	-0.60872	0.54864
H	-5.17451	0.36500	0.58580
H	-4.36843	2.57164	-3.07969
H	-2.04091	1.62644	-3.16253
H	-6.32026	2.54667	-1.86622
B	0.63262	-0.94348	0.66556
C	0.72796	-2.37552	0.07132
C	-0.53726	-0.50894	1.62104
C	1.73344	0.12110	0.29012
C	1.98351	-2.93166	-0.23181
C	2.10188	-4.21806	-0.74400
C	0.95718	-4.97002	-0.99880
C	-0.30229	-4.43536	-0.73330
C	-0.40915	-3.15883	-0.19494
C	-1.27451	-1.44481	2.36536
C	-2.36799	-1.05880	3.14507
C	-2.74909	0.27955	3.19435

C	-2.02112	1.23459	2.47903
C	-0.92552	0.84059	1.71423
C	2.18445	0.28263	-1.02247
C	3.14847	1.21779	-1.37403
C	3.71133	2.01796	-0.38690
C	3.29941	1.88639	0.93442
C	2.32085	0.95288	1.24602
F	1.66333	-0.45028	-2.00813
F	3.53198	1.35783	-2.63838
F	4.63452	2.91007	-0.70602
F	3.84025	2.64927	1.87614
F	1.95771	0.85278	2.52688
H	2.88186	-2.34787	-0.04839
H	3.08234	-4.63224	-0.95357
H	1.04560	-5.97104	-1.40851
H	-1.19392	-5.01719	-0.94305
H	-1.39754	-2.75164	0.00620
H	-0.98154	-2.49028	2.34179
H	-2.91127	-1.80077	3.72128
H	-3.59168	0.58399	3.80749
H	-2.29542	2.28350	2.53929
H	-0.35825	1.59276	1.16995

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[H-Q-B(C_6F_5)Ph_2]$^{\cdot}$

C	2.401250	0.767170	0.334000
C	3.606280	1.370790	0.543220
C	4.629580	1.277360	-0.432830
C	4.422350	0.568550	-1.640000
C	3.219190	-0.038450	-1.861450
C	2.169390	0.028990	-0.880770
O	1.078970	-0.564640	-1.164930
O	5.778570	1.890830	-0.154370
H	1.605210	0.830010	1.064850
H	3.812830	1.936300	1.444520
H	5.218570	0.514290	-2.377120
H	3.010850	-0.593480	-2.768920
H	6.415570	1.781030	-0.872810
B	-0.169200	-0.824080	-0.214080
C	-0.945930	0.598160	0.037020
C	0.434790	-1.518260	1.120940
C	-1.103360	-1.788690	-1.108040
C	-2.093030	0.571450	0.831780
C	-2.894070	1.678890	1.071430
C	-2.567790	2.893300	0.482490
C	-1.448240	2.970860	-0.328980
C	-0.673730	1.834090	-0.538210
C	0.303320	-1.009200	2.418510
C	0.877080	-1.644690	3.518910
C	1.604480	-2.817830	3.345080
C	1.748470	-3.349960	2.065360
C	1.167870	-2.707000	0.976240
C	-1.291120	-1.520430	-2.471150
C	-2.115230	-2.311310	-3.265540
C	-2.786490	-3.395980	-2.704310
C	-2.624750	-3.675960	-1.350920
C	-1.791740	-2.879810	-0.566370
F	-2.466360	-0.574730	1.414630
F	-3.970840	1.589640	1.850980
F	-3.320710	3.969780	0.697060
F	-1.121910	4.129240	-0.905350
F	0.388030	2.005290	-1.353650
H	-0.257860	-0.090890	2.580610
H	0.751500	-1.224810	4.512640
H	2.050960	-3.317130	4.199520
H	2.307150	-4.269870	1.919130
H	1.271400	-3.141800	-0.016360
H	-0.775980	-0.671890	-2.918940
H	-2.238550	-2.082350	-4.320250
H	-3.432480	-4.016190	-3.318450
H	-3.146860	-4.517250	-0.904470
H	-1.672210	-3.110010	0.489330

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[H-Q-B(C_6F_5)Ph_2]$^{-}$

C	2.417740	0.812680	0.300970
C	3.640380	1.420630	0.562680
C	4.693230	1.310400	-0.339520
C	4.510650	0.583890	-1.512620
C	3.289390	-0.026740	-1.774050
C	2.218030	0.071200	-0.875510
O	1.074670	-0.530380	-1.215340
O	5.884710	1.932770	-0.031100
H	1.607150	0.909260	1.013580
H	3.792060	1.991300	1.473350
H	5.327770	0.492000	-2.227120
H	3.134390	-0.596930	-2.684140
H	6.500050	1.759630	-0.750720
B	-0.069670	-0.788060	-0.292820
C	-0.923920	0.608320	0.041450
C	0.463750	-1.551330	1.052360
C	-1.088770	-1.732290	-1.155270
C	-2.039550	0.566240	0.876750
C	-2.859200	1.654660	1.145560
C	-2.589240	2.871400	0.538850
C	-1.507300	2.966700	-0.319360
C	-0.710540	1.848800	-0.555540
C	0.333520	-1.107550	2.373270
C	0.848480	-1.825400	3.452680
C	1.518950	-3.024900	3.236540
C	1.671460	-3.491280	1.931820
C	1.151400	-2.761710	0.867250

C	-1.192540	-1.552790	-2.542490
C	-2.064760	-2.310290	-3.320160
C	-2.868830	-3.280030	-2.723900
C	-2.784800	-3.479370	-1.348510
C	-1.906540	-2.714500	-0.581720
F	-2.385970	-0.581890	1.483750
F	-3.909090	1.544230	1.970940
F	-3.365540	3.936110	0.776650
F	-1.244020	4.135240	-0.919960
F	0.295370	2.047910	-1.419430
H	-0.176690	-0.166390	2.571380
H	0.726890	-1.445170	4.464030
H	1.921460	-3.589180	4.073640
H	2.197320	-4.424880	1.747060
H	1.276250	-3.132550	-0.148470
H	-0.558380	-0.804680	-3.012490
H	-2.118080	-2.147400	-4.394260
H	-3.550860	-3.875400	-3.325600
H	-3.402930	-4.236280	-0.871380
H	-1.845770	-2.886920	0.490190

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$[H\text{-}Q\text{-}BPh_3]^+$

C	-2.07923	1.24862	1.62690
C	-3.41036	1.25818	1.40578
C	-4.04542	0.04659	0.97218
C	-3.32944	-1.18022	0.73245
C	-2.00365	-1.22520	0.97302
C	-1.30560	-0.02876	1.54440
O	-0.18213	-0.10761	1.98416
O	-5.32484	0.12577	0.78434
H	-1.52783	2.12771	1.94559
H	-4.02844	2.14279	1.51042
H	-3.86955	-2.04406	0.35424
H	-1.40831	-2.12303	0.82142
H	-5.73128	-0.70669	0.48912
B	1.25087	-0.00868	-0.64126
C	2.64570	0.07356	0.04656
C	0.47881	1.31926	-0.99734
C	0.60209	-1.41853	-0.89859
C	3.66055	-0.85283	-0.26049
C	4.91130	-0.77990	0.34079
C	5.16462	0.20206	1.29774
C	4.17106	1.11719	1.63953
C	2.93392	1.06130	1.00787
C	1.18695	2.51553	-1.20415
C	0.53652	3.71384	-1.49704
C	-0.85283	3.75463	-1.57608
C	-1.58585	2.58653	-1.37884
C	-0.92286	1.38801	-1.11495
C	0.92051	-2.49380	-0.04533
C	0.29712	-3.73360	-0.17044
C	-0.66006	-3.93316	-1.16682
C	-0.97715	-2.89461	-2.04132
C	-0.35176	-1.65636	-1.90572
H	3.46692	-1.63027	-0.99521
H	5.68687	-1.48934	0.07190
H	6.13650	0.25247	1.77809
H	4.36582	1.87515	2.39104
H	2.16614	1.78290	1.27527
H	2.27081	2.50321	-1.14305
H	1.11540	4.61736	-1.65736
H	-1.36068	4.68757	-1.79737
H	-2.66961	2.60699	-1.45430
H	-1.50821	0.47384	-1.03202
H	1.65338	-2.34237	0.74177
H	0.56165	-4.54519	0.49991
H	-1.13952	-4.90120	-1.27434
H	-1.69561	-3.05631	-2.83884
H	-0.59281	-0.86334	-2.60867

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$[H\text{-}Q\text{-}BPh_3]^{\cdot}$

C	2.311690	0.195510	0.208220
C	3.676290	0.241500	0.250310
C	4.430330	0.196350	-0.946250
C	3.791590	0.116010	-2.205700
C	2.426850	0.075620	-2.263470
C	1.637140	0.103480	-1.061820
O	0.370030	0.061730	-1.206570
O	5.757920	0.238920	-0.821810
H	1.717050	0.233380	1.111800
H	4.213390	0.314970	1.188900
H	4.388840	0.087680	-3.112880
H	1.891260	0.012650	-3.203930
H	6.188060	0.202730	-1.686170
B	-0.740500	-0.028920	-0.065680
C	-0.823230	1.432770	0.636030
C	-0.302230	-1.245920	0.918310
C	-2.090280	-0.335270	-0.901760
C	-1.843270	1.643900	1.580030
C	-1.994090	2.857360	2.240530
C	-1.132590	3.918080	1.959990
C	-0.132290	3.746820	1.011450
C	0.013810	2.519720	0.361030
C	-0.196060	-1.133590	2.310550
C	0.190760	-2.212520	3.106490
C	0.487740	-3.440060	2.523480
C	0.386500	-3.581890	1.140440
C	-0.007250	-2.500350	0.358530
C	-2.399490	0.424680	-2.039570
C	-3.568450	0.219350	-2.763710

C	-4.478240	-0.754730	-2.353470
C	-4.202330	-1.513460	-1.221350
C	-3.019520	-1.305510	-0.510500
H	-2.536990	0.832070	1.791510
H	-2.789420	2.981830	2.969680
H	-1.250110	4.869820	2.468820
H	0.533940	4.569890	0.768720
H	0.795490	2.432700	-0.391220
H	-0.413640	-0.179030	2.784550
H	0.261090	-2.091940	4.183820
H	0.790440	-4.281250	3.139680
H	0.607410	-4.538310	0.674990
H	-0.102280	-2.629970	-0.718570
H	-1.704580	1.199520	-2.359160
H	-3.777860	0.821370	-3.643570
H	-5.395440	-0.916600	-2.911910
H	-4.905650	-2.273120	-0.891970
H	-2.812490	-1.916020	0.365590

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[H-Q-BPh_3]$^-$

C	2.340940	0.323670	0.227140
C	3.726280	0.358960	0.340980
C	4.535820	0.179720	-0.776040
C	3.943590	-0.035670	-2.016910
C	2.558580	-0.074790	-2.133670
C	1.724200	0.103140	-1.018700
O	0.407070	0.071420	-1.225280
O	5.904740	0.226400	-0.606170
H	1.723320	0.470540	1.104980
H	4.197490	0.527950	1.304120
H	4.567120	-0.176850	-2.899140
H	2.085170	-0.245720	-3.095170
H	6.310340	0.065350	-1.464080
B	-0.644870	0.002450	-0.143400
C	-0.840590	1.460070	0.575640
C	-0.298270	-1.218900	0.897260
C	-2.032840	-0.344980	-0.939370
C	-1.836070	1.671090	1.544750
C	-2.048360	2.912550	2.138030
C	-1.267270	4.005730	1.766790
C	-0.286750	3.834860	0.793930
C	-0.084720	2.583370	0.211750
C	-0.287190	-1.131090	2.294920
C	-0.005820	-2.233050	3.105790
C	0.282900	-3.466930	2.533390
C	0.288500	-3.584510	1.143340
C	-0.000100	-2.478940	0.350620
C	-2.232420	0.100980	-2.254350
C	-3.421410	-0.131560	-2.941130
C	-4.463030	-0.822880	-2.324390
C	-4.292750	-1.279810	-1.020330
C	-3.093710	-1.045190	-0.348110
H	-2.473270	0.835040	1.830660
H	-2.829010	3.031540	2.885980
H	-1.427390	4.978440	2.224710
H	0.323660	4.680500	0.485180
H	0.680750	2.472540	-0.552410
H	-0.491670	-0.171900	2.766220
H	-0.006530	-2.123560	4.188010
H	0.504980	-4.327090	3.159800
H	0.518330	-4.541810	0.681190
H	0.005170	-2.579420	-0.733410
H	-1.421430	0.636040	-2.742230
H	-3.539460	0.226550	-3.961700
H	-5.393390	-1.006930	-2.855820
H	-5.092910	-1.828790	-0.528730
H	-2.968530	-1.432180	0.662320

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[H-Q-BEt_3]$^+$

C	1.34661	-0.53294	0.53092
C	2.56159	-1.08081	0.71487
C	3.72374	-0.37972	0.22498
C	3.65563	0.89383	-0.45897
C	2.45047	1.45928	-0.64544
C	1.21006	0.78524	-0.15406
O	0.14308	1.30631	-0.30434
O	4.84915	-0.96783	0.43437
H	0.42494	-1.00706	0.85782
H	2.72300	-2.03164	1.21123
H	4.57523	1.36107	-0.80066
H	2.31802	2.41489	-1.14424
H	5.62819	-0.48937	0.09796
B	-2.12635	-0.08306	-0.25337
C	-1.60591	-0.96808	-1.46035
C	-2.08910	-0.67577	1.21970
C	-2.89000	1.26838	-0.52838
C	-2.85306	2.32259	0.58387
C	-3.51965	-0.97591	1.71798
C	-2.68561	-2.03203	-1.75808
H	-1.41617	-0.38217	-2.36675
H	-0.67326	-1.50047	-1.21350
H	-1.50903	-1.60844	1.28694
H	-1.62945	0.04802	1.90914
H	-3.93831	0.96820	-0.70311
H	-2.57002	1.71018	-1.47959
H	-3.44991	3.20195	0.33051
H	-1.82751	2.66358	0.76220
H	-3.23247	1.92965	1.53138
H	-4.01991	-1.70014	1.06853
H	-4.13296	-0.07159	1.73038

H	-3.51225	-1.38973	2.72898
H	-2.40406	-2.66072	-2.60608
H	-2.84379	-2.68793	-0.89648
H	-3.64501	-1.56525	-2.00027

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$[H\text{-}BQ\text{-}BEt_3]^{\cdot}$

C	1.257290	-0.843840	-0.289040
C	2.599220	-1.036420	-0.489280
C	3.511330	0.013040	-0.251770
C	3.059360	1.271520	0.194950
C	1.718670	1.475100	0.395440
C	0.772490	0.427530	0.159460
O	-0.463680	0.704650	0.364240
O	4.807210	-0.250110	-0.468300
H	0.545320	-1.640220	-0.459000
H	2.992180	-1.988390	-0.827490
H	3.774410	2.069880	0.373950
H	1.328580	2.428380	0.733860
H	5.348730	0.525780	-0.276220
B	-1.759010	-0.135390	0.100530
C	-1.840240	-0.210340	-1.548990
C	-1.663790	-1.622870	0.784260
C	-2.930540	0.772970	0.757310
C	-3.086400	2.167320	0.145370
C	-0.987460	-1.663080	2.157760
C	-3.143370	-0.859990	-2.009850
H	-1.757560	0.798040	-1.974500
H	-0.983690	-0.783060	-1.935450
H	-1.214550	-2.382940	0.126770
H	-2.706490	-1.947850	0.903090
H	-3.883630	0.232630	0.671980
H	-2.753100	0.873030	1.838600
H	-3.821230	2.783800	0.673870
H	-3.405490	2.105610	-0.901200
H	-2.132620	2.707190	0.158310
H	-1.058370	-2.648110	2.630880
H	-1.443840	-0.935360	2.836410
H	0.080100	-1.415880	2.098230
H	-3.198470	-0.946000	-3.100890
H	-3.254000	-1.866610	-1.592850
H	-4.008860	-0.274870	-1.682150

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$[H\text{-}Q\text{-}BEt_3]^{-}$

C	1.254930	-0.811690	-0.266970
C	2.610680	-1.018620	-0.500950
C	3.536750	-0.010240	-0.259010
C	3.088810	1.215810	0.225330
C	1.735340	1.427070	0.458530
C	0.774110	0.423020	0.220360
O	-0.487210	0.697970	0.490050
O	4.873380	-0.267530	-0.508940
H	0.546740	-1.608620	-0.454330
H	2.967990	-1.973680	-0.875060
H	3.804300	2.015060	0.419930
H	1.378240	2.380690	0.834470
H	5.364820	0.530060	-0.288470
B	-1.725610	-0.125720	0.078280
C	-1.781790	-0.243040	-1.559850
C	-1.745720	-1.607650	0.810580
C	-2.962760	0.782290	0.663670
C	-3.052130	2.181110	0.048700
C	-1.140870	-1.610160	2.218070
C	-3.093550	-0.845520	-2.073750
H	-1.645840	0.751960	-2.011710
H	-0.949340	-0.850210	-1.947000
H	-1.252030	-2.392680	0.212850
H	-2.794890	-1.936940	0.881410
H	-3.922510	0.260910	0.521870
H	-2.843430	0.885890	1.753990
H	-3.806520	2.826530	0.520770
H	-3.296800	2.125280	-1.019700
H	-2.081420	2.682810	0.127230
H	-1.246420	-2.572290	2.738680
H	-1.613350	-0.843450	2.842910
H	-0.072330	-1.369250	2.182360
H	-3.123690	-0.967270	-3.165500
H	-3.268270	-1.834220	-1.630980
H	-3.949320	-0.219770	-1.792280

20) References

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