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SUPPORTING INFORMATION

Bonding and Stability of Donor Ligand-Supported Heavier Analogues of Cyanogen Halides (L′)PSi(X)(L)

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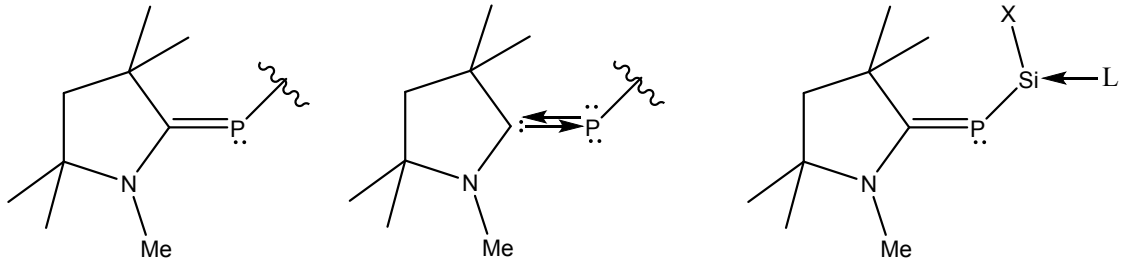
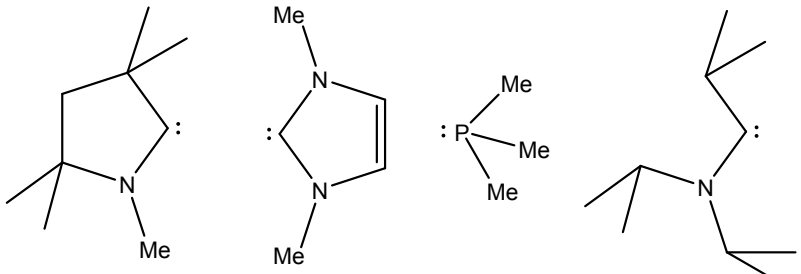
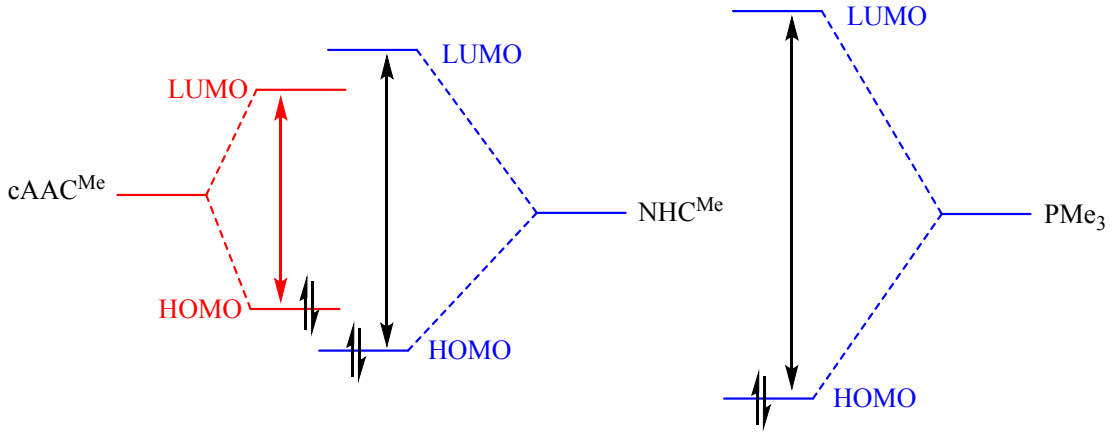




L = cAAC^{Me} L = NHC^{Me} L = PMe_3 L = aAAC

1-Cl; L = cAAC^{Me}, X = Cl
2-Cl; L = NHC^{Me}, X = Cl
3-Cl; L = PMe_3, X = Cl
4-Cl; L = aAAC, X = Cl

1-F; L = cAAC^{Me}, X = F
2-F; L = NHC^{Me}, X = F
3-F; L = PMe_3, X = F
4-F; L = aAAC, X = F



cAAC^{Me} possesses one N-atom bonded to the carbene carbon while NHC^{Me} has two adjacent N-atoms. The energy of HOMO of cAAC^{Me} is higher in energy and LUMO of cAAC^{Me} is lower in energy. In contrust the energy of HOMO of NHCC^{Me} is lower in energy and LUMO of NHC^{Me} is higher in energy. This is due to replacement of one of the σ-withdrawing and π-donating N-atoms of of NHC^{Me} by a σ-donating quarternary C-atom in cAAC^{Me}. The cAAC^{Me} ligand is thus superior σ-donor and π-acceptor than NHC^{Me}.

Scheme S1. cAAC^{Me} possesses one N-atom bonded to the carbene carbon while NHC^{Me} has two adjacent N-atoms. The energy of HOMO of cAAC^{Me} is higher in energy and LUMO of cAAC^{Me} is lower in energy. In contrast the energy of HOMO of NHC^{Me} is lower in energy and LUMO of NHC^{Me} is higher in energy. This is due to replacement of one of the s-withdrawing and p-donating N-atoms of NHC^{Me} by a s-donating quaternary C-atom in cAAC^{Me}. The cAAC^{Me} ligand is thus superior s-donor and p-acceptor than NHC^{Me}.

Abbreviations

cAAC^{Me}: cyclic alkyl(amino)carbene

NHC^{Me}: N-heterocyclic carbene

aAAC^{Me}: acyclic alkyl(amino)carbene

Mes* = 2,4,6-triteriarybutylphenyl

Tip = 2,4,6-triisopropylphenyl

EDA: Energy decomposition analysis.

NOCV: Natural orbital for chemical valence

NBO: Natural bond orbital

HOMO: Highest occupied molecular orbital

LUMO: Lowest un-occupied molecular orbital

SOMO: Singly occupied molecular orbital

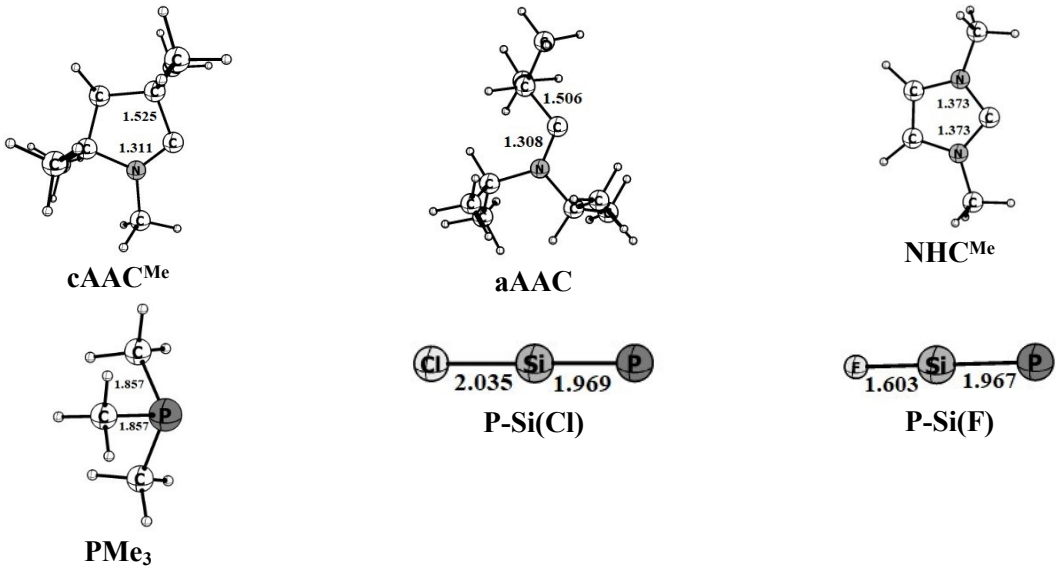


Figure S0. Optimized geometries of ligands cAAC^{Me}, aAAC, NHC^{Me}, PMe_3, and P-Si(Cl/F) at BP86(D3BJ)/def2-TZVPP level.

Table S1. Dissociation energy (D_e), change in Gibbs free energy (ΔG^{298}) and HOMO-LUMO gap (Δ_{H-L}) of cAAC-P-Si(Cl/F)-L complexes (L = cAAC^{Me}, NHC^{Me}, PMe_3 and aAAC).

Complex	D_e (kcal/mol)	ΔG^{298} (kcal/mol)	Δ_{H-L} (kcal/mol)
1-Cl	127.40	111.52	46.0
2-Cl	114.0	100.7	47.73
3-Cl	102.20	87.26	60.0
4-Cl	120.5	104.4	46.2
1-F	129.02	113.7	46.12
2-F	115.35	101.75	51.2

3-F	100.0	86.3	57.2
4-F	122.6	106.4	47.5

Table S2. NBO results of the complexes cAAC-P-Si(F)-L (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes (**1-F to 4-F**) at the BP86/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the C_{cAAC}–P, P–Si and Si–C_L bonds and partial charges q.

Complex	Bond	ON	Polarization and hybridization (%)		*WBI*	*q*	
						P	Si
1-F	C_{cAAC}–P	1.97	C: 65.13 s(38.7), p(61.0)	P: 34.9 s(19.0), p(80.2)	1.49	-0.12	0.97
		1.91	C: 42.3 s(0.00), p(99.9)	P: 57.7 s(0.0), p(99.5)			
	P–Si	1.90	P: 59.5 s(13.7), p(85.3)	Si: 40.5 s(33.1), p(66.1)	0.92		
	Si–C_L	1.66	Si: 39.4 s(42.4), p(56.9)	C: 60.6 s(25.5), p(69.7)	1.13		
		1.51	Si: 60.0 s(3.8), p(95.7)	C: 40.0 s(15.6), p(76.3)			
2-F	C_{cAAC}–P	1.97	C: 65.3 s(39.0), p(60.7)	P: 34.7 s(20.7), p(79.0)	1.51	-0.15	0.24
		1.91	C: 40.7 s(0.0), p(99.8)	P: 59.3 s(0.0), p(99.4)			
	P–Si	1.86	P: 64.4 s(13.7), p(85.4)	Si: 35.6 s(11.1), p(88.4)	0.88		
	Si–C_L	1.94	Si: 21.9 s(10.9), p(88.3)	C: 78.1 s(42.57), p(57.26)	0.79		
3-F	C_{cAAC}–P	1.97	C:65.1 S(38.9), p(60.8)	P: 34.9 s(20.8), p(78.4)	1.51	-0.18	0.57
		1.91	C: 40.7 s(0.0), p(99.8)	P: 59.3 S(0.0), p(99.5)			
	P–Si	1.90	P: 64.6 s(13.6), p(85.8)	Si: 35.4 s(10.0), p(88.5)	0.91		
	Si–P_L	1.93	Si: 23.7 S(6.0), p(92.0)	P: 76.3 s(29.2), p(70.8)	0.70		
4-F	C_{cAAC}–P	1.96	C:65 S(38.6), p(61.4)	P: 35 s(19), p(80), d(1)	1.47	-0.12	1.1
		1.90	C: 38.6 s(0.0), p(99.8)	P: 61.4 S(0.0), p(99.5)			
	P–Si	1.91	P: 59 s(14.1), p(85.9)	Si: 41 s(38.7), p(61.3)	0.95		
	Si– C_L	1.91	Si: 33.5 S(51.2), p(48.8)	C: 66.5 s(28.5), p(71.5)	1.24		
		1.84	Si: 39.6 S(3), p(97)	C: 60.4 s(9.8), p(90.2)			

Table S3. EDA-NOCV results of cAACP–Si(F)L bond of cAAC-P-Si(F)-L (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes using three different sets of fragments with different charges and electronic states (S = singlet, D = doublet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
cAAC-P-Si(F)-cAAC	E	$cAAC^{Me}$-P (D) + Si(F)-$cAAC^{Me}$ (D)	-62.8	200.6	-119.9	-13.7	**-129.8**
	D	$[cAAC^{Me}\text{-}P]^-$ (S) + $[Si(F)\text{-}cAAC^{Me}]^+$ (S)	-191.3	260.3	-236.4	-13.7	-203.4
	D	$[cAAC^{Me}\text{-}P]^+$ (S) + $[Si(F)\text{-}cAAC^{Me}]^-$ (S)	-215.3	226.4	-206.4	-13.7	-223.4
cAAC-P-Si(F)-NHC	E	$cAAC^{Me}$-P (D) + Si(F)-NHC^{Me} (D)	-59.2	182.8	-110.5	-11.1	**-120.4**
	D	$[cAAC^{Me}\text{-}P]^-$ (S) + $[Si(F)\text{-}NHC^{Me}]^+$ (S)	-172.0	225.6	-219.9	-11.1	-166.6
	D	$[cAAC^{Me}\text{-}P]^+$ (S) + $[Si(F)\text{-}NHC^{Me}]^-$ (S)	-242.7	230.6	-217.5	-11.1	-244.7
cAAC-P-Si(F)-PMe_3	E	$cAAC^{Me}$-P (D) + Si(F)-PMe_3 (D)	-64.4	192.5	-120.4	-12.4	**-124.1**
	D	$[cAAC^{Me}\text{-}P]^-$ (S) + $[Si(F)\text{-}PMe_3]^+$ (S)	-186.5	216.9	-226.2	-12.4	-164.7
	D	$[cAAC^{Me}\text{-}P]^+$ (S) + $[Si(F)\text{-}PMe_3]^-$ (S)	-238.2	260.2	-235.3	-12.4	-250.7
cAAC-P-Si(F)-aAAC	E	$cAAC^{Me}$-P (D) + Si(F)-aAAC (D)	-64.6	204.9	-123.2	-12.4	**-133.8**
	D	$[cAAC^{Me}\text{-}P]^-$ (S) + $[Si(F)\text{-}aAAC]^+$ (S)	-203.5	266.5	-242.4	-12.4	-215.1
	D	$[cAAC^{Me}\text{-}P]^+$ (S) + $[Si(F)\text{-}aAAC]^-$ (S)	-233.3	369.3	-259.5	-12.4	-330.7

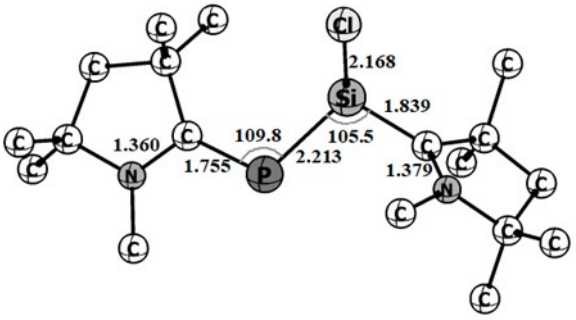
[a]D = Dative bond; E = Electron-sharing bond.

Table S4. The EDA-NOCV results at the BP86-D3(BJ)/TZ2P level of cAACP–Si(F)L bond of cAAC-P-Si(F)-L complexes (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) using (cAAC-P) and (Si(F)-L) in the electronic doublet (D) states as interacting fragments. Energies are in kcal/mol.

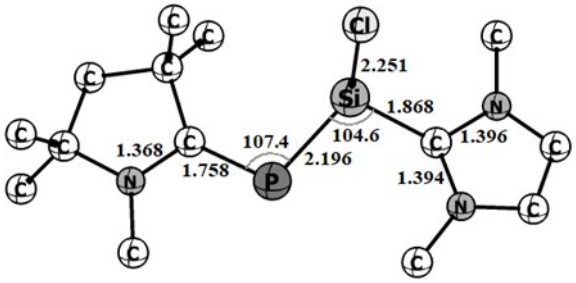
Energy	**Interaction**[c]	**cAAC-P (D) + Si(F)-cAAC (D)**	**cAAC-P (D) + Si(F)-NHC (D)**	**cAAC-P (D) + Si(F)-PMe_3 (D)**	**cAAC-P (D) + Si(F)-aAAC (D)**
ΔE_{int}		-62.8	-59.2	-64.4	-64.6
ΔE_{Pauli}		200.6	182.8	192.5	204.9
ΔE_{disp}[a]		-13.7 (5.2%)	-11.1 (4.6%)	-12.4 (4.8%)	-12.4 (4.6%)
ΔE_{elstat}[a]		-119.9 (45.5%)	-110.5 (45.6%)	-120.4 (46.9%)	-123.2 (45.7%)
ΔE_{orb}[a]		-129.8 (49.3%)	-120.4 (49.8%)	-124.1 (48.3%)	-133.8 (49.7%)
$\Delta E_{orb(1)}$[b]	cAACP–Si(F)L σ e^- sharing	-101.1 (77.9%)	-97.5 (81%)	-101.1 (81.4%)	-103.4 (77.3%)
$\Delta E_{orb(2)}$[b]	cAACP→Si(F)L π donation	-12.0 (9.2%)	-8.4 (7%)	-7.9 (6.3%)	-10.2 (7.6%)
$\Delta E_{orb(3)}$[b]	cAACP→Si(F)L π donation	-7.9 (6.0%)			-10.7 (4.0%)
	cAACP←Si(F)L σ back donation		-7.0 (5.8%)	-6.7 (5.4%)	
$\Delta E_{orb(4)}$[b]	cAACP→Si(F)L σ donation	-4.6 (3.5%)	-3.6 (3%)	-4.1 (3.3%)	-5.0 (3.7%)
$\Delta E_{orb(rest)}$[b]		-4.2 (3.2%)	-3.9 (3.2%)	-4.3 (3.4%)	-4.5 (3.3%)

[a]The values in the parentheses show the contribution to the total attractive interaction $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

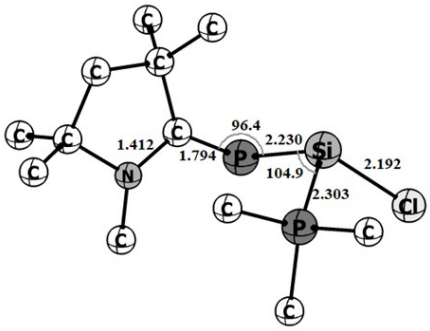
[b]The values in parentheses show the contribution to the total orbital interaction ΔE_{orb}.



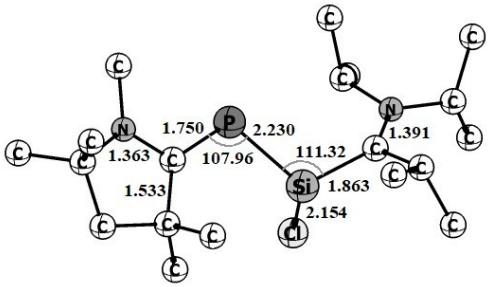
1T-Cl (23.6 kcal/mol)



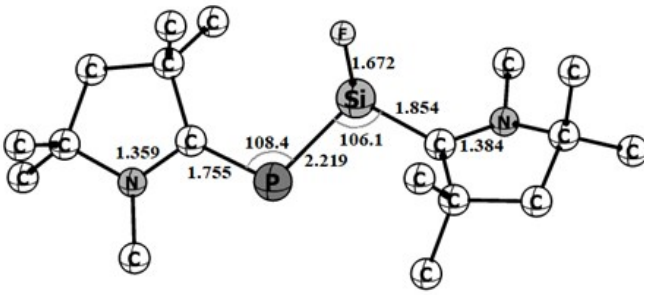
2T-Cl (32.1 kcal/mol)



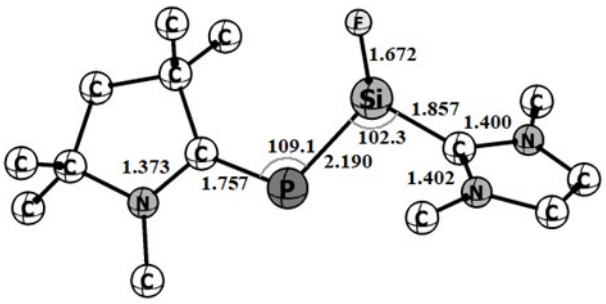
3T-Cl (37.6 kcal/mol)



4T-Cl (21.2 kcal/mol)



1T-F (24.4 kcal/mol)



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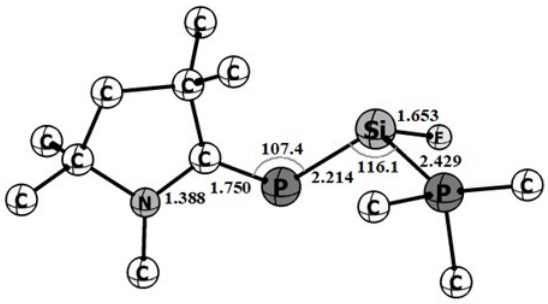
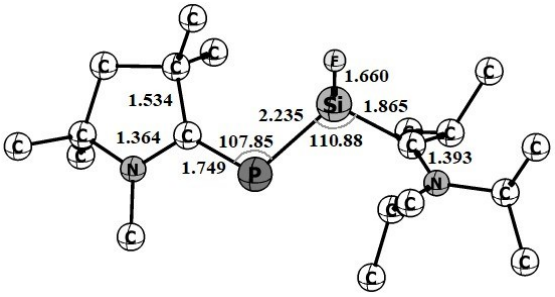
T-F (32.4 kcal/mol)



3T-F (40.7 kcal/mol)



4T-F (22.5 kcal/mol)

Figure S1. Optimized geometries of triplet state cAAC-PSi(Cl/F)-L complexes **1T-Cl** to **4T-Cl** and **1T-F** to **4T-F** with L = $cAAC^{Me}$ (**1T-Cl**, **1T-F**), NHC^{Me} (**2T-Cl**, **2T-F**), PMe_3 (**3T-Cl**, **3T-F**) and aAAC (**4T-Cl**,**4T-F**) at BP86(D3BJ)/def2-TZVPP level.

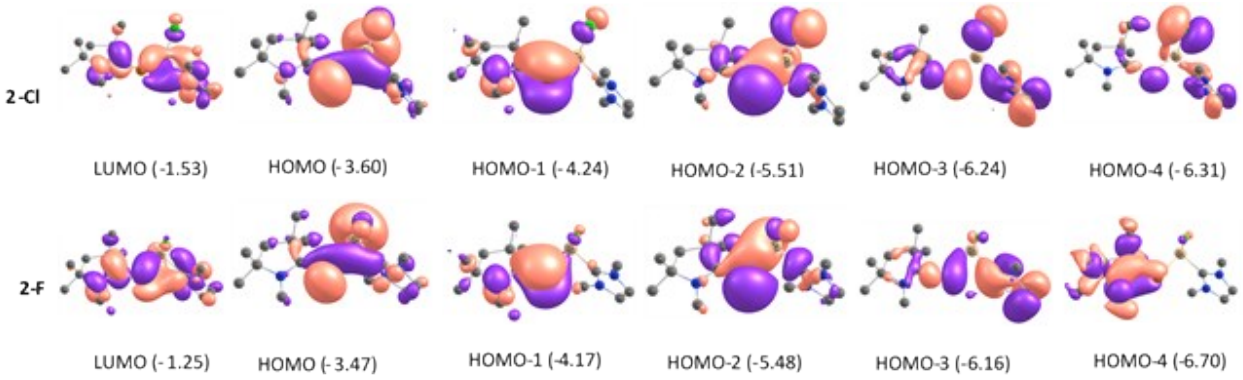


Figure S2. Molecular orbitals of complex **2-Cl** and **2-F** at BP86(D3BJ)/def2-TZVPP. Energy values in eV are given in parenthesis.

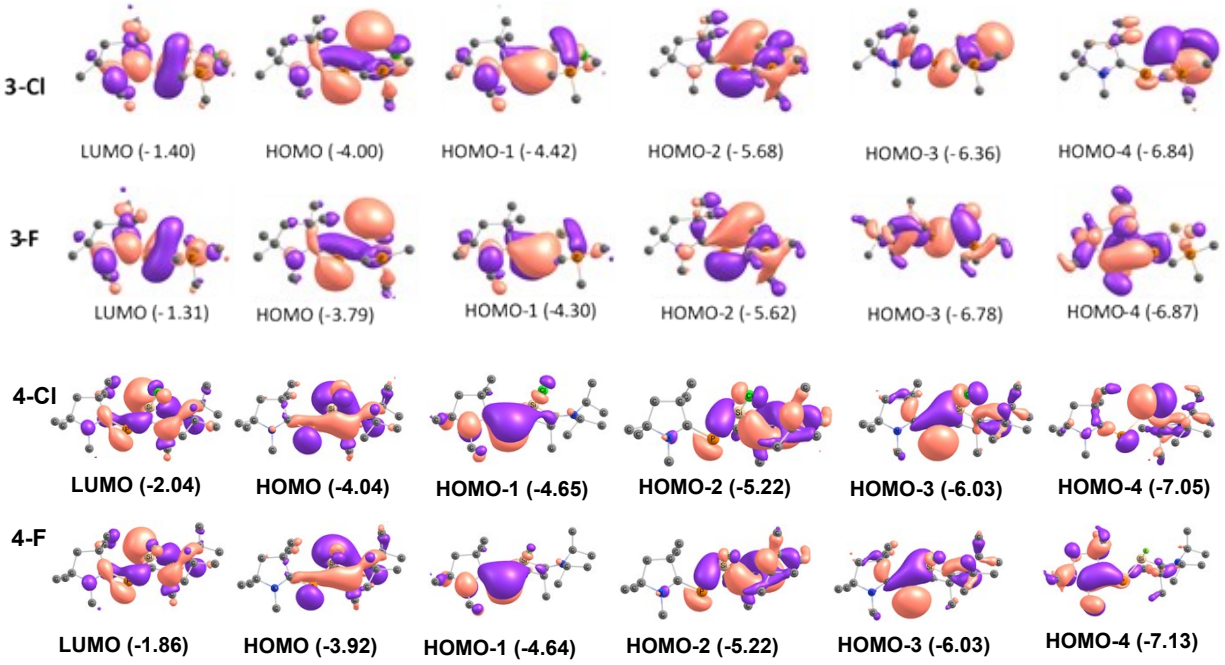
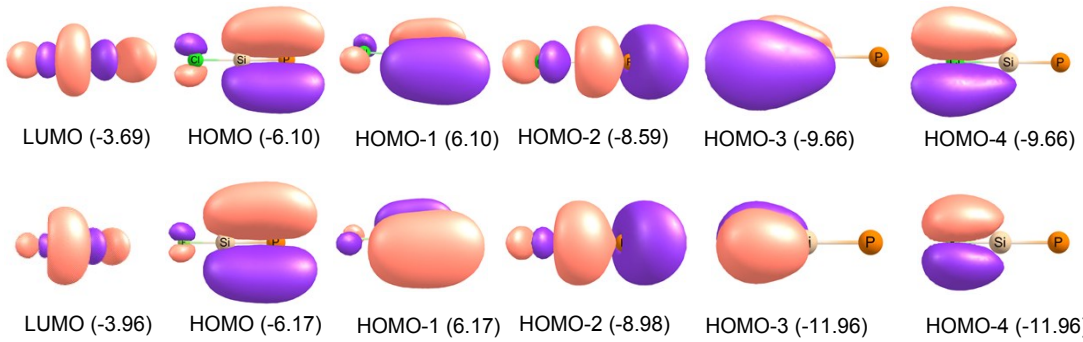


Figure S3. Molecular orbitals of complex **3-Cl** and **3-F** at BP86(D3BJ)/def2-TZVPP. Energy values in eV are given in parenthesis.



Molecular orbitals of complex **P-Si-Cl** at BP86(D3BJ)/def2-TZVPP. Energy values in eV are given in parenthesis.

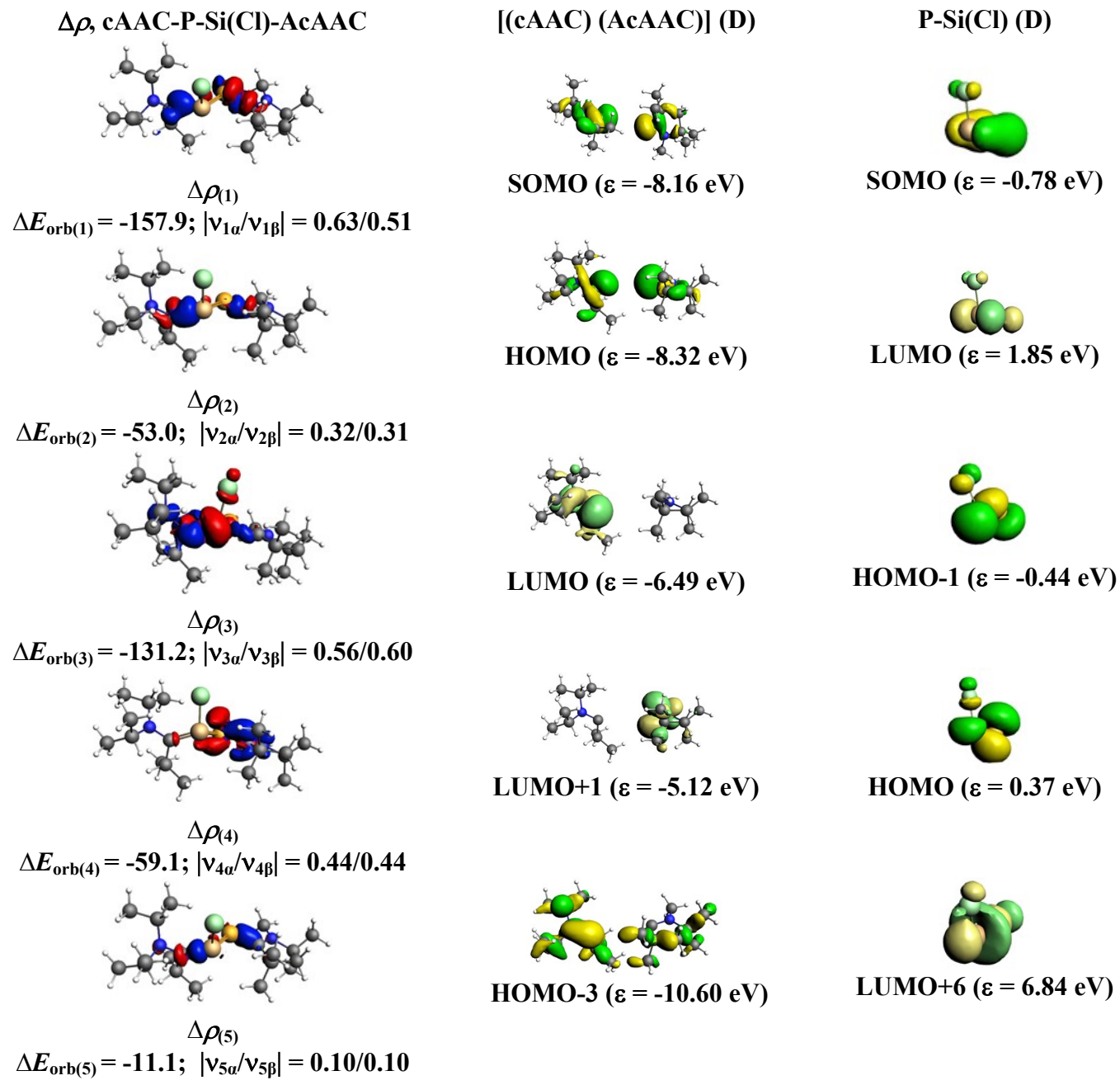


Figure S4. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of cAAC-P-Si(Cl)-AcAAC and the fragments orbitals of [(cAAC)(AcAAC)]$^+$ and [P-Si-Cl]$^-$ in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(7)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

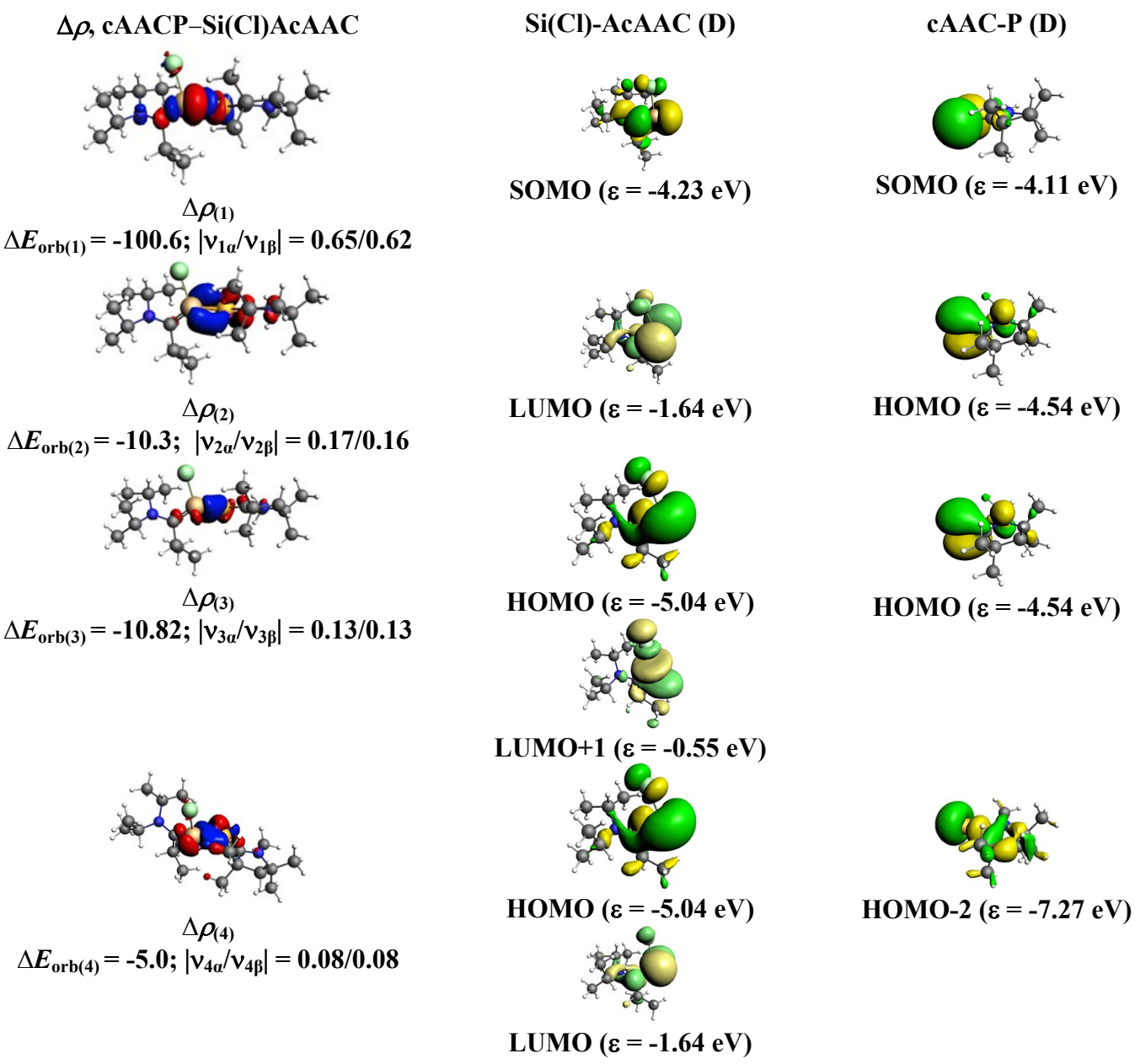


Figure S5. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(Cl)-AcAAC and the fragments orbitals of cAAC-P and (Cl)Si-AcAAC in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(3)}$ and isosurface value 0.0003 for $\Delta\rho_{(4)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

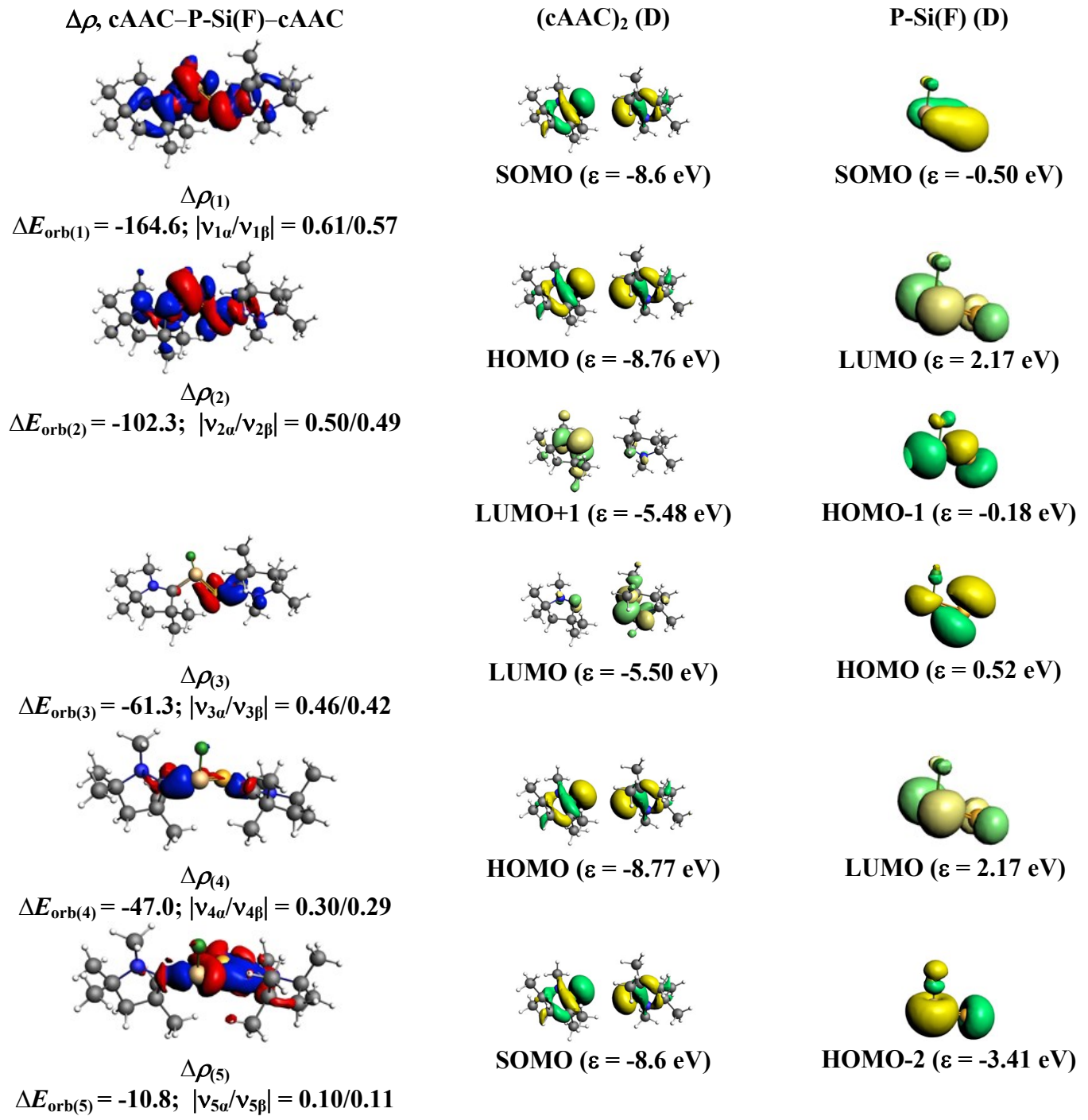


Figure S6. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of cAAC-P-Si(F)-cAAC and the fragments orbitals of $[(cAAC)_2]^+$ and $[P\text{-}Si\text{-}F]^-$ in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(4)}$ and isosurface value 0.0003 for $\Delta\rho_{(5)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

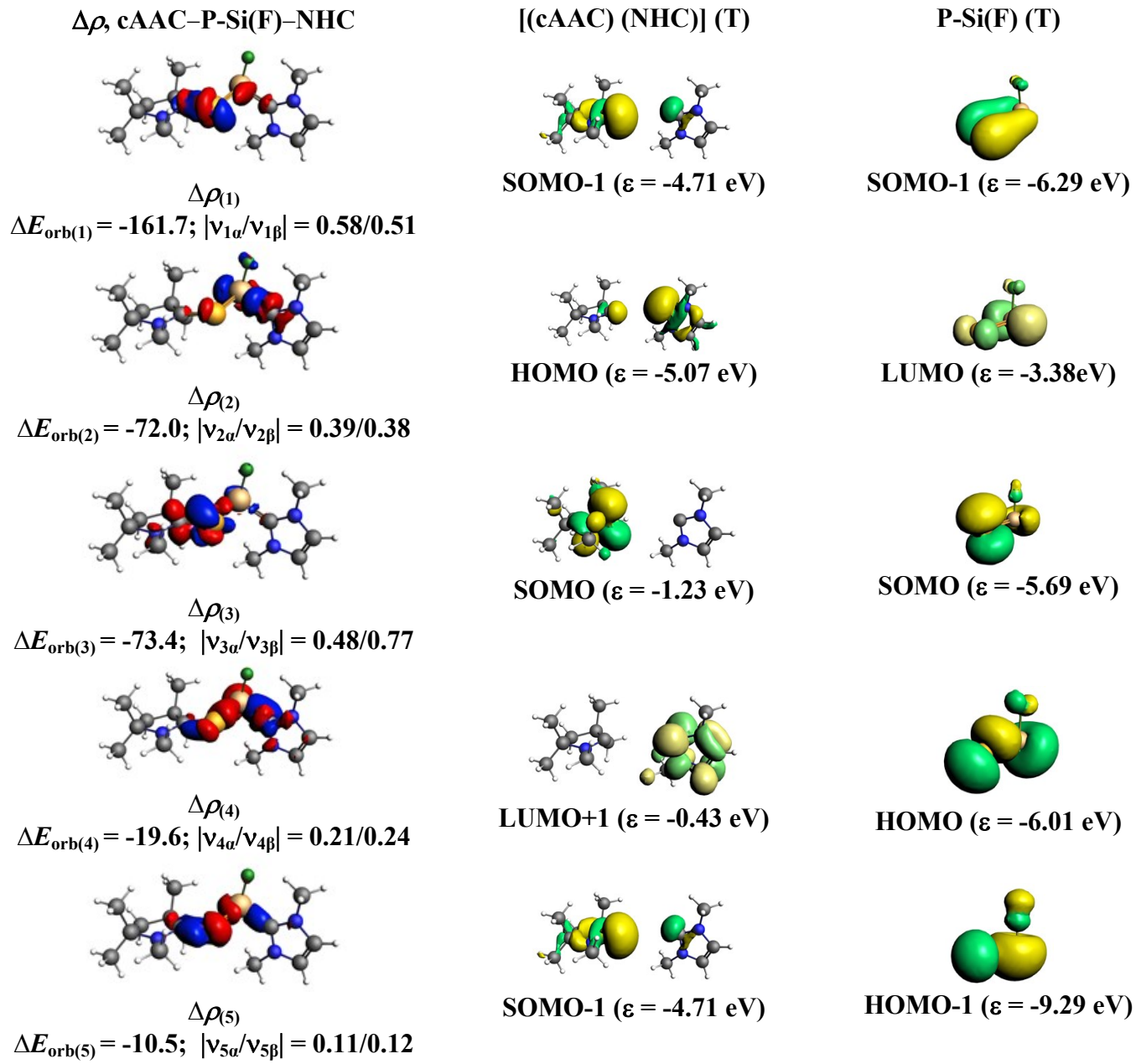


Figure S7. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of cAAC-P-Si(F)-NHC and the fragments orbitals of $[(cAAC)(NHC)]^{+}$ and $[P\text{-}Si\text{-}F]^{-}$ in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(3)}$ and isosurface value 0.001 for $\Delta\rho_{(4)-(5)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

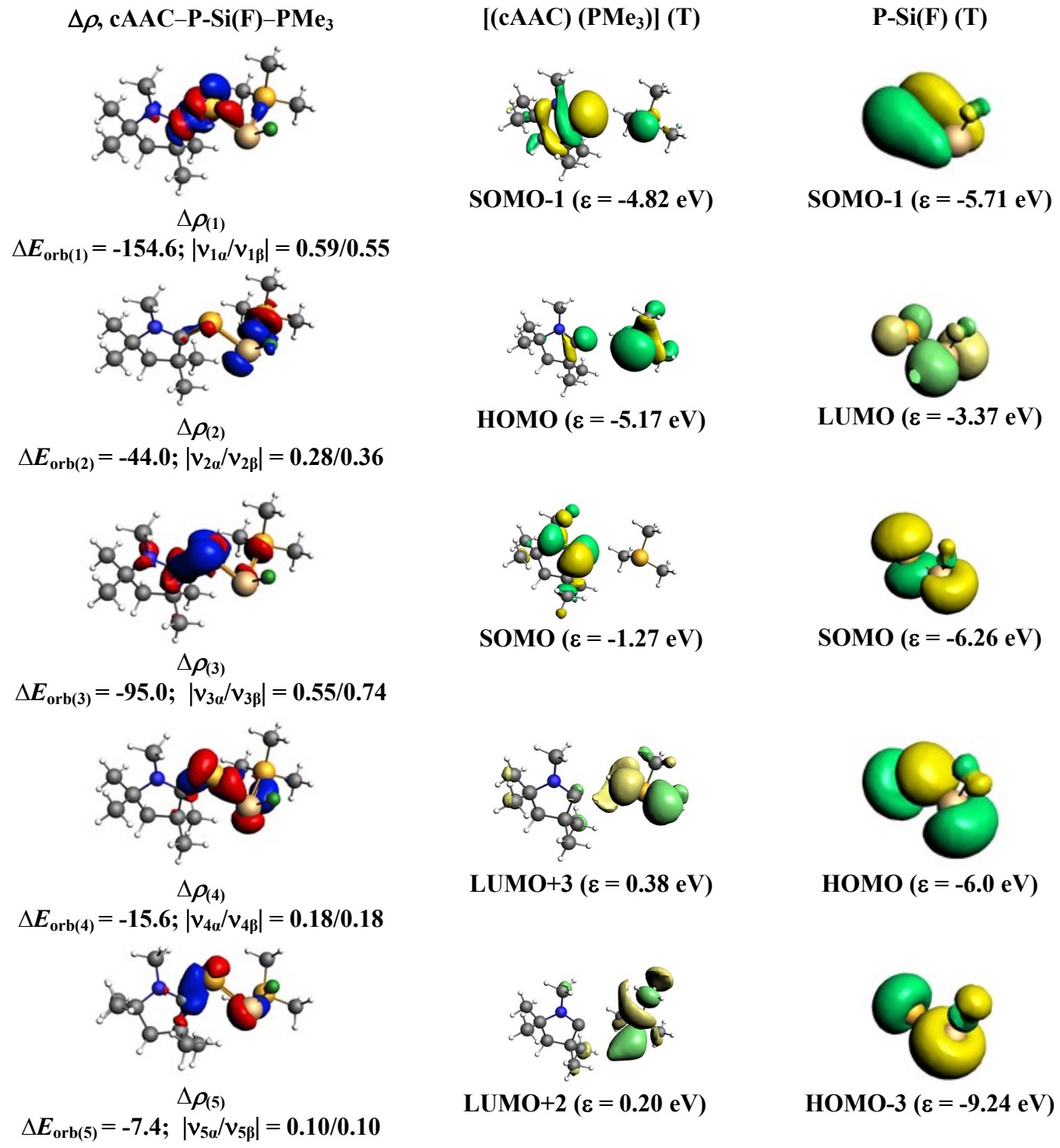


Figure S8. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of cAAC-P-Si(F)-PMe_3 and the fragments orbitals of [(cAAC) (PMe_3)] and [P-Si-F] in the triplet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

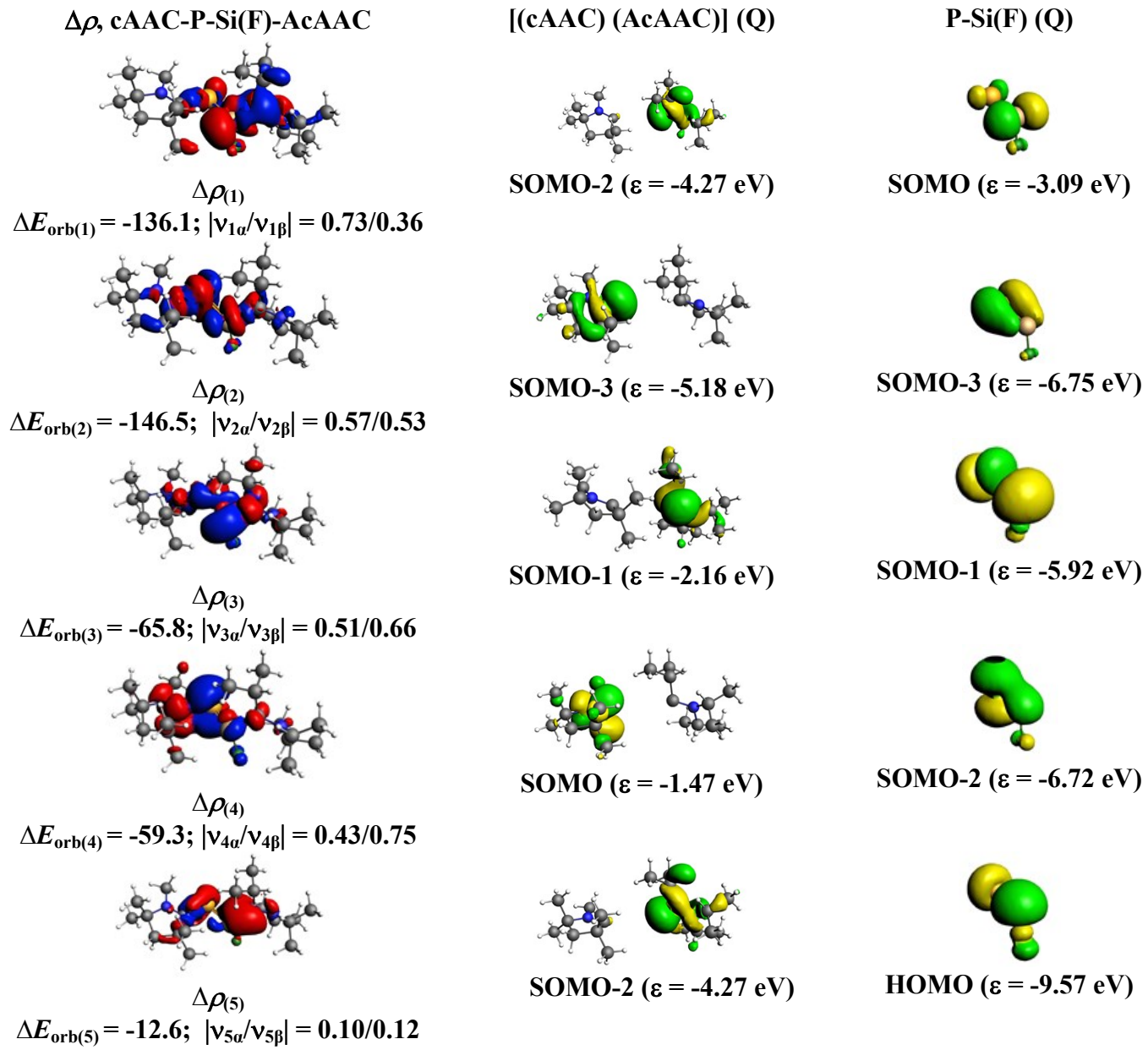


Figure S9. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of cAAC-P-Si(F)-AcAAC and the fragments orbitals of [(cAAC) (AcAAC)] and [P-Si-F] in the quartet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

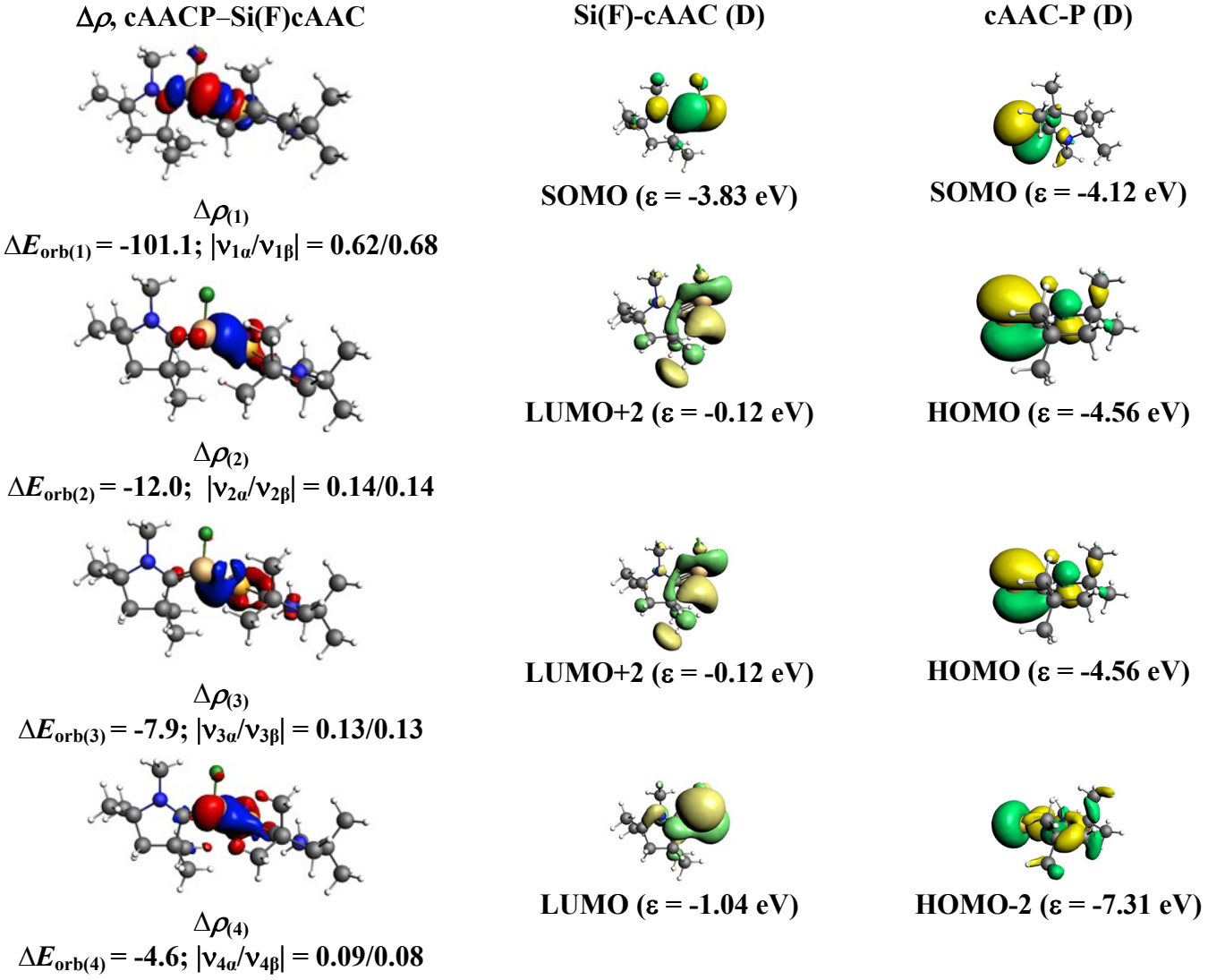


Figure S10. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(F)-cAAC and the fragments orbitals of cAAC-P and (F)Si-cAAC in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(3)}$ and isosurface value 0.0003 for $\Delta\rho_{(4)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

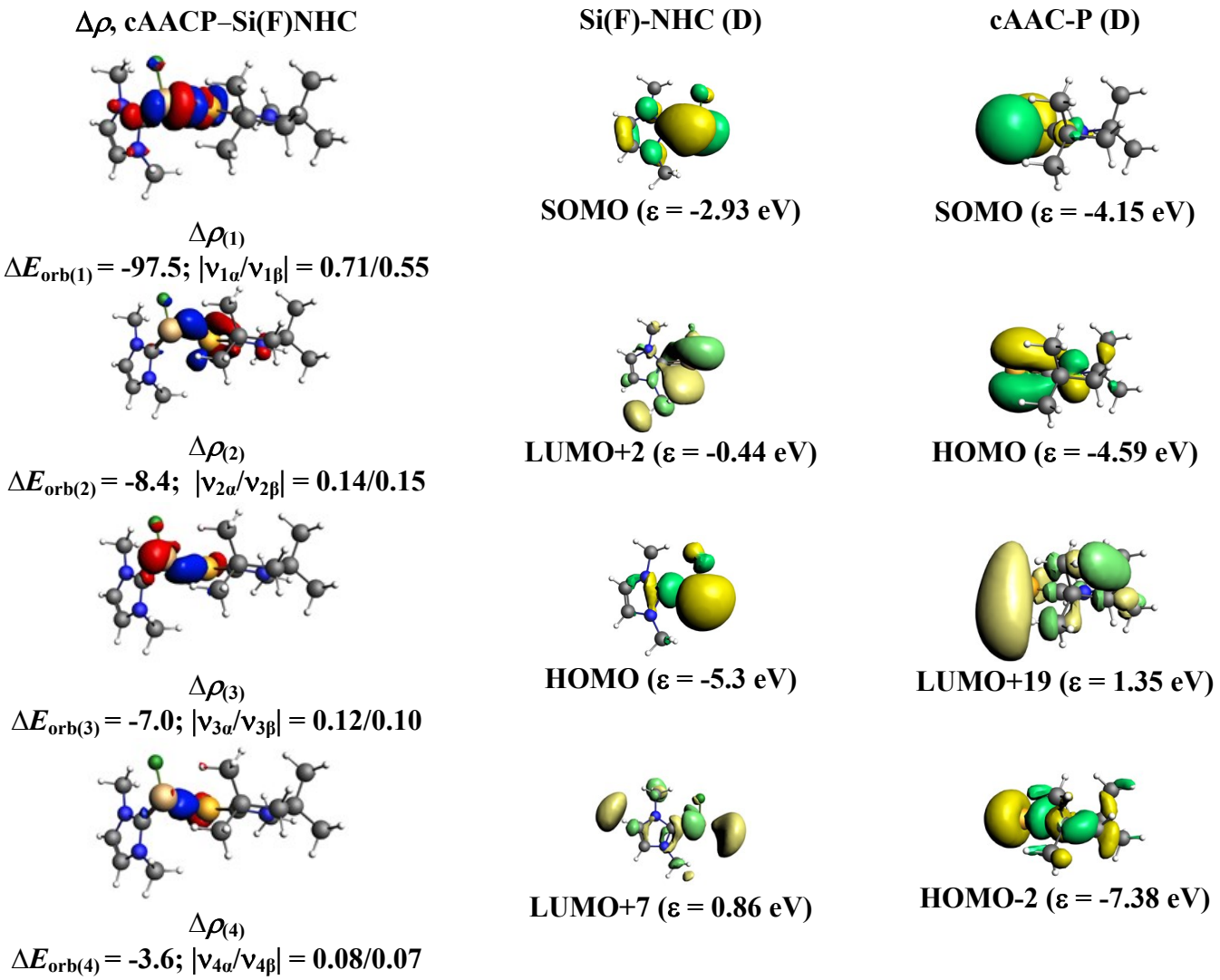


Figure S11. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(F)-NHC and the fragments orbitals of cAAC-P and (F)Si-NHC in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(3)}$ and isosurface value 0.0003 for $\Delta\rho_{(4)}$. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

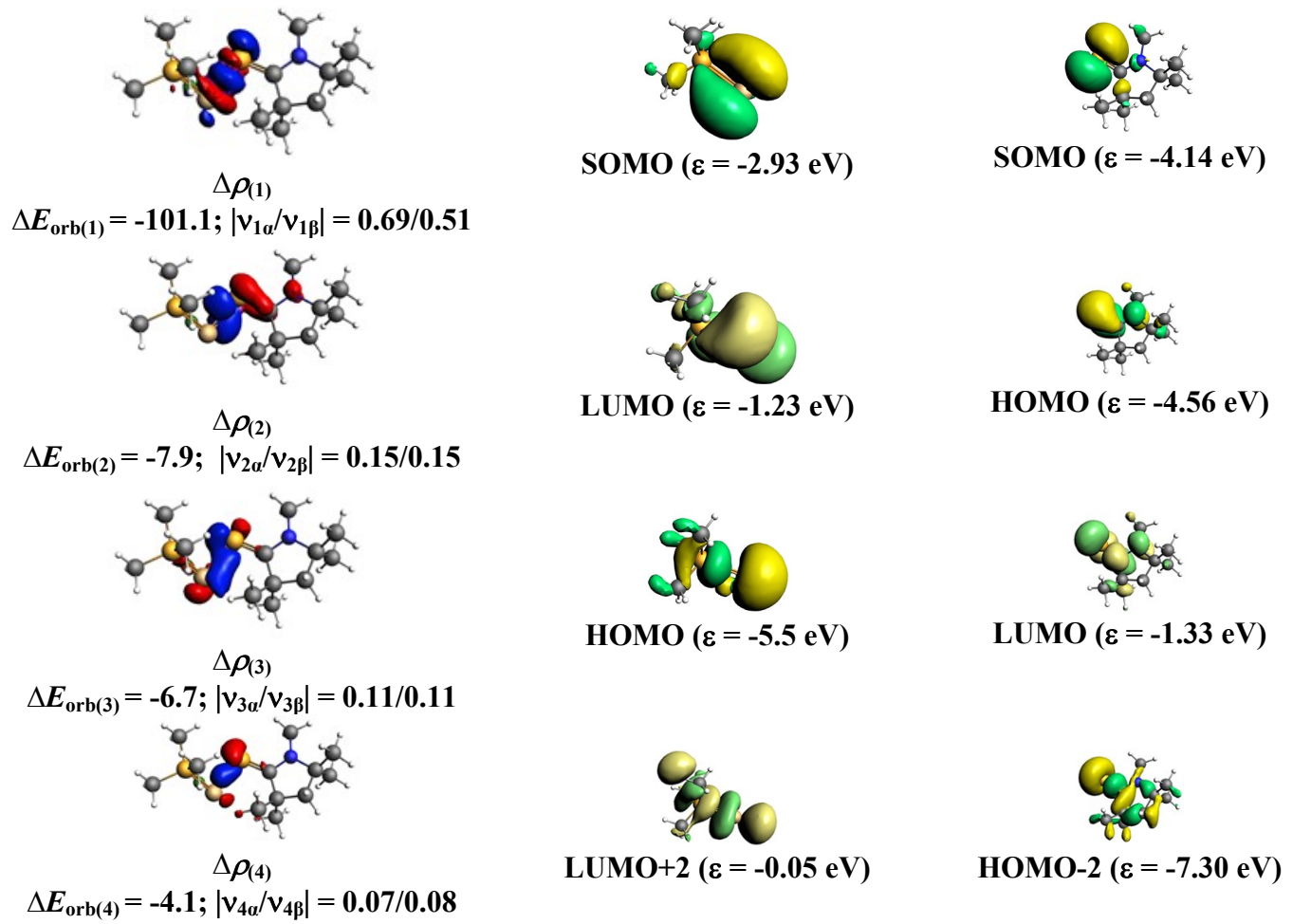


Figure S12. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(F)-PMe_3 and the fragments orbitals of cAAC-P and (F)Si-PMe_3 in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

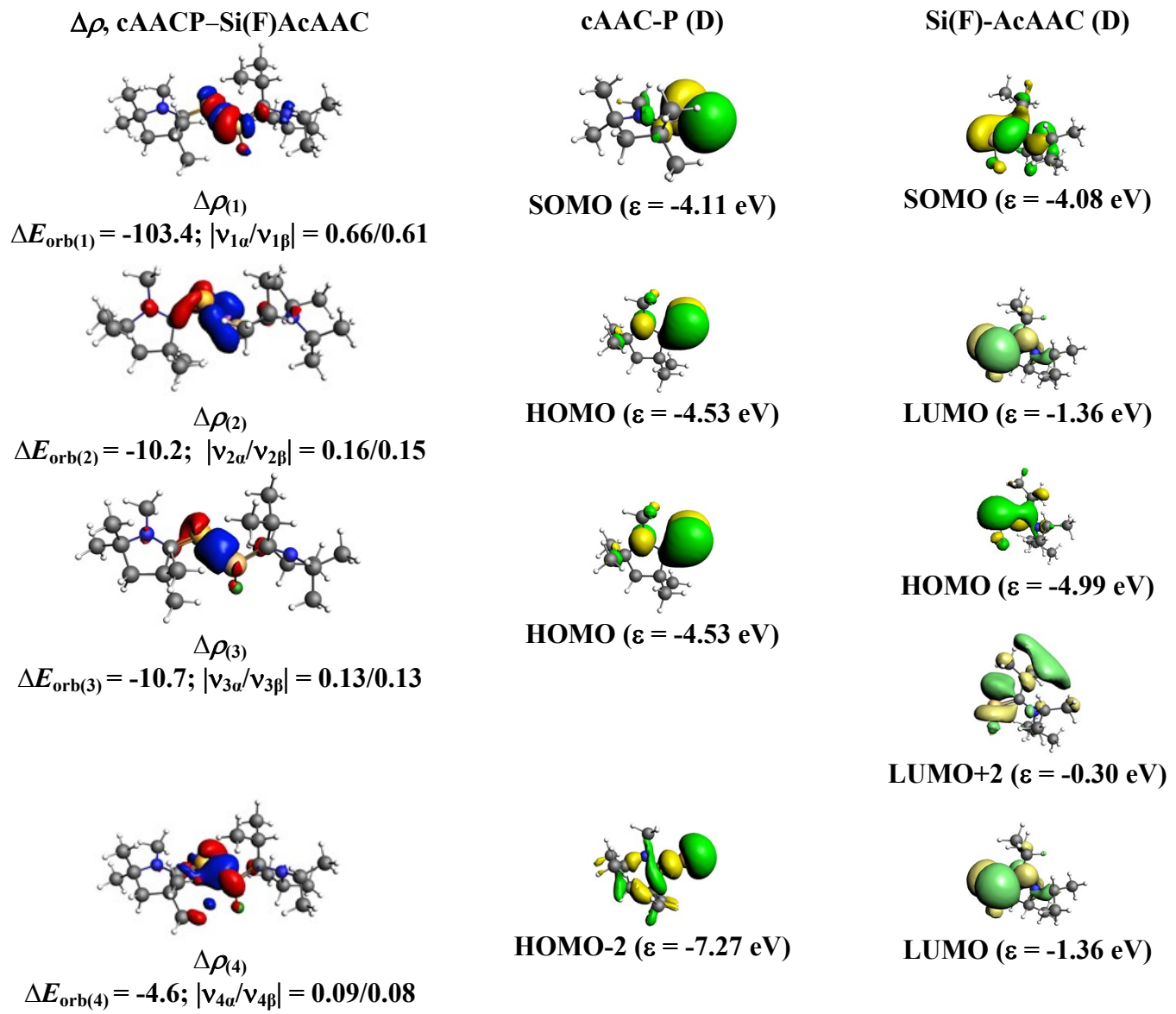


Figure S13. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(F)-AcAAC and the fragments orbitals of cAAC-P and (F)Si-AcAAC in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

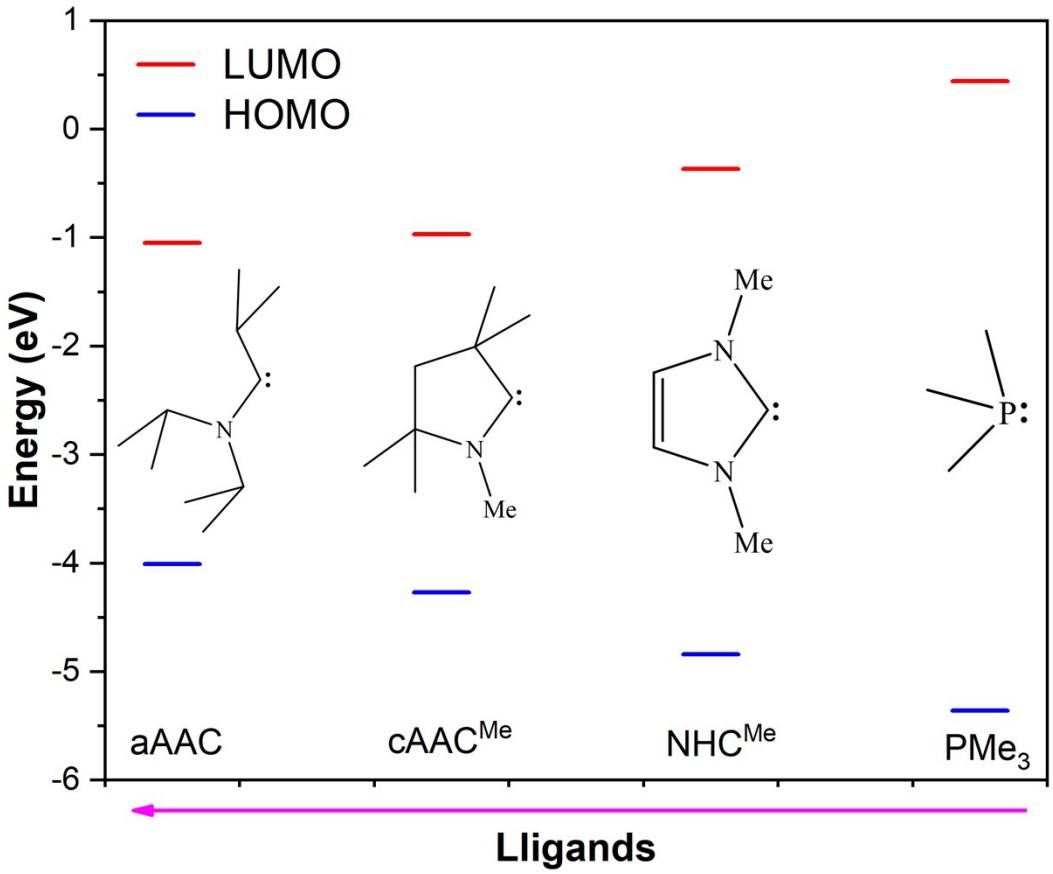
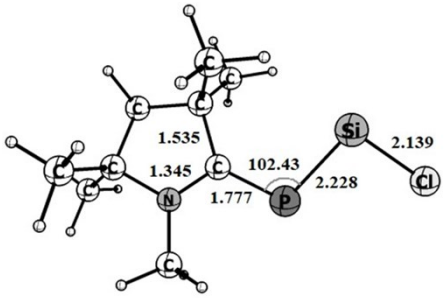
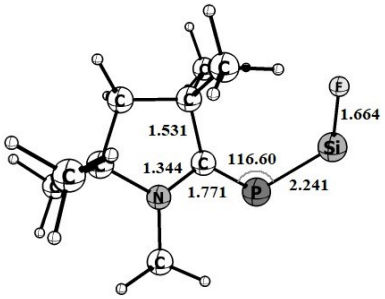


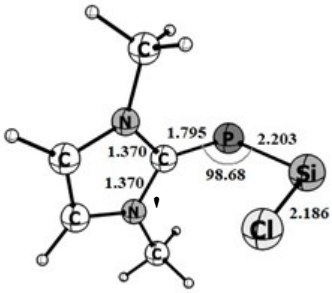
Figure S14. HOMO-LUMO energy gaps of ligands.



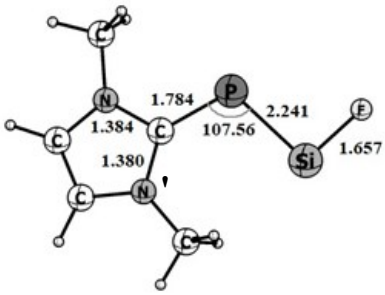
cAAC-P-Si(Cl)
a(C-P-Si) = 102.4°
t(N-C-P-Si) = 18.3°
t(C-P-Si-Cl) = 2.0°



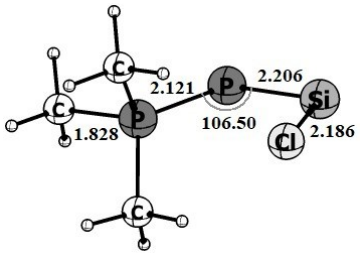
cAAC-P-Si(F)
a(C-P-Si) = 116.6°
t(N-C-P-Si) = 23.7°
t(C-P-Si-F) = 3.41°



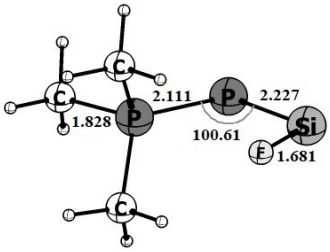
NHC-P-Si(Cl)
a(C-P-Si) = 98.7°
t(N'-C-P-Si) = 90.4°
t(C-P-Si-Cl) = 0.0°



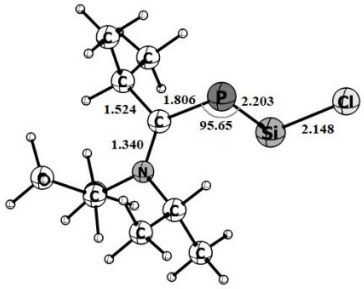
NHC-P-Si(F)
a(C-P-Si) = 107.5°
t(N'-C-P-Si) = 0.0°
t(C-P-Si-F) = 0.0°



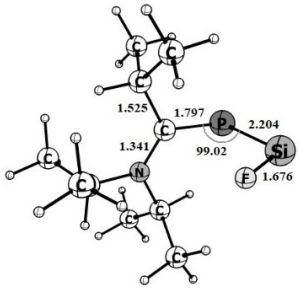
PMe_3-P-Si(Cl)
a(P-P-Si) = 106.5°
t(P-P-Si-Cl) = 0.0°



PMe_3-P-Si(F)
a(P-P-Si) = 100.6°
t(P-P-Si-F) = 0.0°

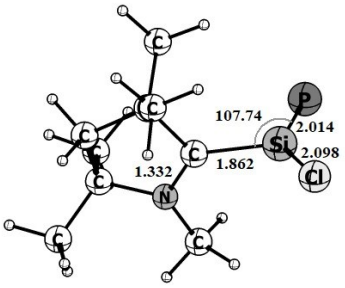


aAAC-P-Si(Cl)
a(C-P-Si) = 96.6°
t(N-C-P-Si) = 75.8°
t(C-P-Si-Cl) = 177.1°

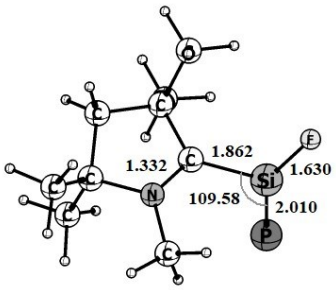


aAAC-P-Si(F)
a(C-P-Si) = 99.0°
t(N-C-P-Si) = 94.9°
t(C-P-Si-Cl) = 5.2°

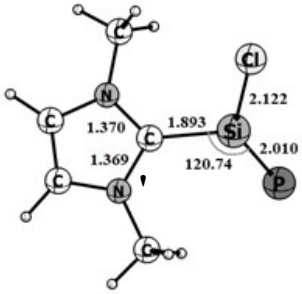
Figure S15. Optimized geometries of L-PSi(Cl/F) complexes with L = $cAAC^{Me}$, NHC^{Me}, PMe_3 and aAAC at BP86(D3BJ)/def2-TZVPP level.



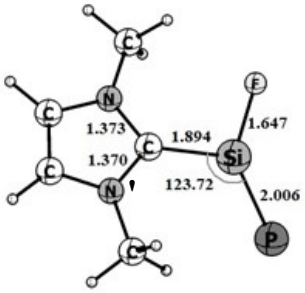
cAAC-Si(Cl)P
a(C-Si-P) = 107.4°
t(N-C-Si-P) = 78.0°
t(N-C-Si-Cl) = 73.8°



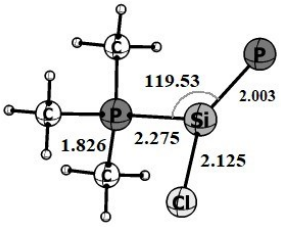
cAAC-Si(F)P
a(C-Si-P) = 109.6°
t(N-C-Si-P) = 72.2°
t(N-C-Si-F) = 63.8°



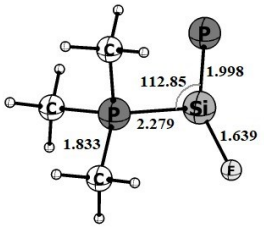
NHC-Si(Cl)P
a(C-Si-P) = 120.7°
t(N'-C-Si-P) = 45.7°
t(N-C-Si-Cl) = 43.6°



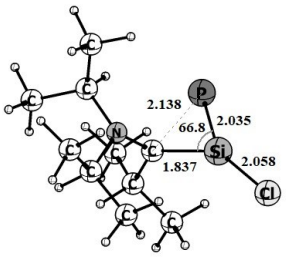
NHC-Si(F)P)
a(C-Si-P) = 123.7°
t(N'-C-Si-P) = 31.3°
t(N-C-Si-F) = 27.2°



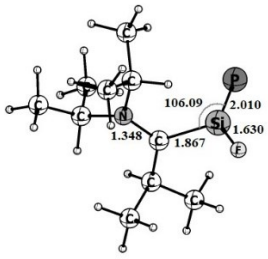
PMe_3-Si(Cl)P
a(P-Si-P) = 119.5°



PMe_3-Si(F)P
a(P-Si-P) = 112.8°



aAAC-P-Si(Cl)
a(C-Si-P) = 66.8°
t(N-C-Si-P) = 77.7°
t(N-C-Si-Cl) = 80.5°



aAAC-P-Si(F)
a(C-Si-P) = 106.1°
t(N-C-Si-P) = 94.9°
t(N-C-Si-F) = 99.4°

Figure S16. Optimized geometries of L-Si(Cl/F)P complexes with L = $cAAC^{Me}$, NHC^{Me}, PMe_3 and aAAC at BP86(D3BJ)/def2-TZVPP level.

Table S5. Dissociation energy (D_e), change in Gibbs free energy (ΔG^{298}) and HOMO-LUMO gap (Δ_{H-L}) of L-PSi(Cl/F) complexes (L = $cAAC^{Me}$, NHC^{Me}, PMe_3 and aAAC).

Complex	D_e (kcal/mol)	ΔG^{298} (kcal/mol)	Δ_{H-L} (kcal/mol)
cAAC-PSiCl	78.54	68.19	40.58
NHC-PSiCl	70.54	60.37	58.60
PMe_3-PSiCl	52.85	42.50	56.96
aAAC-PSiCl	73.84	62.44	46.35
cAAC-PSiF	77.54	66.77	41.97
NHC-PSiF	67.86	57.49	52.11
PMe_3-PSiF	55.31	44.78	59.96
aAAC-PSiF	78.62	66.36	53.50

Table S6. Dissociation energy (D_e), change in Gibbs free energy (ΔG^{298}) and HOMO-LUMO gap (Δ_{H-L}) of L-Si(Cl/F)P complexes (L = $cAAC^{Me}$, NHC^{Me}, PMe_3 and aAAC).

Complex	D_e (kcal/mol)	ΔG^{298} (kcal/mol)	Δ_{H-L} (kcal/mol)
cAAC-Si(Cl)P	65.98	55.85	39.20
NHC-Si(Cl)P	55.82	45.37	33.89
PMe_3-Si(Cl)P	35.64	27.23	41.97
aAAC-Si(Cl)P	49.33	37.95	49.12
cAAC-Si(F)P	69.63	59.11	38.05
NHC-Si(F)P	59.88	49.38	32.28
PMe_3-Si(F)P	38.13	28.66	48.88
aAAC-Si(F)P	65.89	53.62	40.81

Table S7. NBO results of the complexes L-PSi(Cl) (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes at the BP86-D3(BJ)/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the C_L–P and P–Si bonds and partial charges q.

Complex	Bond	ON	Contribution and Hybridization (%)		WBI
cAAC-P-Si(Cl)	C-P σ	1.97	P: 34.4 s(18.1), p(80.9), d(0.9)	C: 65.6 s(37.7), p(62.1)	1.34
	P-Si σ	1.94	P: 65.1 s(15.7), p(83.5), d(0.8)	Si: 34.9 s(11.0), p(87.7), d(1.2)	1.23
NHC-PSi(Cl)	C-P σ	1.97	P: 33.5 s(15.1), p(83.9), d(0.9)	C: 66.4 s(40.9), p(58.8)	1.10
	P-Si σ	1.91	P: 75.9 s(0.00), p(99.5), d(0.5)	Si: 24.1 s(0.00), p(98.5), d(1.5)	1.42
	P-Si π	1.85	P: 65.7 s(14.3), p(84.7), d(0.9)	Si: 34.3 s(12.9), p(85.8), d(1.3)	
PMe_3-PSi(Cl)	P-P_L σ	1.96	P: 41.7 s(12.9), p(85.8), d(1.3)	P_L: 58.3 s(28.4), p(71.0), d(0.5)	1.12
	P-Si σ	1.93	P: 66.8 s(17.2), p(81.8), d(1.0)	Si: 33.2 s(12.8), p(85.9), d(1.3)	1.42
	P-Si π	1.87	P: 79.1 s(0.00), p(99.5), d(0.5)	Si: 20.9 s(0.00), p(98.5), d(1.5)	
aAAC-Psi(Cl)	C-P σ	1.95	P: 34.8 s(16.1), p(82.8), d(1.0)	C: 65.2 s(35.4), p(64.4)	1.21
	P-Si σ	1.91	P: 70.5 s(7.4), p(91.9), d(0.7)	Si: 29.5 s(4.7), p(93.9), d(1.3)	1.36
	P-Si π	1.73	P: 70.2 s(5.6), p(93.5), d(0.9)	Si: 29.8 s(6.9), p(91.7), d(1.3)	

Table S8. NBO results of the complexes L-PSi(F) (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes at the BP86-D3(BJ)/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the C_L–P and P–Si bonds and partial charges q.

Complex	Bond	ON	Contribution and Hybridization (%)		WBI
cAAC-PSi(F)	C-P σ	1.97	P: 35.3 s(20.6), p(78.6), d(0.7)	C: 64.7 s(37.3), p(62.4)	1.34
	P-Si σ	1.94	P: 68.8 s(15.6), p(83.5), d(0.8)	Si: 31.2 s(11.3), p(87.9), d(0.7)	1.22
NHC-PSi(F)	C_2-P_1 σ	1.97	P: 33.3 s(16.3), p(82.7), d(0.9)	C: 66.7 s(41.8), p(58.0)	1.23
	P_1-Si_{11} σ	1.94	P: 68.0 s(15.9), p(82.9), d(1.0)	Si: 31.9 s(10.7), p(88.7), d(0.6)	1.29
	P_1-P_{15} σ	1.96	P_1: 41.5 s(13.1), p(85.5), d(1.3)	P_{15}: 58.5 s(28.9), p(70.5), d(0.5)	1.16
PMe_3-PSi(F)	P_1-Si_2 σ	1.92	P: 68.7 s(14.8), p(83.9), d(1.3)	Si: 31.3 s(12.0), p(87.4), d(0.6)	1.31
	P_1-Si_2 π	1.86	P: 82.0 s(0.00), p(99.3), d(0.7)	Si: 18.0 s(0.00), p(98.6), d(1.4)	
aAAC-PSi(F)	C-P σ	1.96	P: 35.7 s(17.5), p(81.7), d(0.9)	C: 64.3 s(35.0), p(64.8)	1.21
	P-Si σ	1.91	P: 75.5 s(1.8), p(97.6), d(0.6)	Si: 24.5 s(1.4), p(96.9), d(1.6)	1.34
	P-Si π	1.74	P: 69.0 s(9.4), p(89.6), d(0.9)	Si: 31.0 s(13.9), p(84.7), d(1.4)	

Table S9. NBO results of the complexes L-Si(Cl)P (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes at the BP86-D3(BJ)/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the C_L–Si and P–Si bonds and partial charges q.

Complex	Bond	ON	Contribution and Hybridization (%)		WBI
P-(Cl)Si-aAAC	Si-C σ	1.95	Si: 30.2 s(36.9), p(62.5)	C: 69.8 s(23.0), p(76.7)	0.89
	Si-P σ	1.94	Si: 46.0 s(38.1), p(61.5)	P: 53.9 s(12.8), p(86.1), d(1.0)	1.69
	Si-P π	1.91	Si: 32.5 s(0.03), p(98.85), d(1.0)	P: 67.5 s(0.05), p(99.1), d(0.8)	
	P-C σ	1.83	C: 61.1 s(12.4), p(87.2)	P: 38.87 s(8.5), p(90.2), d(1.3)	0.82
P-(Cl)Si-cAAC	Si-C σ	1.89	Si: 23.6 s(30.3), p(54.3), d(15.3)	C: 76.4 s(36.9), p(62.9)	0.77
	Si-P σ	1.94	Si: 47.5 s(46.9), p(50.1), d(2.9)	P: 52.5 s(16.1), p(82.7), d(1.2)	2.16
	Si-P π	1.95	Si: 40.5 s(0.09), p(97.0), d(2.8)	P: 59.5 s(0.07), p(99.2), d(0.7)	
	Si-P π	1.53	Si: 17.9 s(0.4), p(60.5), d(39.0)	P: 82.1 s(2.8), p(96.6), d(0.6)	
P-(Cl)Si-NHC	Si-C σ	1.95	Si: 26.3 s(29.1), p(69.3)	C: 73.7 s(41.1), p(58.9)	0.74
	Si-P σ	1.96	Si: 49.4 s(51.3), p(48.2)	P: 50.6 s(15.7), p(83.0), d(1.2)	2.29
	Si-P π	1.95	Si: 39.4 s(0.13), p(98.4), d(1.5)	P: 60.6 s(1.1), p(98.2), d(0.6)	
P-(Cl)Si-PMe_3	Si-P_L σ	1.84	Si: 26.3 s(22.2), p(53.2), d(24.5)	P: 73.7 s(27.2), p(72.4)	0.72
	Si-P σ	1.94	Si: 49.0 s(51.9), p(44.3), d(3.7)	P: 50.9 s(13.9), p(84.8), d(1.2)	2.40
	Si-P π	1.84	Si: 18.9 s(3.1), p(61.3), d(35.6)	P: 81.0 s(4.2), p(95.2), d(0.5)	
	Si-P π	1.94	Si: 49.3 s(0.00), p(99.6)	P: 50.7 s(0.00), p(99.26), d(0.7)	

Table S10. NBO results of the complexes L-Si(F)P (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes at the BP86-D3(BJ)/def2-TZVPP level of theory. Occupation number ON, polarization and hybridization of the C_L–Si and P–Si bonds and partial charges q.

Complex	Bond	ON	Contribution and Hybridization (%)		WBI
P-(F)Si-aAAC	Si-C σ	1.94	Si: 25.4 s(32.2), p(66.5)	C: 74.6 s(34.1), p(65.8)	0.77
	Si-P σ	1.95	Si: 46.2 s(46.0), p(53.2), d(0.7)	P: 53.8 s(15.5), p(83.2), d(1.2)	2.12
	Si-P π	1.96	Si: 35.5 s(0.4), p(98.0), d(1.6)	P: 64.5 s(0.08), p(99.2), d(0.7)	
P-(F)Si-cAAC	Si-C σ	1.94	Si: 24.6 s(42.8), p(55.4)	C: 75.4 s(36.4), p(63.5)	0.77
	Si-P σ	1.97	Si: 47.2 s(54.6), p(44.7), d(0.6)	P: 52.8 s(15.8), p(82.9), d(1.3)	2.17
	Si-P π	1.95	Si: 35.6 s(0.03), p(98.1), d(1.9)	P: 64.4 s(0.03), p(99.3), d(0.7)	
	Si-P π	1.58	Si: 23.3 s(0.9), p(93.5), d(5.5)	P: 76.7 s(2.1), p(97.3), d(0.6)	
P-(F)Si-NHC	$Si-C_1$ σ	1.95	Si: 24.5 s(40.2), p(57.9)	C: 75.5 s(40.7), p(59.3)	0.74
	Si-P σ	1.98	Si: 48.7 s(57.2), p(42.3), d(0.5)	P: 51.3 s(16.3), p(83.4), d(1.3)	2.31
	Si-P π	1.92	Si: 30.3 s(0.6), p(96.2), d(3.2)	P: 69.7 s(0.6), p(98.7), d(0.7)	
	Si-P π	1.79	Si: 31.7 s(0.5), p(96.5), d(3.0)	P: 68.3 s(1.1), p(98.2), d(0.7)	
P-(F)Si-PMe_3	$Si-P_L$ σ	1.85	Si: 24.6 s(23.2), p(52.2), d(24.6)	P: 75.4 s(26.7), p(72.9)	0.72
	Si-P σ	1.95	Si: 48.5 s(52.5), p(45.4), d(2.1)	P: 51.5 s(14.3), p(84.4), d(1.3)	2.42
	Si-P π	1.95	Si: 43.8 s(0.00), p(98.9), d(0.9)	P: 56.2 s(0.00), p(99.3), d(0.7)	
	Si-P π	1.82	Si: 17.6 s(1.6), p(59.8), d(38.6)	P: 82.4 s(3.2), p(96.1), d(0.6)	

Table S11. EDA-NOCV results of L–PSi(Cl) bonds of L-P-Si(Cl) (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes using three different sets of fragments with different charges and electronic states (S = singlet, D = doublet, T = triplet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
cAAC-P-Si(Cl)	D	$cAAC^{Me}$ (S) + P-Si(Cl) (S)	-101.9	421.7	-244.7	-11.0	-267.8
	E (σ, π)	$cAAC^{Me}$ (T) + P-Si(Cl) (T)	-158.4	306.6	-184.0	-11.0	-270.0
	D + E	$[cAAC^{Me}]^+$ (D) + $[P\text{-}Si(Cl)]^-$ (D)	-200.0	324.1	-255.3	-11.0	**-257.7**
NHC-P-Si(Cl)	D	NHC^{Me} (S) + P-Si(Cl) (S)	-94.5	317.5	-201.7	-11.6	**-198.7**
	E (σ, π)	NHC^{Me} (T) + P-Si(Cl) (T)	-185.0	230.6	-149.3	-11.6	-254.7
	D + E	$[NHC^{Me}]^+$ (D) + $[P\text{-}Si(Cl)]^-$ (D)	-212.4	237.8	-219.7	-11.6	-218.9
PMe_3-P-Si(Cl)	D	PMe_3 (S) + P-Si(Cl) (S)	-77.2	249.0	-147.2	-11.0	**-168.1**
	E (σ, π)	PMe_3 (T) + P-Si(Cl) (T)	-190.4	220.4	-137.1	-11.0	-262.8
	D + E	$[PMe_3]^+$ (D) + $[P\text{-}Si(Cl)]^-$ (D)	-188.9	213.8	-209.1	-11.0	-182.7
aAAC-P-Si(Cl)	D	aAAC (S) + P-Si(Cl) (S)	-103.6	371.3	-225.2	-13.2	-236.4
	E (σ, π)	aAAC (T) + P-Si(Cl) (T)	-150.8	292.6	-175.4	-13.2	-254.8
	D + E	$[aAAC]^+$ (D) + $[P\text{-}Si(Cl)]^-$ (D)	-188.6	305.9	-248.5	-13.2	**-232.7**

[a]D = Dative bond; E = Electron-sharing bond.

Table S12. EDA-NOCV results of L–PSi(F) bonds of L-P-Si(F) (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes using three different sets of fragments with different charges and electronic states (S = singlet, D = doublet, T = triplet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
cAAC-P-Si(F)	D	$cAAC^{Me}$ (S) + P-Si(F) (S)	-103.5	330.4	-210.0	-10.3	**-213.6**
	E (σ, π)	$cAAC^{Me}$ (T) + P-Si(F) (T)	-152.9	263.3	-164.1	-10.3	-241.7
	D + E	$[cAAC^{Me}]^+$ (D) + $[P\text{-}Si(F)]^-$ (D)	-200.9	288.1	-238.5	-10.3	-240.1
NHC-P-Si(F)	D	NHC^{Me} (S) + P-Si(F) (S)	-99.4	363.7	-216.5	-8.5	**-238.1**
	E (σ, π)	NHC^{Me} (T) + P-Si(F) (T)	-184.5	299.2	-187.6	-8.5	-287.6
	D + E	$[NHC^{Me}]^+$ (D) + $[P\text{-}Si(F)]^-$ (D)	-213.9	334.8	-265.2	-8.5	-275.1
PMe_3-P-Si(F)	D	PMe_3 (S) + P-Si(F) (S)	-81.1	243.9	-147.7	-9.6	**-167.7**
	E (σ, π)	PMe_3 (T) + P-Si(F) (T)	-190.2	216.9	-137.4	-9.6	-260.2
	D + E	$[PMe_3]^+$ (D) + $[P\text{-}Si(F)]^-$ (D)	-194.6	214.2	-214.5	-9.6	-184.7
aAAC-P-Si(F)	D	aAAC (S) + P-Si(F) (S)	-106.1	343.9	-221.0	-13.7	**-215.3**
	E (σ, π)	aAAC (T) + P-Si(F) (T)	-149.7	268.6	-169.5	-13.7	-235.0
	D + E	$[aAAC]^+$ (D) + $[P\text{-}Si(F)]^-$ (D)	-193.1	299.6	-248.3	-13.7	230.2

[a]D = Dative bond; E = Electron-sharing bond

Table S13. EDA-NOCV results of L–Si(Cl)P bonds of L-Si(Cl)-P (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes using three different sets of fragments with different charges and electronic states (S = singlet, D = doublet, T = triplet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
cAAC-Si(Cl)-P	D	$cAAC^{Me}$ (S) + Si(Cl)-P (S)	-75.4	330.9	-210.3	-12.7	**-183.3**
	E (σ, π)	$cAAC^{Me}$ (T) + Si(Cl)-P (T)	-148.1	195.9	-142.1	-12.7	-189.2
	D + E	$[cAAC^{Me}]^+$ (D) + $[Si(Cl)\text{-}P]^-$ (D)	-189.8	270.0	-231.0	-12.7	-216.1
NHC-Si(Cl)-P	D	NHC^{Me} (S) + Si(Cl)-P (S)	-64.9	289.7	-186.0	-9.8	**-158.8**
	E (σ, π)	NHC^{Me} (T) + Si(Cl)-P (T)	-179.0	192.3	-130.7	-9.8	-230.9
	D + E	$[NHC^{Me}]^+$ (D) + $[Si(Cl)\text{-}P]^-$ (D)	-194.6	217.7	-209.8	-9.8	-192.7
PMe_3-Si(Cl)-P	D	PMe_3 (S) + Si(Cl)-P (S)	-44.9	208.7	-129.7	-10.1	**-113.8**
	E (σ, π)	PMe_3 (T) + Si(Cl)-P (T)	-184.8	148.6	-102.1	-10.1	-221.3
	D + E	$[PMe_3]^+$ (D) + $[Si(Cl)\text{-}P]^-$ (D)	-174.2	182.1	-192.5	-10.1	-153.7
aAAC-Si(Cl)-P	D	aAAC (S) + Si(Cl)-P (S)	-183.8	359.6	-204.4	-15.2	-323.8
	E (σ, π)	aAAC (T) + Si(Cl)-P (T)	-126.9	354.5	-221.7	-15.2	**-244.4**
	D + E	$[aAAC]^+$ (D) + $[Si(Cl)\text{-}P]^-$ (D)	-258.5	366.7	-275.4	-15.2	-334.5

[a]D = Dative bond; E = Electron-sharing bond

Table S14. EDA-NOCV results of L–Si(F)P bonds of L-Si(F)-P (L = $cAAC^{Me}$, NHC^{Me}, PMe_3, aAAC) complexes using three different sets of fragments with different charges and electronic states (S = singlet, D = doublet, T = triplet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
cAAC-Si(F)-P	D	$cAAC^{Me}$ (S) + Si(F)-P (S)	-79.0	326.3	-210.1	-11.2	**-183.9**
	E (σ, π)	$cAAC^{Me}$ (T) + Si(F)-P (T)	-152.4	232.1	-153.0	-11.2	-220.3
	D + E	$[cAAC^{Me}]^+$ (D) + $[Si(F)\text{-}P]^-$ (D)	-193.4	275.3	-237.1	-11.2	-220.4
NHC-Si(F)-P	D	NHC^{Me} (S) + Si(F)-P (S)	-68.8	280.4	-184.9	-8.3	**-156.0**
	E (σ, π)	NHC^{Me} (T) + Si(F)-P (T)	-788.3	229.9	-115.3	-8.3	-894.5
	D + E	$[NHC^{Me}]^+$ (D) + $[Si(F)\text{-}P]^-$ (D)	-332.9	228.6	-238.3	-8.3	-314.9
PMe_3-Si(F)-P	D	PMe_3 (S) + Si(F)-P (S)	-45.2	202.4	-127.2	-8.6	**-111.7**
	E (σ, π)	PMe_3 (T) + Si(F)-P (T)	-185.3	142.9	-100.7	-8.6	-218.9
	D + E	$[PMe_3]^+$ (D) + $[Si(F)\text{-}P]^-$ (D)	-179.1	185.0	-196.9	-8.6	-158.6
aAAC-Si(F)-P	D	aAAC (S) + Si(F)-P (S)	-80.6	342.9	-217.5	-12.9	**-193.0**
	E (σ, π)	aAAC (T) + Si(F)-P (T)	-144.8	262.0	-166.2	-12.9	-227.8
	D + E	$[aAAC]^+$ (D) + $[Si(F)\text{-}P]^-$ (D)	-187.0	304.8	-250.5	-12.9	-228.3

[a]D = Dative bond; E = Electron-sharing bond

Table S15. The EDA-NOCV results at the BP86-D3(BJ)/TZ2P level of cAAC–PSi(X)/Si(X)P bonds of cAAC-P-Si(X) and cAAC-Si(X)P complex. Energies are in kcal/mol.

Energy	**Interaction**[c]	**$[cAAC^{Me}]^+$ (D) + $[P\text{-}Si(Cl)]^-$ (D)**	**$cAAC^{Me}$ (S) + P-Si(F) (S)**	**$cAAC^{Me}$ (S) + Si(Cl)-P (S)**	**$cAAC^{Me}$ (S) + Si(F)-P (S)**
ΔE_{int}		-200.0	-103.5	-75.4	-79.0
ΔE_{Pauli}		324.1	330.4	330.9	326.3
ΔE_{disp}[a]		-11.0 (2.1%)	-10.3 (2.4%)	-12.7 (3.1%)	-11.2 (2.8%)
ΔE_{elstat}[a]		-255.3 (48.7%)	-210.0 (48.4%)	-210.3 (51.8%)	-210.1 (51.8%)
ΔE_{orb}[a]		-257.7 (49.2%)	-213.6 (49.2%)	-183.3 (45.1%)	-183.9 (45.4%)
$\Delta E_{orb(1)}$[b]	cAAC–P-Si(Cl) σ e^- sharing	-181.6 (70.4%)			
	cAAC→P-Si(X)/Si(X)P σ donation		-155.5 (72.8%)	-131.3 (71.6%)	-129.5 (70.4%)
$\Delta E_{orb(2)}$[b]	cAAC←P-Si(X) π back donation	-42.0 (16.3%)	-28.6 (13.4%)		
	cAAC→Si(X)P σ donation			-34.2 (18.6%)	-36.7 (20.0%)
$\Delta E_{orb(3)}$[b]	cAAC–P-Si(X) σ polarization	-16.3 (6.3%)	-11.6 (5.4%)		
	cAAC←Si(X)P π back donation			-7.3 (4%)	-7.6 (4.1%)
$\Delta E_{orb(4)}$[b]	cAAC→P-Si(Cl) donation	-5.3 (2.0%)			
	cAAC←P-Si(F) back donation		-10.4 (4.8%)		
$\Delta E_{orb(rest)}$[b]		-12.5 (4.8%)	-7.5 (3.5%)	-10.5 (5.7%)	-10.1 (5.5%)

[a]The values in the parentheses show the contribution to the total attractive interaction $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses show the contribution to the total orbital interaction ΔE_{orb}.

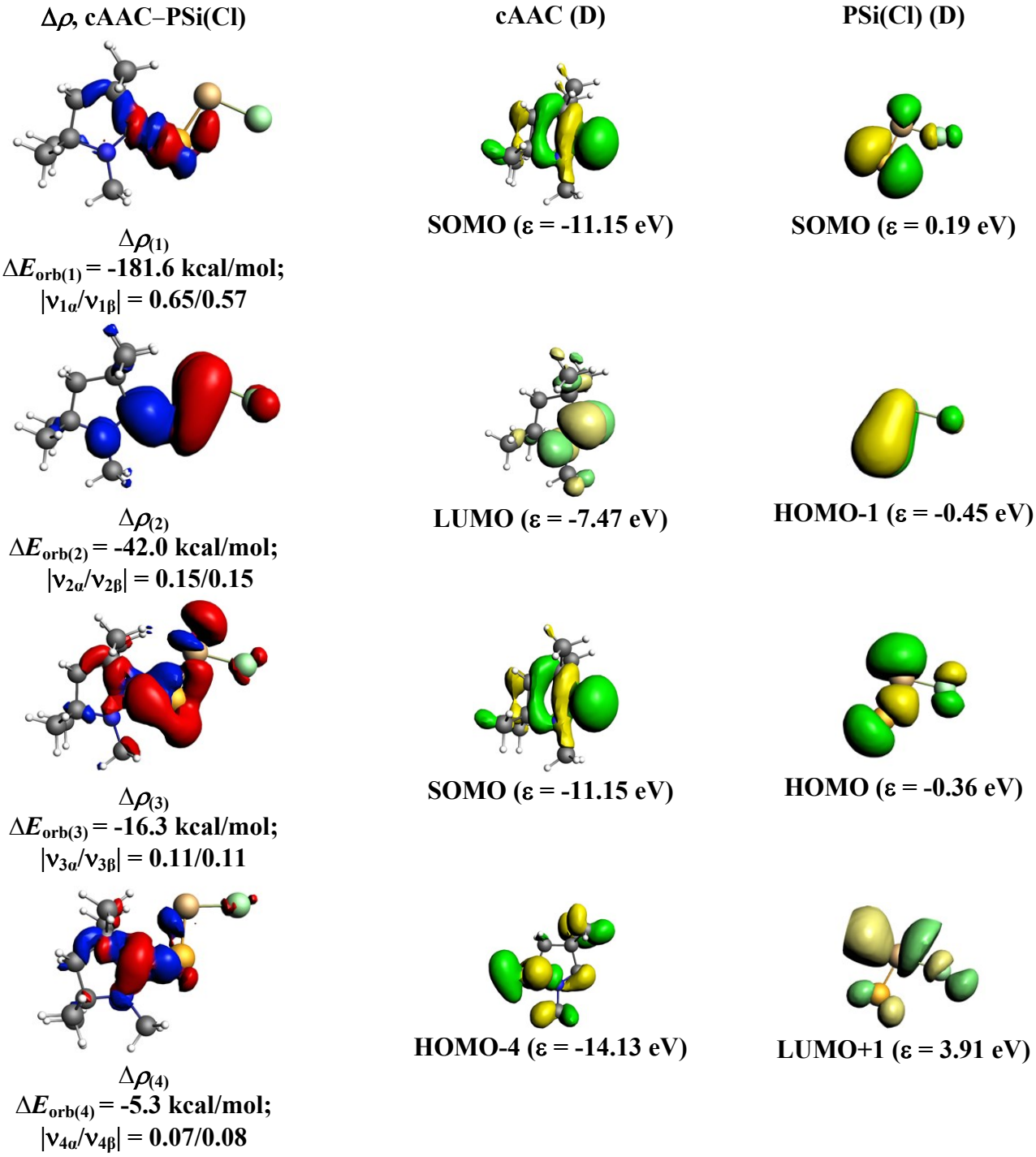


Figure S17. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(Cl) and the fragments orbitals of $[cAAC]^+$ and $[P\text{-}Si(Cl)]^-$ in the doublet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

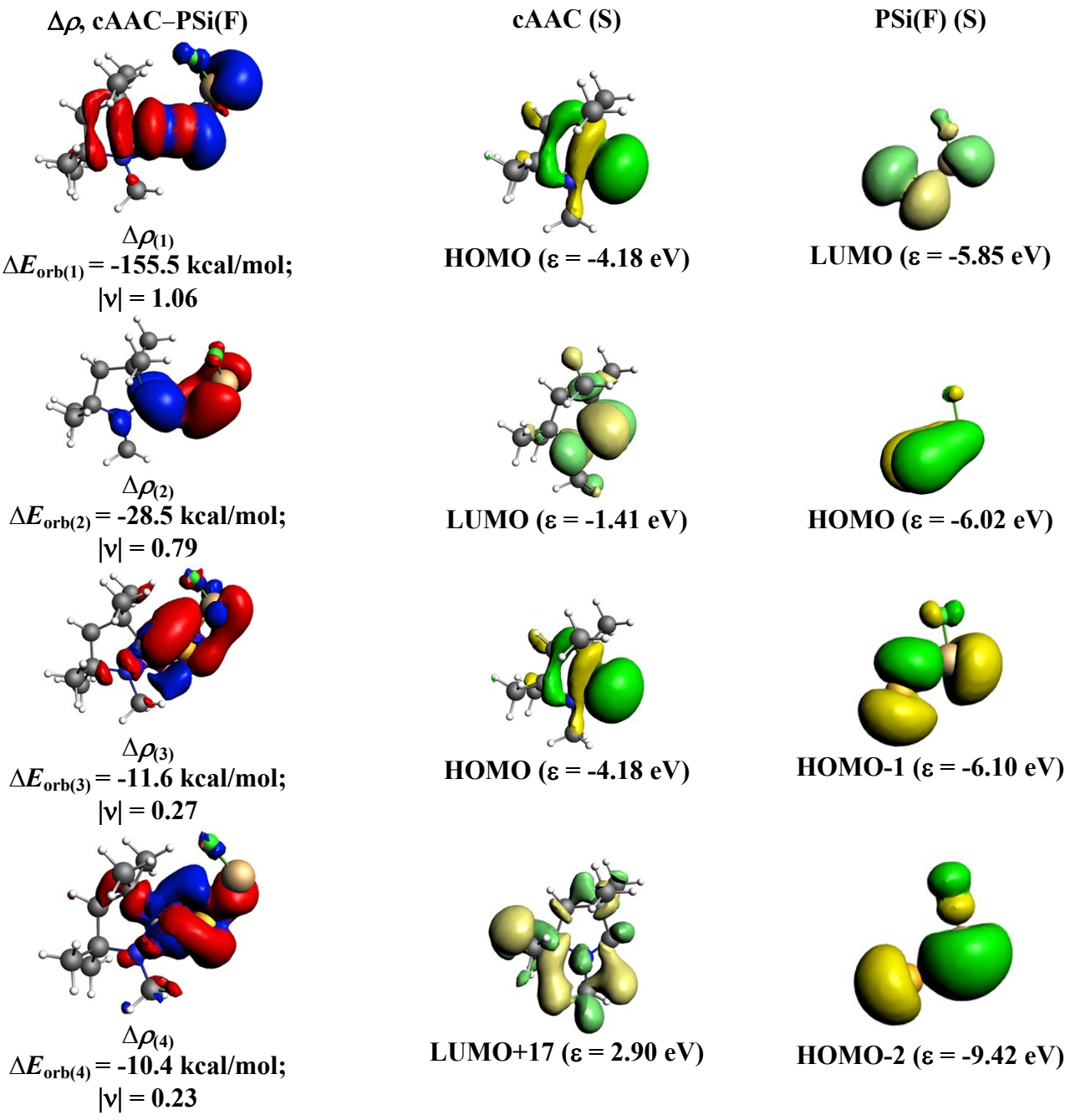


Figure S18. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of cAAC-P-Si(F) and the fragments orbitals of cAAC and P-Si(F) in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

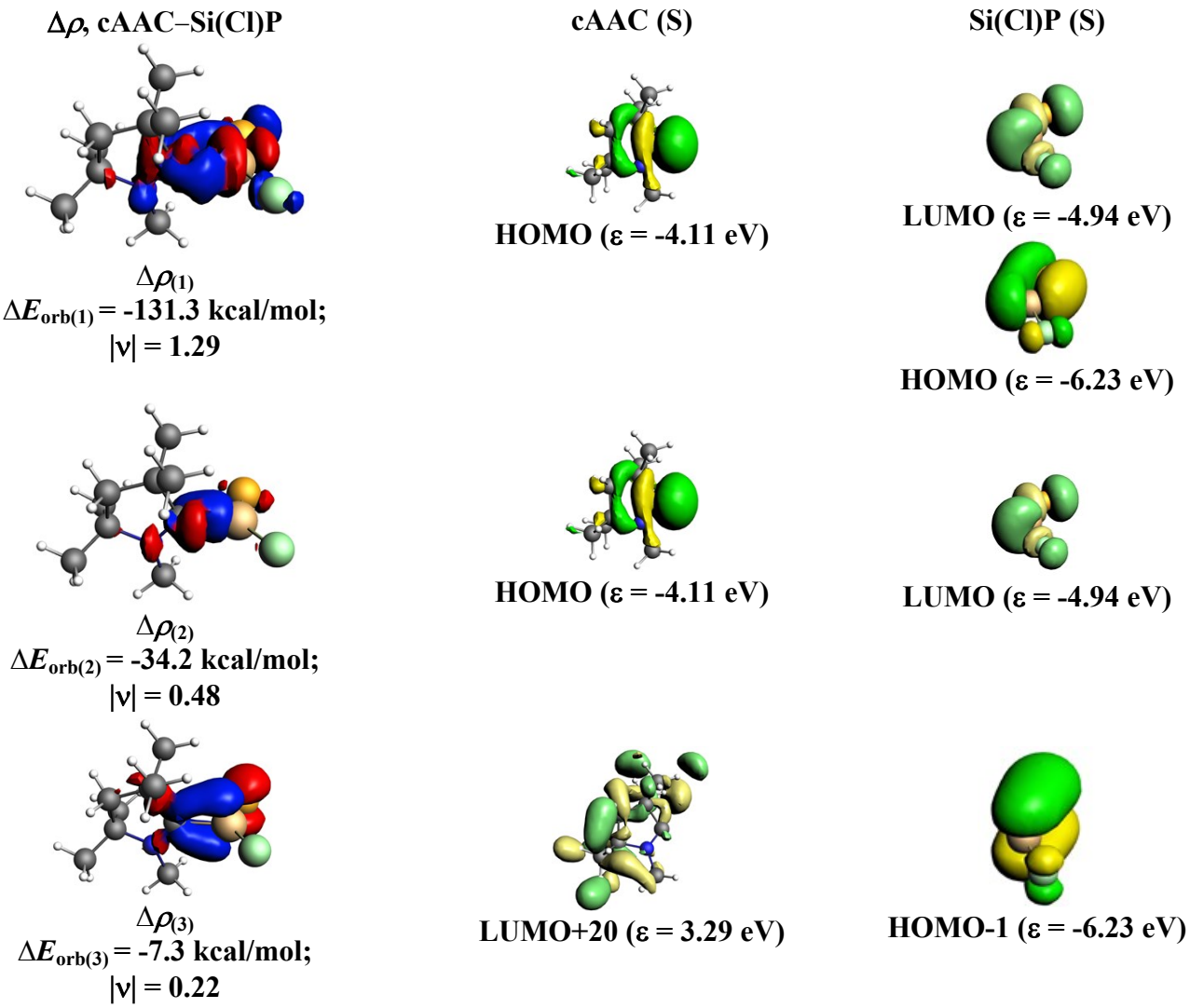


Figure S19. The shape of the deformation densities $\Delta\rho_{(1)\text{-}(3)}$ that correspond to $\Delta E_{\text{orb}(1)\text{-}(3)}$, and the associated MOs of cAAC-Si(Cl)P and the fragments orbitals of cAAC and Si(Cl)P in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

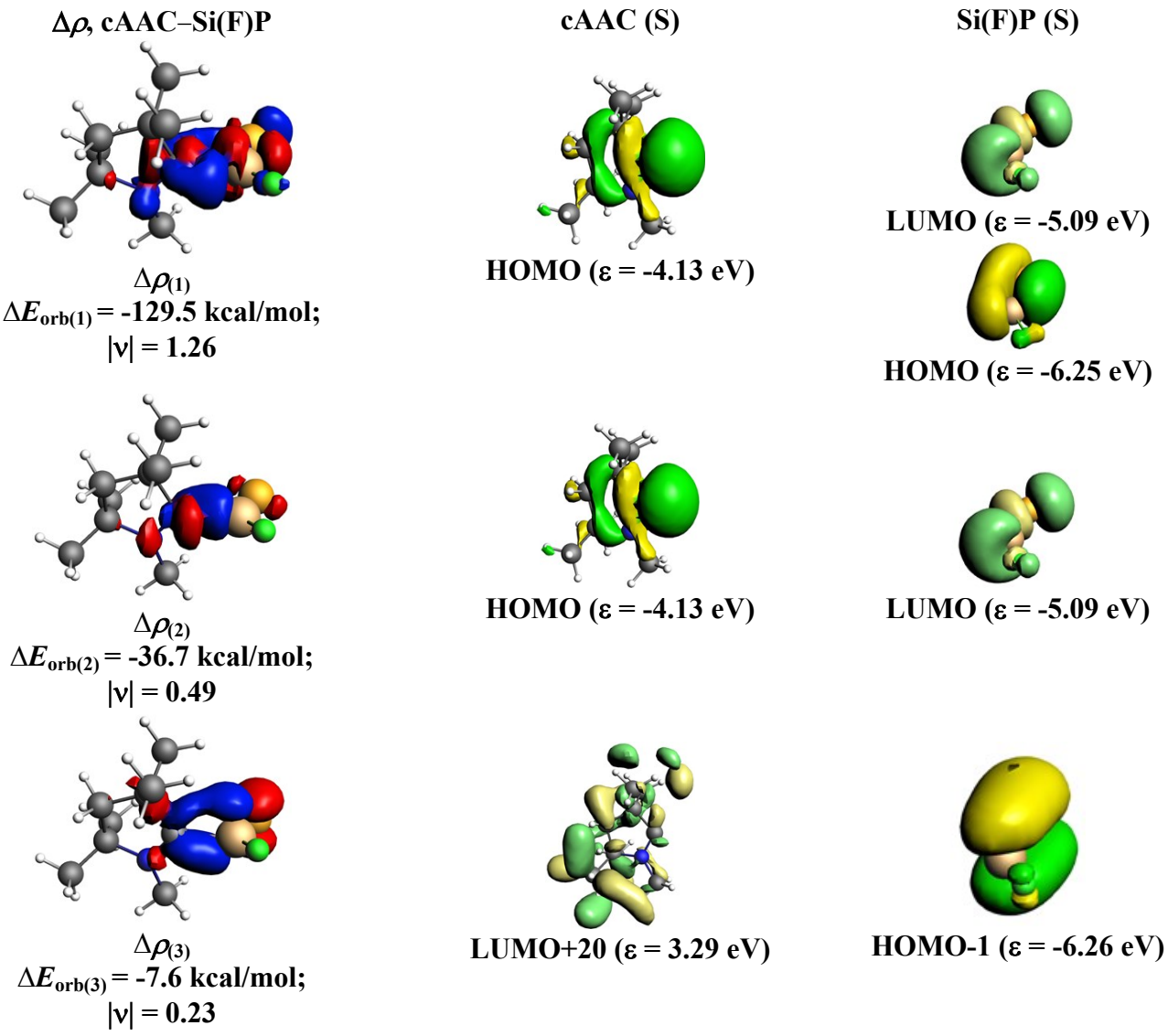


Figure S20. The shape of the deformation densities $\Delta\rho_{(1)-(3)}$ that correspond to $\Delta E_{orb(1)-(3)}$, and the associated MOs of cAAC-Si(F)P and the fragments orbitals of cAAC and Si(F)P in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

Table S16. The EDA-NOCV results at the BP86-D3(BJ)/TZ2P level of NHC–PSi(X)/Si)X)P bonds of NHC-P-Si(X) and NHC-Si(X)P complexes. Energies are in kcal/mol.

Energy	**Interaction[c]**	**NHC^{Me} (S) + P-Si(Cl) (S)**	**NHC^{Me} (S) + P-Si(F) (S)**	**NHC^{Me} (S) + Si(Cl)-P (S)**	**NHC^{Me} (S) + Si(F)-P (S)**
ΔE_{int}		-94.5	-99.4	-64.9	-68.8
ΔE_{Pauli}		317.5	363.7	289.7	280.4
ΔE_{disp}[a]		-11.6 (2.8%)	-8.5 (1.8%)	-9.8 (2.8%)	-8.3 (2.4%)
ΔE_{elstat}[a]		-201.7 (49.0%)	-216.5 (46.8%)	-186.0 (52.4%)	-184.9 (53.0%)
ΔE_{orb}[a]		-198.7 (48.2%)	-238.1 (51.4%)	-158.8 (44.8%)	-156.0 (44.6%)
$\Delta E_{orb(1)}$[b]	NHC→P-Si(X)/Si(X)P σ donation	-149.7 (75.3%)	-182.7 (76.7%)	-112.8 (71.0%)	-108.1 (69.3%)
$\Delta E_{orb(2)}$[b]	NHC←P-Si(X)/Si(X)P π back donation	-21.3 (10.7%)	-20.3 (8.5%)	-21.8 (13.7%)	-22.3 (14.3%)
$\Delta E_{orb(3)}$[b]	NHC←P-Si(X)/Si(X)P π back donation	-9.0 (4.5%)			
	NHC–P-Si(X) σ polarization		-24.1 (10.1%)		-15.8 (10.1%)
	NHC→Si(X)P donation/polarization			-13.4 (8.4%)	
$\Delta E_{orb(4)}$[b]	NHC–P-Si(X) σ polarization	-12.0 (6.0%)			
	NHC→P-Si(X) /Si(X)P donation		-3.4 (1.4%)		-3.0 (19.2%)
	NHC←Si(X)P π back donation			-4.1 (2.6%)	
$\Delta E_{orb(rest)}$[b]		-6.7 (3.4%)	-7.6 (3.2%)	-6.7 (4.2%)	-6.8 (4.3%)

[a]The values in the parentheses show the contribution to the total attractive interaction $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses show the contribution to the total orbital interaction ΔE_{orb}.

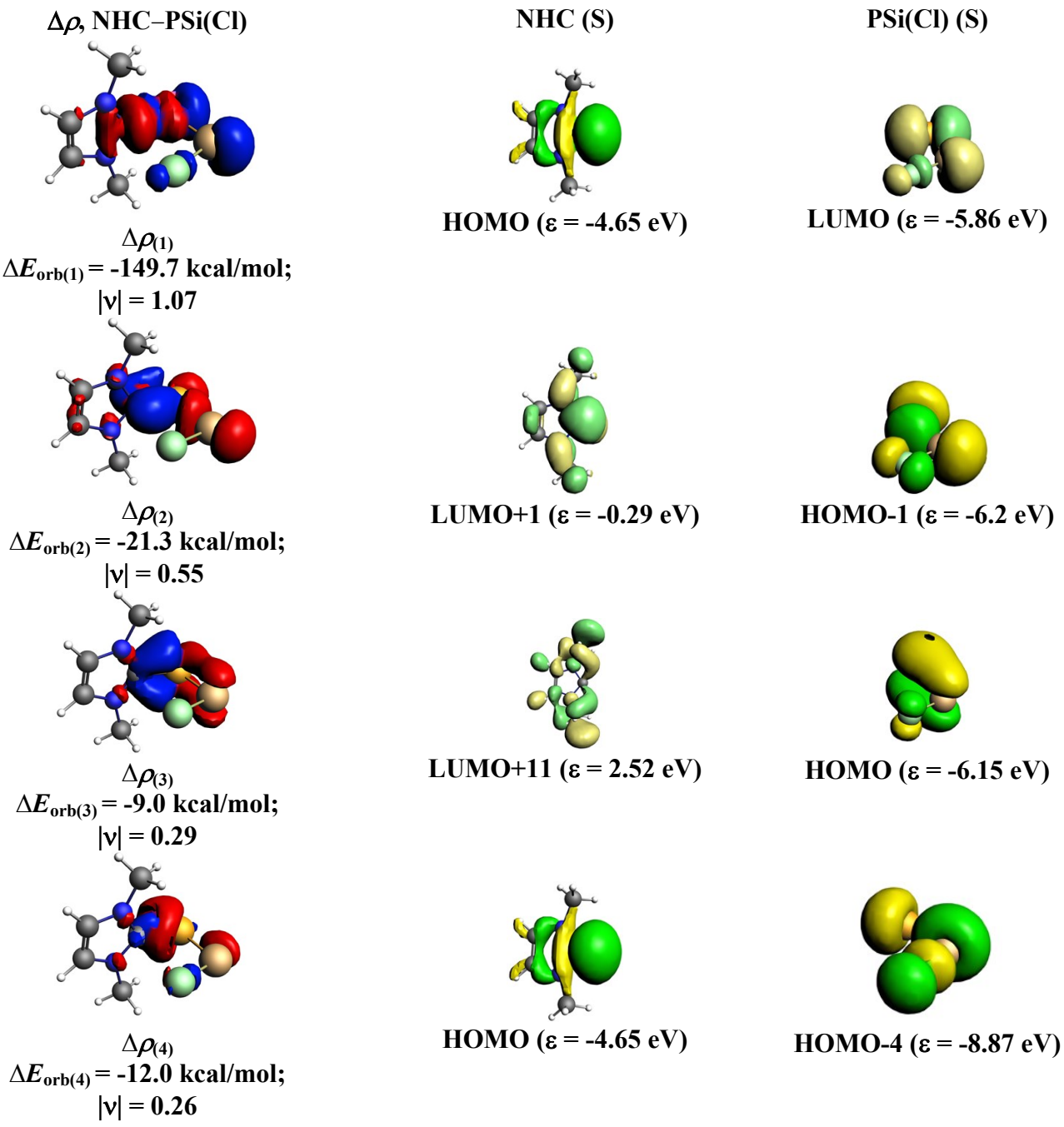


Figure S21. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of NHC-P-Si(Cl) and the fragments orbitals of NHC and P-Si(Cl) in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

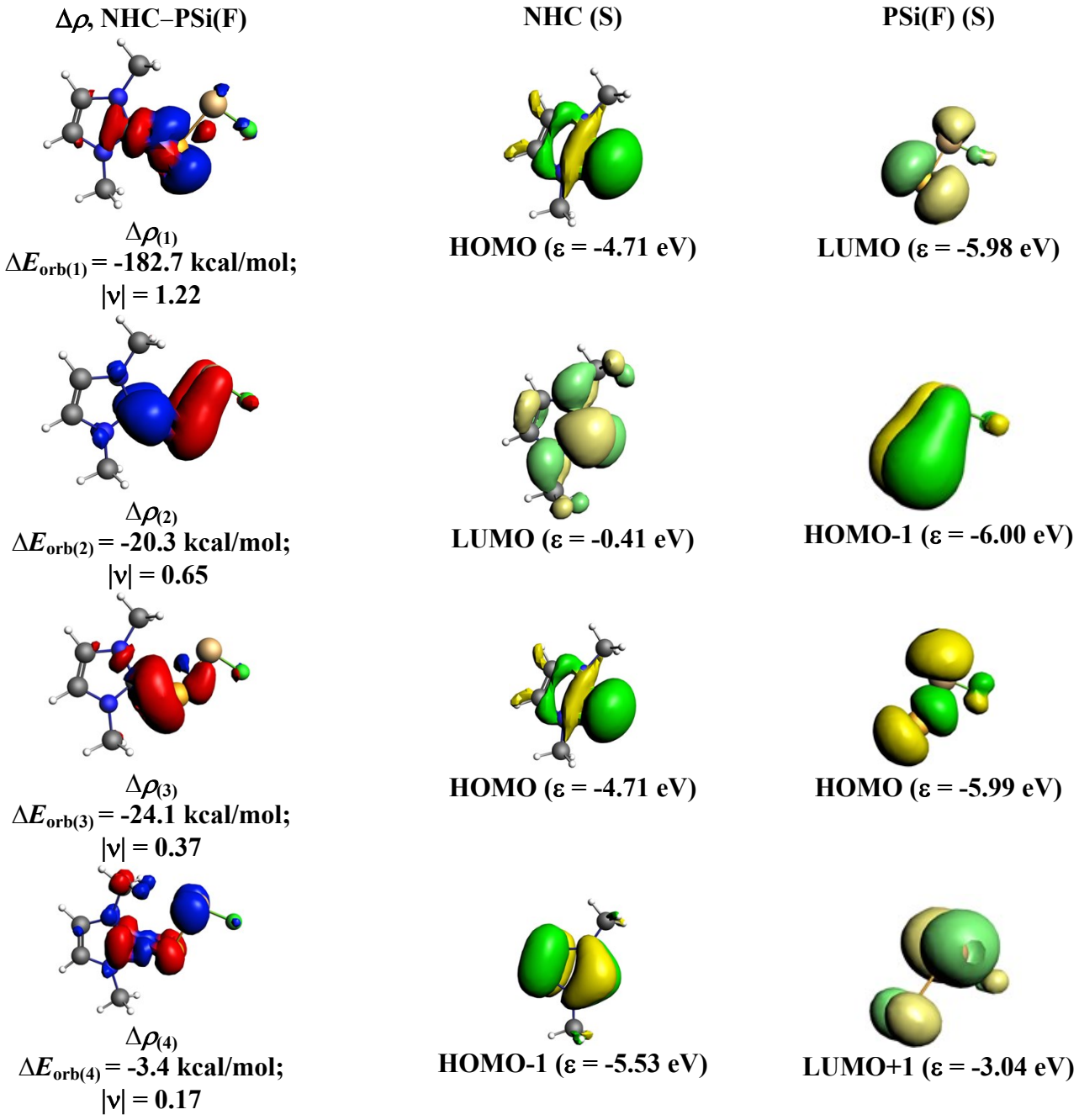


Figure S22. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of NHC-P-Si(F) and the fragments orbitals of NHC and P-Si(F) in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

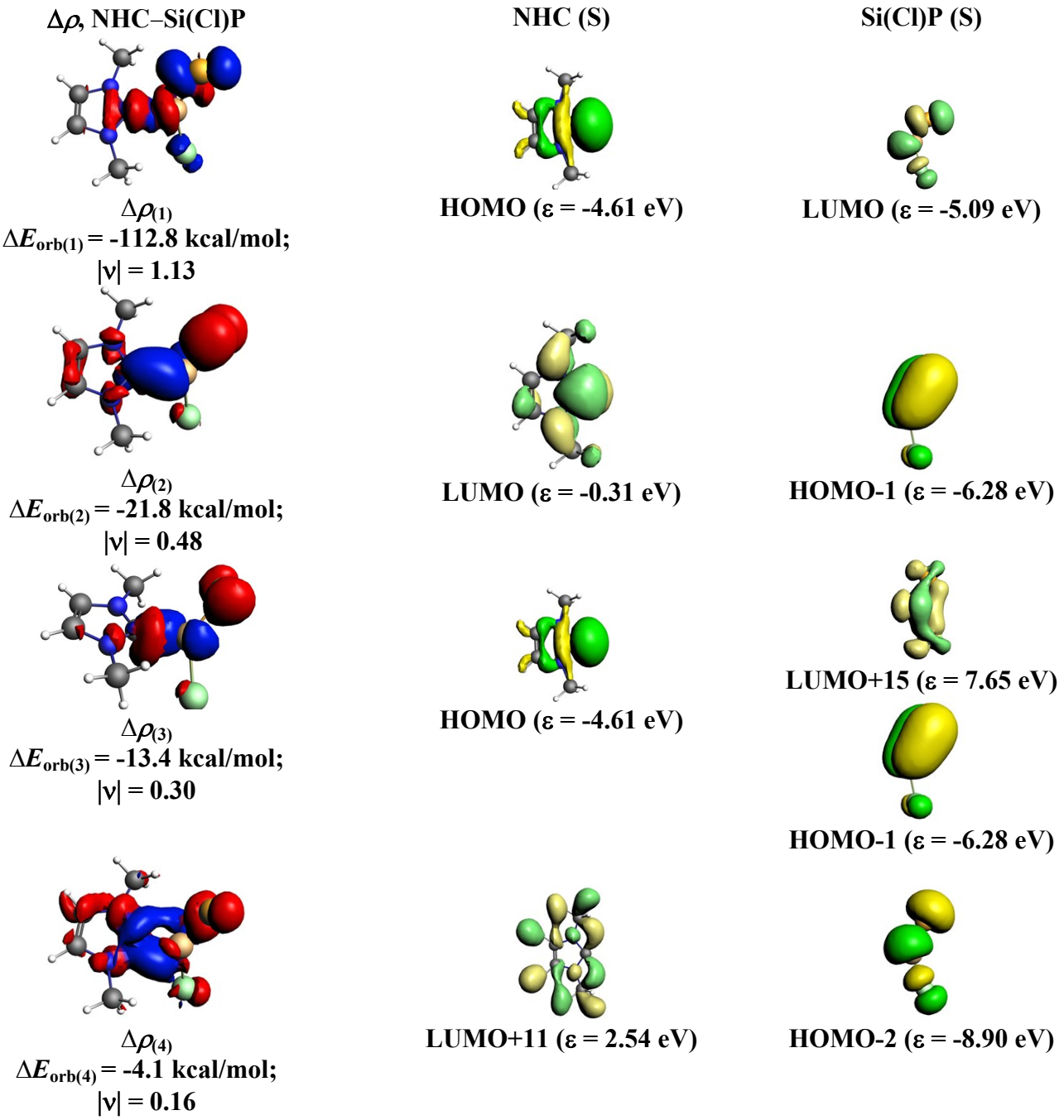


Figure S23. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of NHC-Si(Cl)P and the fragments orbitals of NHC and Si(Cl)P in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

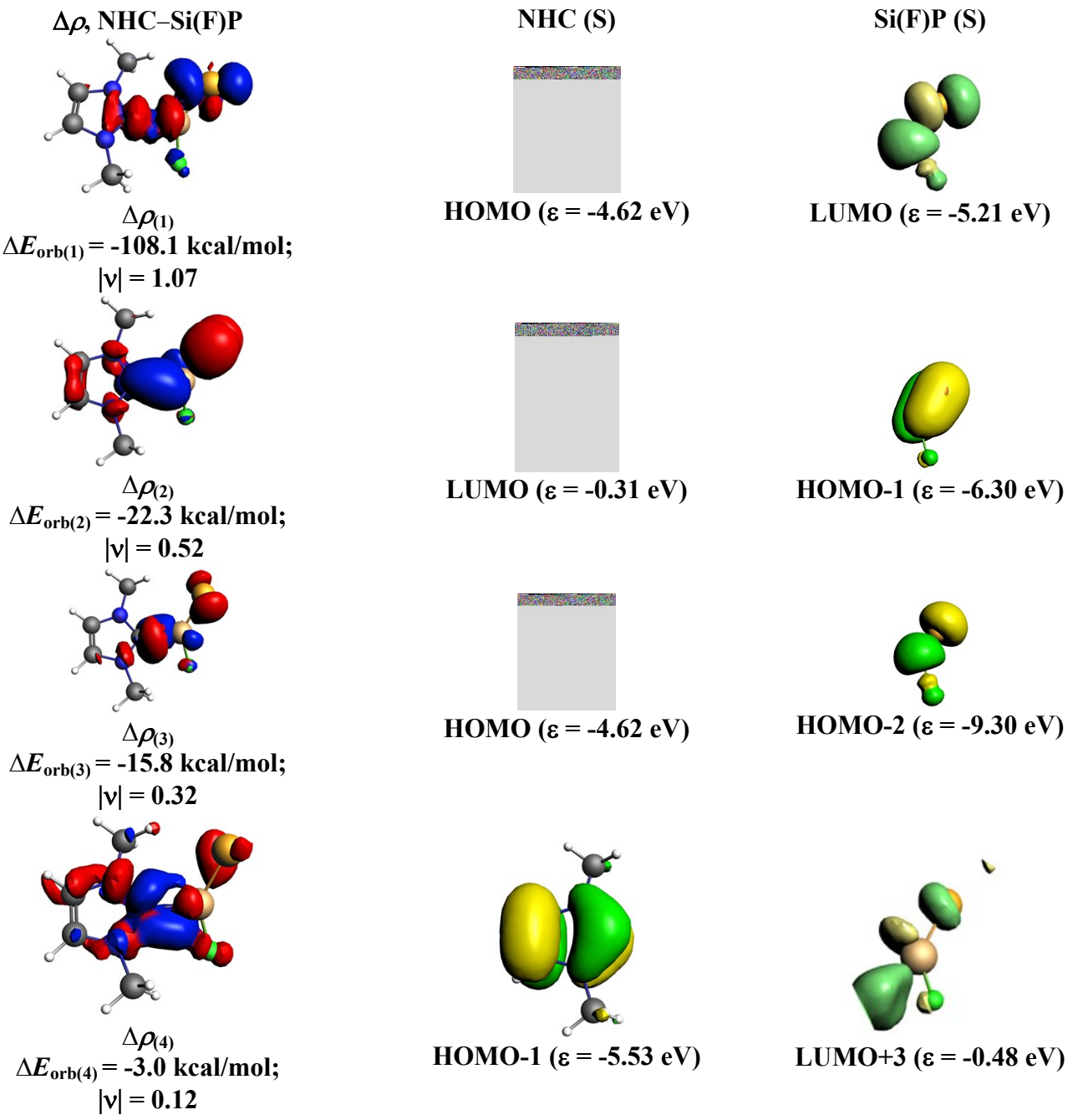


Figure S24. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of NHC-Si(F)P and the fragments orbitals of NHC and Si(F)P in the singlet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

Table S17. EDA-NOCV results of P–Si(Cl) bond of P-Si(Cl) molecule using three different sets of fragments with different charges and electronic states (S = singlet, Q = quartet) and associated bond types at the BP86-D3(BJ)/TZ2P level. Energies are in kcal/mol. The most favourable fragmentation scheme and bond type is given by the smallest ΔE_{orb} value written in red.

Molecule	Bond type[a]	Fragments	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{disp}	ΔE_{orb}
P-Si(Cl)	E	P (Q) + Si(Cl) (Q)	-147.6	157.2	-100.0	-2.8	**-202.1**
	D	$[P]^-$ (S) + $[Si(Cl)]^+$ (S)	-484.4	173.9	-298.7	-2.8	-356.9
	D	$[P]^+$ (S) + $[Si(Cl)]^-$ (S)	-351.5	327.3	-268.0	-2.8	-408.1

[a]D = Dative bond; E = Electron-sharing bond

Table S18. The EDA-NOCV results of best bonding model at the BP86-D3(BJ)/TZ2P level of P–Si(Cl) bond of P-Si(Cl) molecule. Energies are in kcal/mol.

Energy	Interaction[c]	P (Q) + Si(Cl) (Q)
ΔE_{int}		-147.6
ΔE_{Pauli}		157.2
ΔE_{disp}[a]		-2.8 (0.9%)
ΔE_{elstat}[a]		-100.0 (32.8%)
ΔE_{orb}[a]		-202.1 (66.3%)
$\Delta E_{orb(1)}$[b]	P–Si(Cl) σ e^- sharing	-90.2 (44.6%)
$\Delta E_{orb(2)}$[b]	P–Si(Cl) π e^- sharing	-50.8 (25.1%)
$\Delta E_{orb(3)}$[b]	P–Si(Cl) π e^- sharing	-50.8 (25.1%)
$\Delta E_{orb(4)}$[b]	P→Si(Cl) σ donation	-8.8 (4.4%)
$\Delta E_{orb(rest)}$[b]		-1.5 (0.7%)

[a]The values in the parentheses show the contribution to the total attractive interaction $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$. [b]The values in parentheses show the contribution to the total orbital interaction ΔE_{orb}.

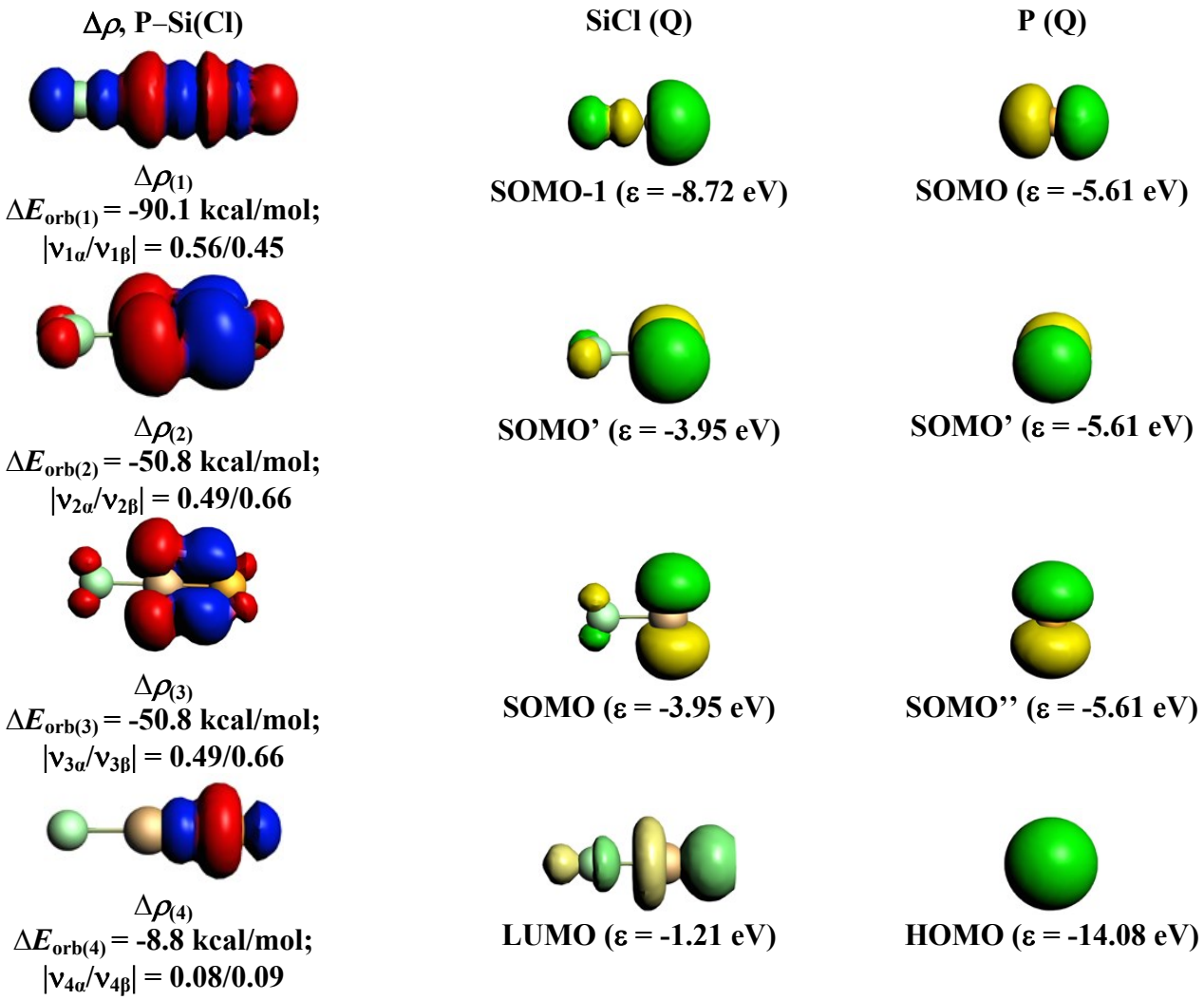


Figure S25. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of P-Si(Cl) and the fragments orbitals of P and Si(Cl) in the quartet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.001 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

Optimized Coordinates

cAAC^{Me}-PSi(Cl)-cAAC^{Me} Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1907.5241838

6	-3.794098000	-1.611060000	0.829540000
6	-2.363086000	-1.511232000	0.246802000
6	-2.258619000	-0.018582000	-0.110005000
6	-4.604192000	-0.443945000	0.230402000
1	-4.258358000	-2.584094000	0.618404000
1	-3.741136000	-1.496011000	1.922078000
6	-1.333982000	-2.032926000	1.255905000
1	-1.556559000	-3.084156000	1.496504000
1	-0.317078000	-1.985540000	0.843105000
1	-1.358031000	-1.446251000	2.184492000
6	-5.384760000	0.313109000	1.314153000
1	-5.954493000	1.154630000	0.895441000
1	-6.098735000	-0.366337000	1.800761000
1	-4.698567000	0.700901000	2.080041000
6	-2.219565000	-2.305518000	-1.071319000
1	-1.201187000	-2.190197000	-1.469356000
1	-2.407946000	-3.374984000	-0.890653000
1	-2.923797000	-1.951460000	-1.835493000
6	-5.551768000	-0.893612000	-0.892008000
1	-6.336102000	-1.541346000	-0.476077000
1	-6.050920000	-0.038824000	-1.369816000
1	-5.014265000	-1.456382000	-1.665333000
7	-3.515489000	0.429136000	-0.311100000
17	-0.777481000	2.878402000	-0.658369000
15	0.827100000	-0.226575000	-1.084723000
6	2.316964000	-0.161453000	-0.166938000
6	2.689655000	0.474809000	1.182468000
6	4.175781000	0.063138000	1.369100000
6	4.706440000	-0.384510000	-0.003434000
1	4.776914000	0.880092000	1.789634000
1	4.232833000	-0.783546000	2.068393000
7	3.438762000	-0.726057000	-0.696166000
6	2.533305000	2.005696000	1.122556000
1	2.901884000	2.452589000	2.058404000
1	3.093718000	2.439726000	0.284070000
1	1.480810000	2.291471000	0.997918000
6	1.853084000	-0.086057000	2.343885000
1	0.802668000	0.226589000	2.257120000
1	1.889261000	-1.184477000	2.359021000
1	2.250484000	0.289167000	3.299738000
6	5.431202000	0.742608000	-0.760142000
1	6.347152000	1.031359000	-0.225333000
1	5.719077000	0.417167000	-1.770192000
1	4.791070000	1.628818000	-0.856467000
6	5.620073000	-1.609089000	0.123845000
1	6.031490000	-1.924678000	-0.845537000
1	6.471245000	-1.366387000	0.775611000
1	5.074750000	-2.453706000	0.566583000
14	-0.679905000	0.890118000	0.185363000
6	-3.849215000	1.747876000	-0.821331000
1	-3.855007000	2.504632000	-0.020296000
1	-3.110559000	2.049605000	-1.567827000
1	-4.842953000	1.718720000	-1.285976000
6	3.439991000	-1.305329000	-2.024489000
1	3.171334000	-0.551537000	-2.784963000
1	2.685767000	-2.104778000	-2.081939000
1	4.428412000	-1.721728000	-2.247092000

cAAC^{Me}-PSi(Cl)-cAAC^{Me} Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1907.4866204

6	-4.647283000	-0.146822000	0.861506000
6	-3.333177000	0.553153000	1.305425000
6	-2.388891000	0.257905000	0.145550000
6	-4.276311000	-1.137019000	-0.263477000
1	-5.152745000	-0.652810000	1.695365000
1	-5.341369000	0.605382000	0.458723000
6	-3.547885000	2.069149000	1.477945000
1	-4.278265000	2.274132000	2.276981000
1	-2.601445000	2.563430000	1.745782000
1	-3.910935000	2.519902000	0.544076000
6	-5.372717000	-1.207553000	-1.330449000
1	-5.135996000	-1.934357000	-2.120533000
1	-6.318197000	-1.524079000	-0.867634000
1	-5.525189000	-0.222303000	-1.792032000
6	-2.783308000	-0.023851000	2.626415000
1	-1.820675000	0.447858000	2.873061000
1	-3.484472000	0.165813000	3.455104000
1	-2.610886000	-1.105536000	2.554006000
6	-3.960841000	-2.545913000	0.272379000
1	-4.848437000	-2.982381000	0.752260000
1	-3.654097000	-3.217184000	-0.542678000
1	-3.146674000	-2.511463000	1.008040000
7	-3.041967000	-0.505513000	-0.799051000
17	-0.637833000	2.403783000	-1.580052000
15	0.659525000	-0.775283000	-0.158316000
6	2.323642000	-0.261571000	0.059544000
6	2.979614000	1.120959000	0.156858000
6	4.423980000	0.781290000	0.611307000
6	4.686740000	-0.692854000	0.248317000
1	5.164295000	1.451619000	0.154928000
1	4.496680000	0.898404000	1.702330000
7	3.299374000	-1.206661000	0.127642000
6	2.967314000	1.787981000	-1.234720000
1	3.500086000	2.750049000	-1.188349000
1	3.457970000	1.160378000	-1.990276000
1	1.939645000	1.976325000	-1.566845000
6	2.318016000	2.049690000	1.181375000
1	1.300520000	2.335372000	0.878228000
1	2.251884000	1.567535000	2.166528000
1	2.910581000	2.971956000	1.278896000
6	5.435418000	-0.866599000	-1.084105000
1	6.450603000	-0.452738000	-1.004992000
1	5.525923000	-1.930212000	-1.348371000
1	4.914872000	-0.353807000	-1.902040000
6	5.444453000	-1.411697000	1.372725000
1	5.654911000	-2.462478000	1.127650000
1	6.410428000	-0.914084000	1.538448000
1	4.872249000	-1.376517000	2.309731000
14	-0.693941000	0.964691000	0.040881000
6	-2.362102000	-1.080104000	-1.941931000
1	-3.094548000	-1.355679000	-2.711462000
1	-1.676236000	-0.334184000	-2.365680000
1	-1.767923000	-1.972166000	-1.675325000
6	3.021137000	-2.612947000	-0.079285000
1	2.637949000	-2.794081000	-1.097573000
1	2.243914000	-2.947176000	0.626457000
1	3.932403000	-3.199604000	0.078087000

cAAC^{Me}-PSi(Cl)-NHC^{Me} Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1804.3675853

6	-4.661850000	-1.459302000	0.700221000
6	-2.866384000	-0.167990000	0.184631000
6	-4.654519000	-1.281152000	-0.652466000
1	-5.338231000	-2.010221000	1.341581000
6	-3.159820000	-0.737673000	2.592902000

1	-2.586005000	0.190607000	2.748238000
1	-4.049524000	-0.755096000	3.233744000
1	-2.512284000	-1.593292000	2.825790000
7	-3.548269000	-0.503490000	-0.952510000
17	-1.657215000	2.416149000	-1.120150000
15	-0.017161000	-0.673391000	-0.370713000
6	1.625317000	-0.286805000	0.095404000
6	2.225405000	0.892304000	0.878305000
6	3.745302000	0.567681000	0.905451000
6	4.003224000	-0.510407000	-0.161066000
1	4.359382000	1.461669000	0.732357000
1	4.016349000	0.166943000	1.892991000
7	2.647608000	-1.099083000	-0.300154000
6	1.949719000	2.226463000	0.161037000
1	2.464921000	3.043828000	0.688316000
1	2.300428000	2.207164000	-0.879642000
1	0.876684000	2.454782000	0.137802000
6	1.686394000	0.950459000	2.318533000
1	0.614663000	1.191272000	2.329286000
1	1.831854000	-0.014132000	2.825660000
1	2.225654000	1.726411000	2.884338000
6	4.453729000	0.084448000	-1.507521000
1	5.437899000	0.562898000	-1.402441000
1	4.538017000	-0.698329000	-2.275397000
1	3.737548000	0.836725000	-1.862832000
6	5.018694000	-1.549221000	0.327026000
1	5.235547000	-2.311252000	-0.435240000
1	5.967482000	-1.049397000	0.568455000
1	4.651697000	-2.051294000	1.232634000
14	-1.328350000	0.993095000	0.545823000
6	-3.131052000	-0.164506000	-2.310957000
1	-3.459541000	0.847619000	-2.575855000
1	-2.037396000	-0.201237000	-2.361866000
1	-3.562590000	-0.903229000	-2.996078000
6	2.415451000	-2.245494000	-1.155655000
1	1.981334000	-1.937829000	-2.123222000
1	1.689649000	-2.920851000	-0.679124000
1	3.357857000	-2.779174000	-1.322769000
7	-3.568270000	-0.770586000	1.195284000
1	-5.329560000	-1.642303000	-1.418427000

cAAC^{Me}-PSi(Cl)-NHC^{Me} Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1804.3164606

6	-5.220284000	-0.431820000	0.557492000
6	-2.952228000	-0.327138000	0.299082000
6	-4.807140000	-1.636999000	0.071175000
1	-6.210799000	-0.079757000	0.817389000
6	-4.088430000	1.734397000	1.172116000
1	-3.669029000	2.406251000	0.408500000
1	-5.117864000	2.036477000	1.396572000
1	-3.477980000	1.813550000	2.084154000
7	-3.435266000	-1.572964000	-0.099445000
17	-1.658935000	1.882600000	-1.774406000
15	0.187067000	-1.025744000	0.129359000
6	1.761438000	-0.243327000	0.159857000
6	2.189805000	1.198760000	0.443332000
6	3.699996000	1.039632000	0.766662000
6	4.173056000	-0.288991000	0.141330000
1	4.287937000	1.892869000	0.402353000
1	3.828931000	0.988279000	1.857551000
7	2.884529000	-0.989627000	-0.068269000
6	1.970324000	2.062400000	-0.816125000
1	2.367900000	3.075554000	-0.649701000
1	2.474261000	1.632356000	-1.691918000
1	0.903208000	2.148511000	-1.058242000

6	1.466414000	1.833288000	1.637378000
1	0.396802000	1.975339000	1.422889000
1	1.549131000	1.197220000	2.529788000
1	1.907102000	2.817219000	1.860204000
6	4.898987000	-0.093150000	-1.200833000
1	5.845962000	0.442978000	-1.044355000
1	5.135816000	-1.059855000	-1.668866000
1	4.284341000	0.485218000	-1.901604000
6	5.069386000	-1.070653000	1.113284000
1	5.412687000	-2.021795000	0.681577000
1	5.961506000	-0.475751000	1.356071000
1	4.531567000	-1.284228000	2.047229000
14	-1.331247000	0.556211000	0.014031000
6	-2.609929000	-2.647006000	-0.606609000
1	-1.954199000	-2.267402000	-1.405157000
1	-1.964626000	-3.052552000	0.186606000
1	-3.259480000	-3.436759000	-1.001157000
6	2.830447000	-2.379201000	-0.465004000
1	2.123983000	-2.505317000	-1.300616000
1	2.480050000	-3.020788000	0.362316000
1	3.826665000	-2.714356000	-0.776640000
7	-4.099188000	0.366879000	0.688104000
1	-5.372103000	-2.529445000	-0.168405000

cAAC^{Me}-PSi(Cl)-PMe$_3$ Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1960.6223543

6	-3.202765000	0.727512000	-1.145755000
6	-1.736145000	0.238295000	-1.288371000
6	-1.348372000	-0.133147000	0.151805000
6	-3.734213000	0.196837000	0.197393000
1	-3.219980000	1.827247000	-1.126907000
1	-3.827803000	0.401587000	-1.987958000
6	-1.637728000	-0.996442000	-2.205695000
1	-1.997304000	-0.741431000	-3.214222000
1	-0.594730000	-1.332949000	-2.285622000
1	-2.237095000	-1.833204000	-1.824307000
6	-4.511134000	-1.123822000	0.054314000
1	-4.799122000	-1.519260000	1.039065000
1	-5.430344000	-0.963589000	-0.527035000
1	-3.906226000	-1.884509000	-0.455221000
6	-0.864227000	1.370083000	-1.855131000
1	0.167303000	1.024946000	-2.021307000
1	-1.269512000	1.706786000	-2.822270000
1	-0.843149000	2.227595000	-1.168030000
6	-4.603875000	1.245127000	0.902942000
1	-5.459828000	1.504444000	0.263705000
1	-5.008270000	0.876732000	1.856525000
1	-4.026697000	2.159768000	1.096271000
7	-2.465662000	-0.033074000	0.930106000
6	-2.459305000	-0.446589000	2.318142000
1	-2.211075000	-1.517620000	2.412667000
1	-1.684980000	0.111000000	2.867699000
1	-3.439027000	-0.251675000	2.768379000
15	0.155316000	-0.674323000	0.861388000
14	1.660418000	-0.738609000	-0.905963000
17	2.976949000	-2.294483000	-0.052634000
15	2.945630000	0.867073000	0.189324000
6	2.184386000	2.523070000	0.066536000
1	2.035438000	2.778378000	-0.990451000
1	1.204145000	2.484167000	0.559937000
1	2.811877000	3.288237000	0.542909000
6	4.601538000	1.032423000	-0.570143000
1	5.208992000	1.796047000	-0.065206000
1	5.103716000	0.058076000	-0.505198000
1	4.486521000	1.291552000	-1.630610000

6	3.281073000	0.621670000	1.968004000
1	2.321838000	0.602334000	2.501461000
1	3.765841000	-0.354987000	2.091855000
1	3.925514000	1.417236000	2.366464000

cAAC^{Me}-PSi(Cl)-PMe$_3$ Triplet

BP86 (D3BJ)/def2-TZVPP

Energy: -1960.5624527

6	-2.955453000	-0.136805000	-1.164106000
6	-1.913890000	-1.244089000	-0.850793000
6	-1.098692000	-0.614649000	0.277119000
6	-3.034283000	0.779226000	0.072325000
1	-2.605628000	0.457586000	-2.021887000
1	-3.938468000	-0.550308000	-1.427901000
6	-2.576613000	-2.558979000	-0.383077000
1	-3.182188000	-2.996440000	-1.192341000
1	-1.801644000	-3.283571000	-0.096218000
1	-3.224116000	-2.404085000	0.489188000
6	-4.095365000	0.305824000	1.083596000
1	-4.167663000	0.993531000	1.938223000
1	-5.083693000	0.264329000	0.604695000
1	-3.857672000	-0.693394000	1.470367000
6	-1.081650000	-1.555831000	-2.105689000
1	-0.314973000	-2.313394000	-1.892777000
1	-1.729325000	-1.937254000	-2.911743000
1	-0.566639000	-0.654851000	-2.469081000
6	-3.307736000	2.234622000	-0.322313000
1	-4.288202000	2.313910000	-0.813621000
1	-3.325179000	2.899148000	0.553904000
1	-2.541629000	2.596968000	-1.021674000
7	-1.657522000	0.635366000	0.621582000
6	-1.378959000	1.213484000	1.922158000
1	-1.901723000	0.692580000	2.746800000
1	-0.303067000	1.124311000	2.123869000
1	-1.662480000	2.274607000	1.933530000
15	0.180053000	-1.409985000	1.252523000
14	1.821053000	-1.156889000	-0.236152000
17	3.792801000	-1.381137000	0.693956000
15	2.097277000	1.120847000	-0.432103000
6	0.699437000	1.993045000	-1.201805000
1	0.563794000	1.611725000	-2.221737000
1	-0.213491000	1.778104000	-0.623086000
1	0.888237000	3.075195000	-1.237714000
6	3.541420000	1.462013000	-1.498216000
1	3.714100000	2.542683000	-1.596131000
1	4.423257000	0.981233000	-1.056197000
1	3.365053000	1.024118000	-2.488963000
6	2.467987000	2.002213000	1.125422000
1	1.582524000	1.975094000	1.770487000
1	3.284404000	1.468432000	1.628438000
1	2.759549000	3.044605000	0.935354000

cAAC^{Me}-PSi(Cl)-AcAAC-Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1948.0396198

6	-1.925065000	-2.058514000	0.579391000
6	-2.040388000	-0.591059000	0.163407000
6	-0.714729000	-2.416697000	1.446242000
1	-0.743298000	-3.483672000	1.712585000
1	0.227242000	-2.230949000	0.909742000
1	-0.699256000	-1.824205000	2.372253000
6	-1.940434000	-2.909562000	-0.709475000
1	-1.039464000	-2.708373000	-1.307588000
1	-1.965914000	-3.982615000	-0.465232000
1	-2.821262000	-2.671947000	-1.321259000
7	-3.338690000	-0.168218000	-0.069887000
17	-1.107169000	2.524699000	-0.087965000

15	1.010259000	-0.247165000	-1.065225000
6	2.534881000	0.104180000	-0.273485000
6	2.881932000	0.687851000	1.104272000
6	4.921459000	-0.124541000	-0.075578000
7	3.690907000	-0.235719000	-0.900060000
6	2.273376000	2.078431000	1.334962000
1	2.703677000	2.520131000	2.246980000
1	2.478967000	2.747915000	0.489077000
1	1.185136000	2.030740000	1.469929000
6	2.412450000	-0.266679000	2.219354000
1	1.315075000	-0.322973000	2.230117000
1	2.802156000	-1.284125000	2.082732000
1	2.752047000	0.108682000	3.196327000
6	6.063420000	0.523553000	-0.866527000
1	6.905148000	0.728662000	-0.190255000
1	6.439518000	-0.128809000	-1.667407000
1	5.736163000	1.473451000	-1.310432000
6	5.344183000	-1.516550000	0.425134000
1	5.595993000	-2.177672000	-0.416571000
1	6.232958000	-1.435213000	1.066610000
1	4.540848000	-1.989615000	1.004039000
14	-0.589474000	0.488728000	0.322101000
6	-3.643598000	0.770481000	-1.181078000
1	-3.505393000	1.812210000	-0.841533000
6	3.691288000	-0.925935000	-2.175092000
1	4.720780000	-1.071208000	-2.519432000
6	-5.091753000	0.613811000	-1.667694000
1	-5.836689000	0.900026000	-0.917481000
1	-5.237884000	1.268701000	-2.537595000
1	-5.290256000	-0.421278000	-1.981158000
6	-2.718665000	0.524973000	-2.376338000
1	-3.026024000	1.182578000	-3.201330000
1	-1.666179000	0.733616000	-2.161711000
1	-2.798345000	-0.518811000	-2.713531000
6	-4.270237000	-0.250606000	1.097592000
6	-4.628109000	1.147931000	1.618839000
1	-5.279299000	1.702239000	0.930098000
1	-5.157377000	1.059708000	2.578315000
1	-3.715407000	1.738374000	1.779690000
1	-2.831750000	-2.326423000	1.150073000
6	-5.487680000	-1.165297000	0.907859000
1	-5.948905000	-1.360614000	1.887817000
1	-6.257586000	-0.732638000	0.259413000
1	-5.180869000	-2.127974000	0.477336000
1	-3.657816000	-0.710101000	1.884686000
6	4.430227000	0.797122000	1.054238000
1	4.711004000	1.833349000	0.816866000
1	4.890203000	0.540743000	2.017769000
1	3.185107000	-1.903016000	-2.093461000
1	3.136736000	-0.333299000	-2.918631000

cAAC^{Me}-PSi(Cl)-AcAAC-Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1948.0058852

6	-2.573631000	1.715120000	1.449620000
6	-2.183201000	0.579326000	0.515813000
6	-3.205148000	2.907605000	0.700512000
1	-3.488633000	3.711065000	1.398121000
1	-2.482070000	3.317704000	-0.020768000
1	-4.098366000	2.608625000	0.135764000
6	-1.376092000	2.200768000	2.286131000
1	-0.610333000	2.659878000	1.641166000
1	-1.698249000	2.960886000	3.014848000
1	-0.903884000	1.368138000	2.824385000
7	-3.079696000	-0.453631000	0.263371000
17	-1.054396000	0.845250000	-2.497520000

15	0.842986000	-0.885252000	0.108149000
6	2.472418000	-0.275266000	-0.078248000
6	3.016808000	1.108521000	-0.452204000
6	4.846030000	-0.419959000	0.278014000
7	3.522879000	-1.089259000	0.223889000
6	2.513707000	1.600098000	-1.816139000
1	3.064007000	2.508127000	-2.107107000
1	2.660099000	0.836374000	-2.591900000
1	1.445269000	1.848370000	-1.787208000
6	2.636818000	2.134150000	0.633716000
1	1.544121000	2.251453000	0.670144000
1	2.975554000	1.821817000	1.630007000
1	3.085858000	3.111147000	0.399905000
6	5.920692000	-1.261480000	-0.421285000
1	6.850166000	-0.679732000	-0.497267000
1	6.155884000	-2.181401000	0.132887000
1	5.598752000	-1.534139000	-1.435481000
6	5.249449000	-0.157277000	1.739662000
1	5.360053000	-1.101373000	2.292549000
1	6.213126000	0.370196000	1.779135000
1	4.499032000	0.454783000	2.255613000
14	-0.570757000	0.763481000	-0.399677000
6	-2.524923000	-1.702405000	-0.291096000
1	-1.558024000	-1.404367000	-0.732944000
6	3.323767000	-2.422288000	0.753322000
1	4.291750000	-2.916508000	0.890260000
6	-3.308035000	-2.330930000	-1.445488000
1	-3.449474000	-1.612822000	-2.262506000
1	-2.722380000	-3.175024000	-1.835466000
1	-4.286332000	-2.725530000	-1.140826000
6	-2.187278000	-2.715194000	0.813302000
1	-1.543768000	-3.508140000	0.405486000
1	-1.634341000	-2.217943000	1.621074000
1	-3.087568000	-3.184890000	1.231475000
6	-4.527362000	-0.277470000	0.486507000
6	-5.295473000	0.049597000	-0.809870000
1	-5.452638000	-0.835968000	-1.436213000
1	-6.283479000	0.463401000	-0.558025000
1	-4.747979000	0.796043000	-1.400363000
1	-3.311951000	1.327053000	2.172986000
6	-5.180702000	-1.418036000	1.275347000
1	-6.225847000	-1.154707000	1.493379000
1	-5.189871000	-2.362754000	0.716846000
1	-4.661921000	-1.585799000	2.228382000
1	-4.611005000	0.613839000	1.117272000
6	4.550600000	0.871443000	-0.506745000
1	4.856164000	0.730768000	-1.553589000
1	5.112291000	1.727306000	-0.109285000
1	2.785090000	-2.390857000	1.716435000
1	2.708494000	-3.011938000	0.055858000

cAAC^{Me}-PSi(F)-cAAC^{Me} Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1547.1535991

6	-3.961053000	-1.170735000	1.065463000
6	-2.492946000	-1.284198000	0.578567000
6	-2.278157000	0.057252000	-0.128397000
6	-4.660517000	-0.145373000	0.145668000
1	-4.474547000	-2.142021000	1.060038000
1	-3.966189000	-0.795681000	2.099282000
6	-1.540932000	-1.561342000	1.747841000
1	-1.794675000	-2.525011000	2.216322000
1	-0.498952000	-1.614136000	1.401124000
1	-1.609384000	-0.769517000	2.506236000
6	-5.449092000	0.891119000	0.958421000
1	-5.940930000	1.629962000	0.309930000

1	-6.230564000	0.388233000	1.545616000
1	-4.782346000	1.421387000	1.652701000
6	-2.327593000	-2.399149000	-0.480028000
1	-1.285693000	-2.436126000	-0.829098000
1	-2.589223000	-3.375685000	-0.044081000
1	-2.970027000	-2.224608000	-1.353277000
6	-5.571494000	-0.805866000	-0.900137000
1	-6.423277000	-1.290255000	-0.402220000
1	-5.978370000	-0.066578000	-1.605354000
1	-5.029818000	-1.567330000	-1.475156000
7	-3.490164000	0.507286000	-0.517128000
15	0.784487000	-0.427675000	-0.974625000
6	2.302447000	-0.114166000	-0.157025000
6	2.702956000	0.862990000	0.960172000
6	4.206484000	0.541970000	1.192124000
6	4.697193000	-0.269364000	-0.019359000
1	4.802794000	1.452927000	1.335440000
1	4.312625000	-0.068406000	2.100483000
7	3.413735000	-0.799923000	-0.542739000
6	2.503012000	2.321716000	0.506914000
1	2.898026000	3.005530000	1.273556000
1	3.014543000	2.527764000	-0.443029000
1	1.437863000	2.546638000	0.362738000
6	1.919465000	0.609353000	2.259098000
1	0.855739000	0.856258000	2.130552000
1	1.997707000	-0.444470000	2.561567000
1	2.330259000	1.235629000	3.066387000
6	5.371513000	0.611787000	-1.085790000
1	6.304273000	1.039556000	-0.691393000
1	5.621639000	0.026667000	-1.982518000
1	4.712467000	1.436100000	-1.387847000
6	5.638169000	-1.400620000	0.408809000
1	6.018430000	-1.974115000	-0.448636000
1	6.507886000	-0.976208000	0.929929000
1	5.126574000	-2.090032000	1.094219000
14	-0.694214000	0.988674000	-0.002250000
6	-3.679623000	1.699808000	-1.325606000
1	-3.605400000	2.616337000	-0.716525000
1	-2.909086000	1.745391000	-2.100411000
1	-4.667433000	1.669655000	-1.801882000
6	3.383753000	-1.727076000	-1.656532000
1	3.096421000	-1.215095000	-2.591229000
1	2.628941000	-2.505643000	-1.469854000
1	4.367567000	-2.194218000	-1.775872000
9	-0.819184000	2.332292000	-0.986557000

cAAC^{Me}-PSi(F)-cAAC^{Me} Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1547.1146947

6	-4.362520000	-1.358305000	-0.267858000
6	-2.812781000	-1.394854000	-0.423449000
6	-2.371000000	-0.100770000	0.262914000
6	-4.747276000	0.072838000	0.154772000
1	-4.875548000	-1.656545000	-1.192246000
1	-4.667975000	-2.059540000	0.522166000
6	-2.247535000	-2.639539000	0.288873000
1	-2.677768000	-3.556062000	-0.146704000
1	-1.154554000	-2.691081000	0.189496000
1	-2.490991000	-2.613769000	1.360288000
6	-5.915801000	0.077450000	1.143768000
1	-6.208851000	1.097209000	1.432719000
1	-6.794041000	-0.395841000	0.682380000
1	-5.655118000	-0.484936000	2.051002000
6	-2.382101000	-1.427345000	-1.902935000
1	-1.285710000	-1.402719000	-1.983587000
1	-2.740157000	-2.350277000	-2.385927000

1	-2.777886000	-0.567215000	-2.458931000
6	-5.063225000	0.969766000	-1.056967000
1	-5.934627000	0.582363000	-1.603794000
1	-5.294027000	1.997333000	-0.740177000
1	-4.207503000	1.008118000	-1.744414000
7	-3.484396000	0.521287000	0.801623000
15	0.804565000	-0.837532000	0.383595000
6	2.389948000	-0.107733000	0.203979000
6	2.853647000	1.313265000	-0.142333000
6	4.373528000	1.259790000	0.164310000
6	4.797217000	-0.221653000	0.143601000
1	4.955113000	1.860833000	-0.547190000
1	4.554727000	1.667519000	1.169406000
7	3.489830000	-0.893681000	0.345333000
6	2.590557000	1.587514000	-1.638810000
1	3.007559000	2.569094000	-1.911390000
1	3.059222000	0.826357000	-2.276818000
1	1.515323000	1.593203000	-1.849415000
6	2.193031000	2.402158000	0.711251000
1	1.119657000	2.499606000	0.495142000
1	2.300586000	2.181639000	1.782134000
1	2.667519000	3.372944000	0.501385000
6	5.418122000	-0.655476000	-1.195107000
1	6.374062000	-0.136918000	-1.355124000
1	5.617774000	-1.736848000	-1.205540000
1	4.752594000	-0.421574000	-2.034982000
6	5.760116000	-0.536709000	1.296548000
1	6.076345000	-1.589496000	1.298526000
1	6.665844000	0.077985000	1.196001000
1	5.292467000	-0.308468000	2.263976000
14	-0.727687000	0.748805000	0.142563000
6	-3.401163000	1.845928000	1.382822000
1	-2.578363000	1.870323000	2.110252000
1	-3.205440000	2.628803000	0.625082000
1	-4.336451000	2.084291000	1.904512000
6	3.392368000	-2.326023000	0.542327000
1	2.834310000	-2.793424000	-0.285643000
1	2.843662000	-2.547819000	1.471470000
1	4.396091000	-2.760518000	0.600782000
9	-0.650837000	1.586674000	-1.302174000

cAAC^{Me}-PSi(F)-NHC^{Me} Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: - -1443.9966159

6	4.366902000	-1.792013000	-0.186438000
6	2.924019000	-0.038211000	-0.105559000
6	4.923764000	-0.839601000	0.614422000
1	4.727385000	-2.768313000	-0.485842000
6	2.202392000	-1.964271000	-1.489120000
1	1.904749000	-1.267025000	-2.289651000
1	2.673940000	-2.856657000	-1.915507000
1	1.299468000	-2.232766000	-0.921791000
7	4.031975000	0.225362000	0.656125000
15	0.087413000	-0.083905000	0.830946000
6	-1.522858000	-0.096740000	0.148257000
6	-2.086682000	0.429806000	-1.181427000
6	-3.590325000	0.042658000	-1.114649000
6	-3.909986000	-0.295023000	0.351919000
1	-4.237091000	0.844516000	-1.495566000
1	-3.766505000	-0.847537000	-1.736270000
7	-2.557632000	-0.628051000	0.864123000
6	-1.905308000	1.955636000	-1.291562000
1	-2.405455000	2.324889000	-2.200029000
1	-2.327142000	2.478770000	-0.423064000
1	-0.839763000	2.216007000	-1.357143000

6	-1.428408000	-0.259621000	-2.389683000
1	-0.372461000	0.031511000	-2.473646000
1	-1.489239000	-1.353060000	-2.290220000
1	-1.948967000	0.034184000	-3.314940000
6	-4.478728000	0.908355000	1.125078000
1	-5.460426000	1.194054000	0.721030000
1	-4.608677000	0.666259000	2.189856000
1	-3.806391000	1.772839000	1.050181000
6	-4.861665000	-1.491662000	0.457269000
1	-5.115163000	-1.731512000	1.499984000
1	-5.801782000	-1.259812000	-0.063079000
1	-4.417408000	-2.381218000	-0.010085000
14	1.416277000	1.028030000	-0.719904000
6	4.211273000	1.405421000	1.495954000
1	3.516307000	2.181193000	1.161952000
1	3.997653000	1.158135000	2.544913000
1	5.246084000	1.760372000	1.407769000
6	-2.369374000	-1.109993000	2.217496000
1	-2.050074000	-0.296370000	2.891854000
1	-1.570443000	-1.866222000	2.228929000
1	-3.301707000	-1.553586000	2.585243000
7	3.151440000	-1.290310000	-0.618644000
1	5.863950000	-0.825743000	1.151785000
9	1.768833000	2.462866000	0.103870000

cAAC^{Me}-PSi(F)-NHC^{Me} Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1443.9449112

6	-5.233806000	-0.335447000	0.686352000
6	-3.051074000	-0.040610000	0.071604000
6	-4.890464000	-1.386424000	-0.111569000
1	-6.170434000	-0.104816000	1.178971000
6	-4.029987000	1.677061000	1.609069000
1	-3.665315000	2.526618000	1.010151000
1	-5.019903000	1.916428000	2.014869000
1	-3.320159000	1.515775000	2.436890000
7	-3.576343000	-1.202611000	-0.509929000
15	0.015837000	-0.793997000	0.182025000
6	1.641673000	-0.128133000	0.155243000
6	2.179655000	1.249360000	-0.240603000
6	3.683608000	1.154743000	0.134254000
6	4.033464000	-0.339646000	0.267376000
1	4.322321000	1.657312000	-0.604473000
1	3.848111000	1.646436000	1.104161000
7	2.697196000	-0.919492000	0.536803000
6	1.988261000	1.479786000	-1.754654000
1	2.437200000	2.442296000	-2.044976000
1	2.465222000	0.686147000	-2.344985000
1	0.923581000	1.500868000	-2.016144000
6	1.526304000	2.399632000	0.539891000
1	0.460289000	2.507663000	0.289647000
1	1.599378000	2.229026000	1.622974000
1	2.028086000	3.349118000	0.296483000
6	4.626546000	-0.932719000	-1.024241000
1	5.592539000	-0.459612000	-1.251930000
1	4.798223000	-2.013607000	-0.916739000
1	3.955071000	-0.776521000	-1.877979000
6	4.990701000	-0.583203000	1.441001000
1	5.267542000	-1.642876000	1.538053000
1	5.919319000	-0.016691000	1.282806000
1	4.536773000	-0.250200000	2.384210000
14	-1.422942000	0.816325000	-0.183448000
6	-2.817374000	-2.126560000	-1.324719000
1	-2.123565000	-1.560428000	-1.963606000
1	-2.218623000	-2.812980000	-0.707504000
1	-3.509856000	-2.702407000	-1.952077000

6	2.530328000	-2.329269000	0.812156000
1	2.255852000	-2.897285000	-0.095127000
1	1.713274000	-2.462834000	1.538390000
1	3.457088000	-2.738872000	1.229948000
7	-4.130740000	0.493752000	0.785477000
1	-5.475122000	-2.237493000	-0.439102000
9	-1.376787000	1.558596000	-1.680937000

cAAC^{Me}-PSi(F)-PMe$_3$ Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1600.2456115

6	2.963845000	-1.058154000	0.920044000
6	1.545238000	-1.259337000	0.322061000
6	1.191669000	0.134804000	-0.219056000
6	3.545245000	0.226829000	0.301990000
1	2.882768000	-0.926179000	2.009164000
1	3.612732000	-1.925857000	0.739918000
6	1.553238000	-2.285109000	-0.828641000
1	1.885737000	-3.265263000	-0.454101000
1	0.542174000	-2.399010000	-1.244429000
1	2.224386000	-1.977214000	-1.641217000
6	4.461857000	-0.051197000	-0.902471000
1	4.783208000	0.886521000	-1.378309000
1	5.363423000	-0.590354000	-0.578228000
1	3.946551000	-0.658383000	-1.657474000
6	0.579308000	-1.729443000	1.420485000
1	-0.415566000	-1.942979000	1.001588000
1	0.960149000	-2.654185000	1.881961000
1	0.478155000	-0.965044000	2.203651000
6	4.294570000	1.055838000	1.353636000
1	5.128716000	0.467026000	1.761194000
1	4.719407000	1.977643000	0.931296000
1	3.623843000	1.325672000	2.180894000
7	2.309776000	0.913652000	-0.142168000
6	2.343342000	2.247217000	-0.705131000
1	2.115459000	2.223394000	-1.784187000
1	1.573524000	2.875654000	-0.229790000
1	3.330884000	2.694126000	-0.544485000
15	-0.280704000	0.784836000	-0.897129000
14	-1.788099000	-0.996418000	-0.970157000
15	-3.142811000	0.253143000	0.520088000
6	-2.407415000	0.382828000	2.186000000
1	-2.233142000	-0.624722000	2.584939000
1	-1.440236000	0.892581000	2.085159000
1	-3.060908000	0.940398000	2.870567000
6	-4.787096000	-0.511757000	0.789474000
1	-5.406173000	0.068240000	1.488174000
1	-5.299166000	-0.582872000	-0.179364000
1	-4.646308000	-1.529199000	1.177277000
6	-3.530291000	1.969346000	0.016288000
1	-2.586785000	2.524873000	-0.063622000
1	-3.997581000	1.939163000	-0.976570000
1	-4.204549000	2.462181000	0.730505000
9	-2.687120000	-0.442534000	-2.289955000

cAAC^{Me}-PSi(F)-PMe$_3$ Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1600.1807799

6	3.015820000	-0.313781000	1.385846000
6	1.636595000	-0.904931000	0.973385000
6	1.294306000	-0.113896000	-0.291676000
6	3.538142000	0.497611000	0.184736000
1	2.887118000	0.361602000	2.244335000
1	3.724911000	-1.097415000	1.684902000
6	1.716576000	-2.416500000	0.697043000
1	1.986753000	-2.957465000	1.616878000
1	0.745775000	-2.791629000	0.344082000
1	2.464762000	-2.644528000	-0.073446000

6	4.395615000	-0.360046000	-0.763969000
1	4.721107000	0.221842000	-1.638421000
1	5.295700000	-0.723075000	-0.247840000
1	3.825995000	-1.227243000	-1.124211000
6	0.609722000	-0.651870000	2.091670000
1	-0.375730000	-1.067184000	1.821472000
1	0.931863000	-1.140158000	3.024730000
1	0.496521000	0.424659000	2.281228000
6	4.315382000	1.736162000	0.636053000
1	5.168128000	1.431348000	1.259029000
1	4.719030000	2.303487000	-0.215054000
1	3.671590000	2.400632000	1.228902000
7	2.256261000	0.871061000	-0.469740000
6	2.269643000	1.678279000	-1.670875000
1	2.479104000	1.080742000	-2.579151000
1	1.280044000	2.137974000	-1.805619000
1	3.024201000	2.468586000	-1.577178000
15	0.017297000	-0.354688000	-1.464359000
14	-1.725394000	-1.191558000	-0.384700000
15	-3.391825000	0.411425000	0.360132000
6	-2.380503000	1.495297000	1.443227000
1	-2.222148000	1.006097000	2.413323000
1	-1.403691000	1.662157000	0.971206000
1	-2.884642000	2.457921000	1.605512000
6	-5.069704000	0.525228000	1.191351000
1	-5.387484000	1.571087000	1.332219000
1	-5.807031000	0.000429000	0.570456000
1	-5.019555000	0.026143000	2.167775000
6	-3.668522000	1.420295000	-1.151558000
1	-2.702579000	1.602883000	-1.638368000
1	-4.310805000	0.861554000	-1.844377000
1	-4.149525000	2.376044000	-0.899182000
9	-2.690916000	-1.840473000	-1.559692000

cAAC^{Me}-PSi(F)-AcAAC-Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -1587.6699234

6	2.003097000	1.896384000	0.801305000
6	2.104996000	0.504037000	0.183019000
6	0.815385000	2.123334000	1.742160000
1	0.855064000	3.138267000	2.164989000
1	-0.138991000	2.022397000	1.204583000
1	0.817414000	1.397539000	2.567923000
6	1.976984000	2.914362000	-0.359987000
1	1.058908000	2.786402000	-0.952216000
1	2.005994000	3.945459000	0.024929000
1	2.839412000	2.766108000	-1.023793000
7	3.403941000	0.082949000	-0.080764000
15	-0.987096000	0.441283000	-1.050128000
6	-2.481337000	-0.099411000	-0.309594000
6	-2.773351000	-1.001145000	0.899543000
6	-4.867945000	-0.001207000	-0.008349000
7	-3.661930000	0.364390000	-0.793081000
6	-2.114061000	-2.383326000	0.792469000
1	-2.498538000	-3.037231000	1.590222000
1	-2.323983000	-2.850607000	-0.178926000
1	-1.023850000	-2.320998000	0.910447000
6	-2.307137000	-0.310451000	2.196821000
1	-1.212037000	-0.216203000	2.201530000
1	-2.733129000	0.696043000	2.304454000
1	-2.610356000	-0.912046000	3.067034000
6	-5.999418000	-0.482610000	-0.924759000
1	-6.821195000	-0.881364000	-0.313402000
1	-6.412218000	0.330786000	-1.538152000
1	-5.645363000	-1.280574000	-1.591509000
6	-5.336865000	1.203050000	0.826096000

1	-5.630480000	2.041514000	0.178131000
1	-6.209231000	0.926658000	1.434979000
1	-4.541888000	1.551137000	1.497532000
14	0.647122000	-0.564935000	0.111381000
6	3.642603000	-0.800011000	-1.254432000
1	3.309967000	-1.828026000	-1.021957000
6	-3.716302000	1.348711000	-1.856413000
1	-4.759607000	1.587985000	-2.088108000
6	5.123769000	-0.848690000	-1.649021000
1	5.761911000	-1.315614000	-0.891170000
1	5.219409000	-1.445009000	-2.566742000
1	5.507087000	0.160639000	-1.856902000
6	2.850165000	-0.301019000	-2.467711000
1	3.075647000	-0.941609000	-3.331603000
1	1.766731000	-0.319020000	-2.313637000
1	3.141983000	0.731224000	-2.711805000
6	4.277409000	-0.058166000	1.127251000
6	4.402838000	-1.524819000	1.560027000
1	5.007113000	-2.121880000	0.864426000
1	4.880180000	-1.581056000	2.548693000
1	3.406290000	-1.983221000	1.634184000
1	2.926159000	2.091434000	1.375413000
6	5.619089000	0.681494000	1.052297000
1	5.472276000	1.699401000	0.666509000
1	6.047102000	0.757131000	2.063345000
1	6.358105000	0.179074000	0.418213000
1	3.701111000	0.434583000	1.920797000
6	-4.317835000	-1.152408000	0.852909000
1	-4.572488000	-2.109913000	0.375805000
1	-4.759930000	-1.155243000	1.858092000
1	-3.180862000	2.267685000	-1.563856000
1	-3.221691000	0.957098000	-2.758585000
9	1.030902000	-2.028792000	-0.564684000

cAAC^{Me}-PSi(F)-AcAAC-Triplet

BP86 (D3BJ)/def2-TZVPP
Energy: -1587.6339886

6	2.630685000	1.849591000	-1.182141000
6	2.246828000	0.670889000	-0.298986000
6	3.257709000	3.009104000	-0.380122000
1	3.540972000	3.843906000	-1.040226000
1	2.531280000	3.385619000	0.356170000
1	4.151075000	2.687833000	0.172347000
6	1.431780000	2.368488000	-1.997481000
1	0.656823000	2.781967000	-1.333300000
1	1.750427000	3.169290000	-2.683289000
1	0.970605000	1.561491000	-2.582210000
7	3.138825000	-0.385888000	-0.129046000
15	-0.789095000	-0.817701000	-0.184390000
6	-2.426400000	-0.274588000	0.106388000
6	-2.983634000	1.003446000	0.746094000
6	-4.799471000	-0.368569000	-0.268334000
7	-3.472232000	-1.026971000	-0.342470000
6	-2.473807000	1.219653000	2.178037000
1	-3.015934000	2.058626000	2.641230000
1	-2.628811000	0.320807000	2.790344000
1	-1.403223000	1.458595000	2.196274000
6	-2.627324000	2.231174000	-0.115624000
1	-1.535875000	2.369070000	-0.136816000
1	-2.975481000	2.121709000	-1.150980000
1	-3.084899000	3.135241000	0.313774000
6	-5.873098000	-1.338354000	0.239857000
1	-6.805183000	-0.787592000	0.429566000
1	-6.101792000	-2.124848000	-0.493359000
1	-5.553436000	-1.813251000	1.177292000
6	-5.196674000	0.180235000	-1.650451000

1	-5.308536000	-0.636255000	-2.378555000
1	-6.157378000	0.711019000	-1.588587000
1	-4.439064000	0.876236000	-2.031772000
14	0.600639000	0.759904000	0.573650000
6	2.588008000	-1.661801000	0.365881000
1	1.608372000	-1.394904000	0.798825000
6	-3.262357000	-2.231971000	-1.116935000
1	-4.224771000	-2.711390000	-1.326657000
6	3.361674000	-2.327904000	1.506912000
1	3.495886000	-1.639466000	2.350276000
1	2.776434000	-3.187544000	1.862207000
1	4.344104000	-2.708232000	1.197400000
6	2.279732000	-2.636980000	-0.780736000
1	1.627350000	-3.442859000	-0.414409000
1	1.744766000	-2.114326000	-1.584363000
1	3.189667000	-3.093250000	-1.192489000
6	4.586037000	-0.199298000	-0.345837000
6	5.355069000	0.084339000	0.960666000
1	5.511766000	-0.820823000	1.558894000
1	6.343507000	0.505220000	0.722820000
1	4.808980000	0.812955000	1.574429000
1	3.371019000	1.501245000	-1.923200000
6	5.245005000	-1.308685000	-1.172956000
1	4.723409000	-1.451432000	-2.128328000
1	6.286564000	-1.028380000	-1.387032000
1	5.266737000	-2.270102000	-0.644137000
1	4.667729000	0.713571000	-0.945515000
6	-4.513901000	0.740553000	0.761423000
1	-4.808840000	0.383955000	1.759187000
1	-5.090220000	1.651377000	0.550974000
1	-2.743652000	-2.011398000	-2.066230000
1	-2.622722000	-2.928003000	-0.551971000
9	0.882057000	0.619473000	2.203651000

cAAC^{Me} Singlet

BP86 (GD3BJ)/def2-TZVPP
Energy: -408.0690298

6	-0.448626000	-1.114953000	-0.429047000
6	-1.442500000	0.025176000	-0.049568000
6	-0.605778000	1.293143000	0.079856000
6	0.955145000	-0.577973000	-0.093546000
1	-0.659329000	-2.056513000	0.096974000
1	-0.515437000	-1.321893000	-1.507407000
6	-2.525593000	0.219679000	-1.120716000
1	-3.134032000	-0.692439000	-1.225647000
1	-3.186358000	1.054293000	-0.849925000
1	-2.077147000	0.448397000	-2.098496000
6	1.964122000	-0.824527000	-1.219104000
1	2.962608000	-0.436734000	-0.971167000
1	2.065114000	-1.905201000	-1.394046000
1	1.627464000	-0.357796000	-2.155513000
6	-2.116199000	-0.218291000	1.316866000
1	-2.732983000	0.646286000	1.597085000
1	-2.760325000	-1.109831000	1.267353000
1	-1.376670000	-0.373698000	2.115224000
6	1.500209000	-1.112924000	1.238543000
1	1.685934000	-2.193455000	1.159428000
1	2.451816000	-0.632563000	1.507152000
1	0.786069000	-0.945502000	2.055128000
7	0.647217000	0.909676000	0.043760000
6	1.758039000	1.849404000	0.183163000
1	2.380767000	1.855558000	-0.722738000
1	1.326991000	2.841816000	0.341429000
1	2.392086000	1.579139000	1.040167000

PSi(Cl) Singlet

BP86 (D3BJ)/def2-TZVPP

Energy: -1091.1745429

15	0.013172000	2.078961000	0.000000000
14	0.000000000	0.109808000	0.000000000
17	-0.011622000	-1.924807000	0.000000000

PSi(F) Singlet

BP86 (D3BJ)/def2-TZVPP
Energy: -730.8013775

15	-0.003521000	-1.570030000	0.000000000
14	0.000000000	0.396511000	0.000000000
9	0.005869000	1.999922000	0.000000000

[(cAAC) cAAC]

BP86 (D3BJ)/def2-TZVPP
Energy: -816.1466191

6	-3.571253000	-1.431006000	0.313089000
6	-2.057183000	-1.055346000	0.287814000
6	-2.004931000	0.464163000	0.227570000
6	-4.327972000	-0.175846000	-0.156284000
1	-3.801652000	-2.301842000	-0.316323000
1	-3.871735000	-1.680823000	1.341743000
6	-1.315350000	-1.562639000	1.534143000
1	-1.407697000	-2.658297000	1.609428000
1	-0.248611000	-1.305067000	1.463318000
1	-1.733628000	-1.120659000	2.451073000
6	-5.527383000	0.160811000	0.733902000
1	-6.051239000	1.066469000	0.395529000
1	-6.250099000	-0.667279000	0.708830000
1	-5.211146000	0.305027000	1.776647000
6	-1.332884000	-1.586498000	-0.967960000
1	-0.271943000	-1.299201000	-0.928880000
1	-1.396881000	-2.685838000	-0.994155000
1	-1.776531000	-1.195636000	-1.895624000
6	-4.756321000	-0.251723000	-1.628904000
1	-5.511923000	-1.039681000	-1.758103000
1	-5.202677000	0.693321000	-1.970980000
1	-3.901187000	-0.485725000	-2.276235000
7	-3.229293000	0.871179000	-0.002769000
6	2.004630000	-0.463625000	0.227691000
6	2.057515000	1.055874000	0.287666000
6	3.571755000	1.430841000	0.313028000
6	4.327925000	0.175351000	-0.156316000
1	3.802608000	2.301620000	-0.316295000
1	3.872257000	1.680432000	1.341733000
7	3.228801000	-0.871197000	-0.002651000
6	1.333589000	1.586984000	-0.968364000
1	1.397975000	2.686294000	-0.994836000
1	1.777208000	1.195723000	-1.895871000
1	0.272546000	1.300044000	-0.929383000
6	1.315827000	1.563953000	1.533746000
1	0.248867000	1.307311000	1.462895000
1	1.733744000	1.122040000	2.450872000
1	1.409011000	2.659572000	1.608712000
6	4.756260000	0.250929000	-1.628952000
1	5.512205000	1.038546000	-1.758216000
1	5.202214000	-0.694330000	-1.970956000
1	3.901232000	0.485251000	-2.276303000
6	5.527235000	-0.161820000	0.733825000
1	6.050578000	-1.067782000	0.395478000
1	6.250374000	0.665896000	0.708631000
1	5.210994000	-0.305793000	1.776602000
6	-3.569446000	2.282358000	-0.168904000
1	-4.266601000	2.611515000	0.614926000
1	-2.638924000	2.852439000	-0.097686000
1	-4.038094000	2.459090000	-1.148295000
6	3.568364000	-2.282554000	-0.168547000
1	4.037657000	-2.459505000	-1.147585000

1	2.637509000	-2.852177000	-0.098011000
1	4.264762000	-2.612074000	0.615805000

[(cAAC) NHC]

BP86 (D3BJ)/def2-TZVPP
Energy: -713.0114171

6	2.608336000	-1.238046000	1.067659000
6	3.278298000	-0.162405000	-0.856838000
6	3.317054000	-0.137360000	1.451359000
1	2.102310000	-1.994365000	1.656075000
6	1.907805000	-2.220405000	-1.130739000
1	2.130449000	-1.999654000	-2.179830000
1	2.259975000	-3.233295000	-0.887432000
1	0.824600000	-2.131206000	-0.942440000
7	3.705940000	0.494041000	0.273044000
6	-0.992665000	-0.655373000	-0.131322000
6	-0.836201000	0.799862000	-0.551873000
6	-2.283153000	1.377191000	-0.639798000
6	-3.181877000	0.389844000	0.126301000
1	-2.357463000	2.394255000	-0.230824000
1	-2.599407000	1.424006000	-1.692389000
7	-2.247701000	-0.812958000	0.209663000
6	0.007282000	1.503650000	0.531946000
1	0.173264000	2.554956000	0.250582000
1	-0.489101000	1.485675000	1.513002000
1	0.981376000	1.010072000	0.638482000
6	-0.105156000	0.895515000	-1.900125000
1	0.932548000	0.541632000	-1.817547000
1	-0.618424000	0.300123000	-2.669847000
1	-0.080087000	1.942747000	-2.241055000
6	-3.526063000	0.868732000	1.544027000
1	-4.157043000	1.767111000	1.490629000
1	-4.084053000	0.106383000	2.106695000
1	-2.617976000	1.119475000	2.107135000
6	-4.457252000	0.032901000	-0.642140000
1	-5.085308000	-0.682082000	-0.091269000
1	-5.055553000	0.940660000	-0.804386000
1	-4.214146000	-0.395216000	-1.624742000
6	4.475513000	1.724564000	0.219651000
1	4.608427000	1.979633000	-0.836691000
1	3.942333000	2.541015000	0.728485000
1	5.460941000	1.593415000	0.690252000
6	-2.775322000	-2.081760000	0.706928000
1	-3.233247000	-1.951410000	1.698143000
1	-1.937275000	-2.780671000	0.777362000
1	-3.535695000	-2.483637000	0.022280000
7	2.608360000	-1.233710000	-0.321233000
1	3.562763000	0.237306000	2.438792000

[(cAAC) PMe_3]

BP86 (D3BJ)/def2-TZVPP
Energy: -869.284946

6	2.353049000	-1.354966000	0.128491000
6	0.804762000	-1.193858000	0.037899000
6	0.525502000	0.289084000	0.239780000
6	2.937244000	0.059017000	-0.044506000
1	2.627002000	-1.748274000	1.118720000
1	2.750747000	-2.051788000	-0.622112000
6	0.253373000	-1.578899000	-1.351687000
1	0.453590000	-2.643015000	-1.550738000
1	-0.832806000	-1.416382000	-1.384752000
1	0.715474000	-0.986892000	-2.154860000
6	3.466692000	0.318390000	-1.461976000
1	3.780556000	1.363924000	-1.593016000
1	4.343265000	-0.316200000	-1.654502000
1	2.703785000	0.088041000	-2.216768000
6	0.080698000	-2.020366000	1.111251000
1	-1.006379000	-1.887582000	1.023938000

1	0.313167000	-3.090131000	0.990818000
1	0.389552000	-1.714079000	2.121612000
6	4.010822000	0.386126000	0.996833000
1	4.846808000	-0.320718000	0.898018000
1	4.418711000	1.398901000	0.866924000
1	3.607688000	0.296693000	2.015366000
7	1.684542000	0.897333000	0.189457000
6	1.817638000	2.348180000	0.303174000
1	2.324474000	2.763092000	-0.580144000
1	0.809889000	2.765585000	0.380500000
1	2.398675000	2.617839000	1.196458000
15	-3.188747000	-0.180016000	-0.096908000
6	-2.878022000	0.635444000	1.536086000
1	-3.195781000	-0.024204000	2.355582000
1	-1.792941000	0.799969000	1.609128000
1	-3.404896000	1.598714000	1.624933000
6	-5.039277000	-0.027660000	-0.188371000
1	-5.384466000	1.000450000	0.004606000
1	-5.384927000	-0.336338000	-1.185090000
1	-5.500302000	-0.700386000	0.548595000
6	-2.698415000	1.219804000	-1.206559000
1	-1.615601000	1.364668000	-1.077942000
1	-2.903044000	0.962342000	-2.255167000
1	-3.227239000	2.152905000	-0.955183000

[(cAAC) aAAC]

BP86 (D3BJ)/def2-TZVPP
Energy: -856.6729612

6	1.766159000	-1.877417000	0.443796000
6	2.022326000	-0.396072000	0.504950000
6	1.051988000	-2.177054000	-0.892709000
1	0.845085000	-3.254925000	-0.971027000
1	0.089452000	-1.645432000	-0.923159000
1	1.659317000	-1.878957000	-1.760549000
6	0.866678000	-2.291822000	1.620005000
1	-0.113433000	-1.802068000	1.528159000
1	0.714716000	-3.383102000	1.620295000
1	1.316941000	-2.007338000	2.581888000
7	3.170815000	0.060621000	0.074250000
6	-2.256677000	-0.635903000	0.125354000
6	-2.056207000	0.872379000	0.113755000
6	-4.467603000	0.365229000	-0.132134000
7	-3.544894000	-0.842096000	0.003555000
6	-1.162934000	1.292597000	1.291079000
1	-1.046161000	2.388781000	1.304490000
1	-1.609418000	0.987678000	2.249665000
1	-0.167234000	0.827421000	1.204318000
6	-1.344577000	1.223531000	-1.209430000
1	-0.372758000	0.714677000	-1.258330000
1	-1.935199000	0.922135000	-2.086952000
1	-1.173968000	2.309781000	-1.267354000
6	-5.628948000	0.277090000	0.861953000
1	-6.205161000	1.213158000	0.840952000
1	-6.321358000	-0.541576000	0.617982000
1	-5.256116000	0.129904000	1.885366000
6	-4.996883000	0.442360000	-1.571376000
1	-5.616067000	-0.430283000	-1.824638000
1	-5.623329000	1.337748000	-1.691273000
1	-4.170867000	0.502072000	-2.292052000
6	3.399124000	1.547232000	0.165250000
1	4.412855000	1.732441000	-0.218430000
6	-4.121904000	-2.183248000	-0.058285000
1	-4.798256000	-2.356926000	0.790875000
6	3.332650000	1.993727000	1.624133000
1	4.093698000	1.483276000	2.231018000
1	3.495158000	3.078303000	1.701289000

1	2.342682000	1.743197000	2.028460000	1	-0.808161000	2.969147000	1.255221000
6	2.393007000	2.290786000	-0.709184000	1	-0.886781000	1.380829000	2.061298000
1	2.572547000	3.374400000	-0.662106000	1	0.662696000	1.978897000	1.430508000
1	2.462162000	1.972031000	-1.758539000	6	0.004462000	2.090594000	-1.237598000
1	1.378673000	2.077157000	-0.350162000	1	1.073963000	2.211991000	-1.013857000
6	4.312827000	-0.714218000	-0.523755000	1	-0.084402000	1.585256000	-2.208890000
6	4.583218000	-0.277862000	-1.966056000	1	-0.440389000	3.093994000	-1.318852000
1	4.959745000	0.753388000	-2.024519000	6	-3.385852000	-0.186882000	1.376551000
1	5.343997000	-0.933049000	-2.414984000	1	-4.320229000	0.390850000	1.356547000
1	3.670924000	-0.346492000	-2.573443000	1	-3.635897000	-1.213279000	1.680463000
1	2.689135000	-2.493685000	0.490169000	1	-2.727129000	0.246447000	2.139200000
6	5.559553000	-0.642823000	0.360428000	6	-3.673300000	-0.749419000	-1.063658000
1	6.351916000	-1.282680000	-0.055203000	1	-4.020207000	-1.755348000	-0.789281000
1	5.959969000	0.379225000	0.424795000	1	-4.559839000	-0.106877000	-1.158463000
1	5.336434000	-0.989166000	1.378368000	1	-3.180040000	-0.802559000	-2.043759000
1	3.973377000	-1.755720000	-0.550383000	14	2.687616000	0.608633000	0.287563000
6	-3.482298000	1.499489000	0.204192000	6	-1.437299000	-2.362723000	0.174036000
1	-3.664114000	1.856703000	1.228532000	1	-0.651007000	-2.651651000	0.884495000
1	-3.610574000	2.358591000	-0.469014000	1	-1.223165000	-2.861381000	-0.783248000
1	-4.689742000	-2.322231000	-0.989942000	1	-2.414540000	-2.692824000	0.543944000
1	-3.293452000	-2.896104000	-0.020987000	17	4.445712000	-0.572684000	-0.012003000

cAAC^{Me}-PSi(Cl) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1499.3687374

15	1.248493000	-1.009923000	-0.236302000
6	-0.320373000	-0.185699000	-0.100676000
6	-0.711133000	1.298497000	-0.134364000
6	-2.235566000	1.243672000	-0.419238000
6	-2.726501000	-0.158343000	-0.011366000
1	-2.779071000	2.036276000	0.111497000
1	-2.406253000	1.387374000	-1.495820000
7	-1.443368000	-0.916202000	0.018005000
6	-0.418953000	1.940284000	1.240590000

cAAC^{Me}-PSi(Cl) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1499.3209771

15	1.140319000	-1.042136000	-0.080191000
6	-0.387499000	-0.205198000	-0.154454000
6	-0.710833000	1.290838000	-0.083980000
6	-2.258134000	1.306962000	-0.240531000
6	-2.767036000	-0.117159000	0.057176000
1	-2.726911000	2.051344000	0.416248000
1	-2.516289000	1.567529000	-1.276842000
7	-1.553523000	-0.915116000	-0.252366000
6	-0.267357000	1.883880000	1.266068000

1	-0.522594000	2.952950000	1.307887000
1	-0.749977000	1.377248000	2.111594000
1	0.821577000	1.784981000	1.395697000
6	-0.057447000	2.073940000	-1.232033000
1	1.042176000	2.064053000	-1.155252000
1	-0.327166000	1.643705000	-2.206121000
1	-0.384102000	3.124163000	-1.205083000
6	-3.169216000	-0.312440000	1.529818000
1	-4.025594000	0.329487000	1.780029000
1	-3.462697000	-1.354527000	1.721645000
1	-2.339612000	-0.062474000	2.203484000
6	-3.929554000	-0.498884000	-0.864772000
1	-4.314015000	-1.506444000	-0.651723000
1	-4.761035000	0.204379000	-0.717346000
1	-3.620076000	-0.454630000	-1.917733000
14	2.754736000	0.468972000	-0.073899000
6	-1.558560000	-2.360793000	-0.191107000
1	-1.219733000	-2.730023000	0.794019000
1	-0.866765000	-2.759362000	-0.949945000
1	-2.566000000	-2.740382000	-0.393587000
17	4.610364000	-0.493332000	0.131174000

cAAC^{Me}-PSi(F) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1138.9939827

15	1.353209000	-1.487151000	-0.352734000
6	0.000049000	-0.365147000	-0.134447000
6	-0.076367000	1.159329000	-0.247538000
6	-1.583802000	1.393841000	-0.525624000
6	-2.340831000	0.162324000	0.015351000
1	-1.944435000	2.326067000	-0.071621000
1	-1.743879000	1.467533000	-1.611134000
7	-1.234774000	-0.835076000	0.113314000
6	0.342446000	1.781403000	1.103092000
1	0.205921000	2.872164000	1.057653000
1	-0.264013000	1.394348000	1.932288000
1	1.395248000	1.572676000	1.317215000
6	0.787675000	1.726160000	-1.378465000
1	1.853914000	1.592425000	-1.164177000
1	0.559593000	1.232288000	-2.332921000
1	0.593760000	2.803811000	-1.487171000
6	-2.977763000	0.393746000	1.393990000
1	-3.771366000	1.149291000	1.313116000
1	-3.434823000	-0.527299000	1.782902000
1	-2.238810000	0.746126000	2.123487000
6	-3.400976000	-0.326545000	-0.980821000
1	-3.933366000	-1.214657000	-0.612891000
1	-4.145316000	0.466280000	-1.139680000
1	-2.942870000	-0.567121000	-1.949846000
14	3.403116000	-0.678553000	0.055193000
6	-1.517409000	-2.236295000	0.380536000
1	-0.728075000	-2.649538000	1.021579000
1	-1.534833000	-2.821770000	-0.551493000
1	-2.488973000	-2.322196000	0.880845000
9	3.318428000	0.888800000	0.606724000

cAAC^{Me}-PSi(F) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1138.9439476

15	-1.345266000	1.432776000	-0.575575000
6	0.017655000	0.333524000	-0.303697000
6	0.118641000	-1.196882000	-0.302691000
6	1.654900000	-1.428481000	-0.332787000
6	2.327574000	-0.138685000	0.173447000
1	1.946376000	-2.301224000	0.265774000
1	1.969931000	-1.615905000	-1.369365000
7	1.231772000	0.850168000	-0.029205000

6	-0.509728000	-1.771388000	0.983760000
1	-0.304070000	-2.850948000	1.040745000
1	-0.109714000	-1.292551000	1.887213000
1	-1.597666000	-1.625354000	0.983186000
6	-0.540419000	-1.837664000	-1.531924000
1	-1.628584000	-1.681167000	-1.512343000
1	-0.144126000	-1.406113000	-2.461401000
1	-0.341983000	-2.920034000	-1.534483000
6	2.709172000	-0.199920000	1.661017000
1	3.503101000	-0.944010000	1.813780000
1	3.088494000	0.769358000	2.015337000
1	1.848415000	-0.479505000	2.280956000
6	3.549894000	0.229948000	-0.675885000
1	4.031890000	1.154174000	-0.327219000
1	4.295148000	-0.575289000	-0.613228000
1	3.267130000	0.356766000	-1.729760000
14	-3.206402000	0.214206000	-0.237755000
6	1.457143000	2.275668000	0.134537000
1	0.657487000	2.704024000	0.759335000
1	1.439660000	2.795247000	-0.835800000
1	2.428404000	2.443815000	0.613095000
9	-3.623632000	-0.063300000	1.339570000

NHC^{Me}-PSi(Cl) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1396.2178174

15	0.890269000	-0.002800000	-1.688436000
6	-0.579975000	-0.000822000	-0.658526000
6	-2.319230000	0.683212000	0.618612000
6	-2.319867000	-0.680073000	0.620305000
1	-2.973882000	1.392429000	1.108543000
7	-1.258343000	-1.086736000	-0.171317000
6	-0.819490000	2.461071000	-0.366359000
1	-0.027958000	2.705909000	0.354566000
1	-0.414374000	2.566452000	-1.379505000
1	-1.675966000	3.130426000	-0.227433000
14	2.412218000	-0.001060000	-0.095267000
6	-0.821882000	-2.461771000	-0.360454000
1	-0.030901000	-2.705942000	0.361300000
1	-0.416495000	-2.569785000	-1.373217000
1	-1.679143000	-3.129887000	-0.220392000
17	1.284792000	0.002567000	1.777676000
7	-1.257368000	1.086931000	-0.174044000
1	-2.975172000	-1.387472000	1.111988000

NHC^{Me}-PSi(Cl) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1396.1615206

15	-0.329625000	1.044408000	-1.529595000
6	0.800683000	0.079028000	-0.494445000
6	1.809387000	-1.674161000	0.532936000
6	2.409192000	-0.533101000	0.982848000
1	1.995608000	-2.712380000	0.777120000
7	1.817550000	0.528526000	0.322568000
6	-0.051665000	-2.199103000	-1.089697000
1	-0.320526000	-3.034959000	-0.433963000
1	-0.954850000	-1.636276000	-1.358545000
1	0.427454000	-2.577698000	-2.003359000
14	-1.579218000	1.225891000	0.308394000
6	2.059567000	1.934243000	0.592634000
1	1.319422000	2.308853000	1.317106000
1	1.936925000	2.498162000	-0.340541000
1	3.075547000	2.053108000	0.985855000
17	-2.609815000	-0.565219000	0.893565000
7	0.836518000	-1.295583000	-0.374406000
1	3.199245000	-0.390712000	1.709339000

NHC^{Me}-PSi(F) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1035.8409927

15	0.863712000	-1.009700000	0.000205000
6	-0.679920000	-0.116099000	0.000229000
6	-2.409773000	1.365514000	-0.000021000
6	-2.947584000	0.114011000	-0.000109000
1	-2.881710000	2.339795000	-0.000173000
7	-1.893742000	-0.781870000	0.000004000
6	-0.080656000	2.309855000	-0.000115000
1	0.569988000	2.251957000	0.886059000
1	0.569652000	2.251550000	-0.886514000
1	-0.627837000	3.259042000	-0.000242000
14	2.519404000	0.500978000	0.000020000
6	-2.019118000	-2.230884000	-0.000168000
1	-1.530301000	-2.652130000	0.888263000
1	-1.530057000	-2.651873000	-0.888579000
1	-3.084457000	-2.487090000	-0.000374000
7	-1.030485000	1.219108000	0.000204000
1	-3.980101000	-0.211761000	-0.000083000
9	3.728822000	-0.631413000	-0.000228000

NHC^{Me}-PSi(F) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1035.7859686

15	-0.660905000	-1.262937000	-0.760255000
6	0.648062000	-0.125786000	-0.264177000
6	1.875221000	1.715143000	0.243967000
6	2.679116000	0.625731000	0.428887000
1	2.074252000	2.769781000	0.388142000
7	1.927879000	-0.490317000	0.113948000
6	-0.500141000	2.087340000	-0.493185000
1	-1.031656000	1.670778000	-1.357160000
1	-1.194375000	2.089738000	0.361299000
1	-0.152664000	3.104882000	-0.706917000
14	-2.193231000	-0.580389000	0.691445000
6	2.397115000	-1.865201000	0.181862000
1	2.949874000	-2.137068000	-0.727800000
1	1.512360000	-2.510970000	0.267354000
1	3.045941000	-1.985337000	1.058188000
7	0.652578000	1.253442000	-0.198170000
1	3.709090000	0.556767000	0.755974000
9	-3.439271000	0.393966000	0.187771000

PMe_3-PSi(Cl) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1552.4647073

15	0.052174000	-1.676241000	0.000092000
14	-2.057779000	-1.032618000	-0.000073000
17	-2.154063000	1.151269000	0.000039000
6	1.033150000	1.166465000	-1.461226000
1	1.230518000	0.567992000	-2.359136000
1	0.002341000	1.537399000	-1.493647000
1	1.736363000	2.009658000	-1.411622000
6	2.991413000	-0.364822000	0.000023000
1	3.205001000	-0.968987000	-0.890625000
1	3.626925000	0.532060000	-0.000127000
1	3.204988000	-0.968711000	0.890860000
6	1.033145000	1.166581000	1.461147000
1	1.231432000	0.568342000	2.359009000
1	1.735709000	2.010283000	1.411051000
1	0.002084000	1.536760000	1.494059000
15	1.221583000	0.092971000	-0.000034000

PMe_3-PSi(Cl) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1552.4117134

15	0.112406000	1.493387000	-0.581687000
14	-1.590631000	0.747878000	0.600407000

17	-2.936230000	-0.668888000	-0.243679000
6	1.749865000	-0.243205000	1.773742000
1	2.232892000	0.691974000	2.083010000
1	0.804964000	-0.352477000	2.322059000
1	2.409774000	-1.096769000	1.983227000
6	2.985399000	-0.003080000	-0.838034000
1	3.454859000	0.944503000	-0.545296000
1	3.642525000	-0.839980000	-0.565115000
1	2.832380000	0.001815000	-1.924732000
6	0.748149000	-1.803057000	-0.458132000
1	0.589554000	-1.835515000	-1.543378000
1	1.464406000	-2.581261000	-0.159061000
1	-0.217599000	-1.970529000	0.035972000
15	1.358962000	-0.144380000	-0.005999000

PMe_3-PSi(F) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1192.095462

15	-0.487156000	-1.506832000	0.000116000
14	-2.346617000	-0.280888000	-0.000484000
6	0.969378000	1.120424000	-1.450439000
1	1.028050000	0.510294000	-2.360061000
1	0.024498000	1.675884000	-1.451219000
1	1.817009000	1.819595000	-1.415470000
6	2.650536000	-0.728827000	0.000191000
1	2.760957000	-1.361104000	-0.889683000
1	3.426264000	0.050239000	-0.000026000
1	2.760682000	-1.360033000	0.890886000
6	0.968857000	1.120206000	1.450255000
1	1.029576000	0.509902000	2.359687000
1	1.814893000	1.821188000	1.414778000
1	0.022610000	1.673389000	1.452381000
15	0.979256000	0.011359000	-0.000113000
9	-1.860670000	1.328263000	0.000602000

PMe_3-PSi(F) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1192.0372365

15	0.406787000	-1.441176000	-0.333411000
14	2.035860000	-0.207899000	0.495594000
6	-1.384449000	0.491384000	1.741671000
1	-1.698383000	-0.416627000	2.271472000
1	-0.441099000	0.847351000	2.176589000
1	-2.158526000	1.266763000	1.828590000
6	-2.691844000	-0.484008000	-0.654897000
1	-2.981648000	-1.409412000	-0.141358000
1	-3.464953000	0.280743000	-0.499472000
1	-2.595686000	-0.693603000	-1.727834000
6	-0.767558000	1.672714000	-0.833926000
1	-0.670477000	1.497488000	-1.912781000
1	-1.586081000	2.380274000	-0.639775000
1	0.179064000	2.085667000	-0.461938000
15	-1.069442000	0.073077000	-0.006634000
9	2.879853000	0.834763000	-0.472026000

aAAC^{Me}-PSi(Cl) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1539.8881676

15	1.280639000	0.438051000	1.052674000
6	-0.374061000	0.574763000	0.343059000
6	-0.887489000	1.983986000	0.073815000
7	-1.167586000	-0.474217000	0.088910000
6	-0.951243000	2.779079000	1.391856000
1	-1.361309000	3.780690000	1.197061000
1	-1.590770000	2.278751000	2.132641000
1	0.053027000	2.886122000	1.822744000
6	-0.027247000	2.715215000	-0.970500000
1	0.980703000	2.900655000	-0.579743000
1	0.077941000	2.126023000	-1.892330000

1	-0.497654000	3.676937000	-1.222682000
14	2.252443000	-0.261157000	-0.796380000
6	-0.767136000	-1.846436000	0.528944000
1	0.161766000	-1.682494000	1.094607000
6	-1.807661000	-2.444159000	1.478624000
1	-1.408667000	-3.382055000	1.888071000
1	-2.005910000	-1.766947000	2.320396000
1	-2.761181000	-2.683888000	0.985819000
6	-0.435474000	-2.751699000	-0.654214000
1	0.401079000	-2.330255000	-1.232122000
1	-0.135958000	-3.741028000	-0.281308000
1	-1.290284000	-2.896283000	-1.331692000
6	-2.484984000	-0.434589000	-0.624773000
1	-2.737935000	-1.497331000	-0.724307000
6	-2.363011000	0.096818000	-2.057675000
1	-2.227673000	1.183237000	-2.107279000
1	-1.514646000	-0.375792000	-2.569685000
1	-3.280574000	-0.150751000	-2.609803000
6	-3.626622000	0.188944000	0.190031000
1	-3.560336000	1.280582000	0.265769000
1	-4.581981000	-0.053151000	-0.297127000
1	-3.651510000	-0.222567000	1.206776000
1	-1.906266000	1.931467000	-0.319640000
17	4.271589000	-0.354618000	-0.070843000

aAAC^{Me}-PSi(Cl) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1539.8401024

15	1.104736000	-0.720899000	0.220340000
6	-0.318617000	0.286332000	-0.011902000
6	-0.273887000	1.801984000	-0.176379000
7	-1.547354000	-0.331271000	-0.137883000
6	0.476000000	2.543660000	0.934732000
1	0.383535000	3.629687000	0.790331000
1	0.083128000	2.283653000	1.926971000
1	1.550783000	2.299435000	0.937657000
6	0.263087000	2.159089000	-1.574606000
1	1.302558000	1.815003000	-1.697629000
1	-0.344058000	1.686741000	-2.358842000
1	0.245982000	3.248512000	-1.723682000
14	2.965759000	0.433806000	-0.034360000
6	-1.593322000	-1.804540000	-0.289046000
1	-0.603553000	-2.071155000	-0.698181000
6	-1.753098000	-2.524422000	1.055414000
1	-1.657760000	-3.610389000	0.916907000
1	-0.976332000	-2.202546000	1.762134000
1	-2.739770000	-2.330849000	1.502862000
6	-2.640029000	-2.240672000	-1.317831000
1	-2.490193000	-1.722674000	-2.274312000
1	-2.543675000	-3.321029000	-1.493869000
1	-3.670139000	-2.057657000	-0.978381000
6	-2.836328000	0.281133000	0.291365000
1	-3.492259000	-0.587150000	0.444211000
6	-3.513987000	1.126297000	-0.797935000
1	-2.999985000	2.078916000	-0.979745000
1	-3.549707000	0.576437000	-1.746885000
1	-4.546120000	1.356780000	-0.495309000
6	-2.762318000	0.982414000	1.654407000
1	-2.251281000	1.951508000	1.611903000
1	-3.781257000	1.162041000	2.025501000
1	-2.236578000	0.352400000	2.383688000
1	-1.309070000	2.158136000	-0.145156000
17	4.592974000	-0.900256000	-0.010492000

aAAC^{Me}-PSi(F) Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1179.5226212

15	1.544510000	-0.424182000	-1.412190000

6	0.263404000	0.438216000	-0.493063000
6	0.537589000	1.890007000	-0.116243000
7	-0.910977000	-0.117528000	-0.161706000
6	1.730426000	2.038187000	0.840817000
1	1.826787000	3.091019000	1.143293000
1	1.603364000	1.422766000	1.740020000
1	2.661023000	1.727785000	0.347471000
6	0.747702000	2.727325000	-1.392455000
1	1.641097000	2.385653000	-1.932010000
1	-0.112419000	2.648687000	-2.072339000
1	0.881306000	3.784718000	-1.121169000
14	2.543695000	-1.447410000	0.264917000
6	-1.252482000	-1.482014000	-0.658866000
1	-0.428797000	-1.730641000	-1.344851000
6	-1.244644000	-2.513166000	0.468471000
1	-1.395964000	-3.515029000	0.043129000
1	-0.284891000	-2.501777000	0.999722000
1	-2.048400000	-2.340745000	1.200165000
6	-2.555420000	-1.470708000	-1.460577000
1	-2.511900000	-0.730167000	-2.270581000
1	-2.699875000	-2.460864000	-1.913966000
1	-3.441027000	-1.263330000	-0.841626000
6	-1.944841000	0.474444000	0.742843000
1	-2.654412000	-0.352192000	0.875527000
6	-2.747325000	1.615751000	0.103110000
1	-2.167900000	2.540399000	-0.006251000
1	-3.114842000	1.326241000	-0.889444000
1	-3.617499000	1.840897000	0.736315000
6	-1.410781000	0.785402000	2.147348000
1	-0.834702000	1.716717000	2.194789000
1	-2.261375000	0.885717000	2.836347000
1	-0.767599000	-0.030082000	2.500985000
1	-0.340571000	2.295964000	0.393198000
9	1.658253000	-1.145916000	1.655435000

aAAC^{Me}-PSi(F) Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1179.4735602

15	1.268962000	-0.799612000	-1.550355000
6	0.340080000	0.242368000	-0.377609000
6	0.824917000	1.686516000	-0.206691000
7	-0.982689000	-0.023842000	-0.063611000
6	2.346005000	1.846804000	-0.129039000
1	2.598189000	2.914202000	-0.052614000
1	2.772662000	1.324342000	0.734267000
1	2.834818000	1.450474000	-1.031703000
6	0.260265000	2.527267000	-1.373152000
1	0.726882000	2.218832000	-2.319973000
1	-0.825434000	2.402491000	-1.472814000
1	0.475849000	3.594418000	-1.215230000
14	1.712732000	-1.561448000	0.590741000
6	-1.693039000	-1.136750000	-0.735624000
1	-1.038126000	-1.404919000	-1.583232000
6	-1.846067000	-2.382613000	0.142168000
1	-2.310574000	-3.190327000	-0.440869000
1	-0.866204000	-2.728975000	0.501169000
1	-2.485481000	-2.196992000	1.017716000
6	-3.030046000	-0.661953000	-1.312820000
1	-2.885306000	0.202305000	-1.974743000
1	-3.488065000	-1.472404000	-1.897112000
1	-3.744581000	-0.381878000	-0.524509000
6	-1.666268000	0.526020000	1.138932000
1	-2.531945000	-0.138037000	1.271518000
6	-2.247285000	1.936274000	0.950012000
1	-1.474378000	2.713866000	0.931461000
1	-2.822871000	2.002880000	0.017962000

1	-2.925763000	2.160591000	1.785999000
6	-0.828655000	0.393586000	2.415789000
1	0.053580000	1.046350000	2.410793000
1	-1.444263000	0.666958000	3.284487000
1	-0.476748000	-0.638757000	2.543493000
1	0.406936000	2.084178000	0.728683000
9	3.173058000	-0.941484000	1.071522000

cAAC^{Me}-Si(Cl)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1499.3487263

6	-0.025764000	0.155008000	-0.131801000
7	0.940999000	-0.537181000	-0.732171000
6	2.321845000	-0.184608000	-0.259265000
6	2.078338000	1.234560000	0.292985000
6	0.564576000	1.334640000	0.632125000
6	0.301976000	1.225587000	2.146562000
6	-0.047484000	2.648344000	0.107486000
6	3.318981000	-0.181241000	-1.418673000
6	2.738455000	-1.188828000	0.826267000
6	0.685435000	-1.801588000	-1.402559000
14	-1.796991000	-0.407507000	-0.016766000
15	-1.906869000	-1.794641000	1.438771000
17	-2.982552000	0.716727000	-1.332352000
1	2.709540000	1.438325000	1.167110000
1	2.332340000	1.971974000	-0.482088000
1	-0.775432000	1.221192000	2.356211000
1	0.761691000	2.084849000	2.657717000
1	0.714450000	0.298190000	2.562190000
1	0.442714000	3.506707000	0.590060000
1	0.078384000	2.740312000	-0.980084000
1	-1.122191000	2.697906000	0.330058000
1	4.277180000	0.227578000	-1.069327000
1	3.516346000	-1.192026000	-1.801712000
1	2.957942000	0.447248000	-2.244310000
1	1.982643000	-1.245391000	1.620631000
1	2.865854000	-2.196378000	0.406221000
1	3.696253000	-0.884597000	1.269691000
1	1.572794000	-2.114645000	-1.962347000
1	-0.157713000	-1.687913000	-2.095980000
1	0.406362000	-2.563960000	-0.654467000

cAAC^{Me}-Si(Cl)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1499.3279642

6	0.054183000	0.068718000	-0.154062000
7	1.048047000	-0.868397000	-0.268430000
6	2.402020000	-0.329095000	0.036304000
6	2.191866000	1.165655000	-0.267079000
6	0.674263000	1.468260000	-0.101866000
6	0.382616000	2.169270000	1.240484000
6	0.189985000	2.357055000	-1.262858000
6	3.462964000	-0.944637000	-0.880852000
6	2.750037000	-0.596608000	1.511362000
6	0.785909000	-2.291260000	-0.202744000
14	-1.690782000	-0.376184000	0.019208000
15	-2.651812000	-2.265709000	0.005270000
17	-2.916917000	1.307278000	0.067157000
1	2.807334000	1.801554000	0.382687000
1	2.490816000	1.363409000	-1.306497000
1	-0.693186000	2.345468000	1.364918000
1	0.895351000	3.142738000	1.273089000
1	0.728276000	1.569951000	2.092904000
1	0.755357000	3.301699000	-1.271685000
1	0.344422000	1.852498000	-2.226735000
1	-0.875595000	2.597410000	-1.166351000
1	4.416072000	-0.415624000	-0.742472000
1	3.643967000	-2.004950000	-0.654865000

1	3.166008000	-0.852986000	-1.934428000	1	-3.104061000	-0.142880000	1.916137000
1	1.985202000	-0.180185000	2.179342000	1	-1.387021000	-1.006703000	-1.965768000
1	2.826021000	-1.675544000	1.708124000	1	-2.328564000	-2.236003000	-1.094001000
1	3.717374000	-0.139572000	1.762546000	1	-3.161845000	-0.856259000	-1.841055000
1	1.681524000	-2.850918000	-0.494948000	1	-1.432650000	-2.530052000	1.365373000
1	-0.028896000	-2.545726000	-0.898111000	1	0.172964000	-1.993778000	1.940694000
1	0.476273000	-2.606096000	0.809732000	1	0.012840000	-2.582445000	0.271626000

cAAC^{Me}-Si(F)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1138.9813766

6	0.180296000	0.190275000	0.330276000
7	-0.787582000	-0.678634000	0.619665000
6	-2.109468000	-0.347616000	-0.010872000
6	-1.936539000	1.163898000	-0.263601000
6	-0.408597000	1.443034000	-0.309270000
6	0.104997000	1.633082000	-1.750041000
6	-0.034215000	2.680606000	0.529420000
6	-3.265707000	-0.635910000	0.947780000
6	-2.251520000	-1.160675000	-1.306958000
6	-0.503187000	-2.028670000	1.076679000
14	2.001363000	-0.188802000	0.403247000
15	2.500472000	-1.393901000	-1.126278000
9	2.678754000	0.749402000	1.551698000
1	-2.439185000	1.475575000	-1.187912000
1	-2.389180000	1.723527000	0.567586000
1	1.197312000	1.745831000	-1.764701000
1	-0.350681000	2.535591000	-2.184228000
1	-0.137028000	0.770056000	-2.382254000
1	-0.526660000	3.573806000	0.117359000
1	-0.348932000	2.561369000	1.575414000
1	1.050937000	2.851664000	0.518304000
1	-4.198405000	-0.247690000	0.515644000
1	-3.408082000	-1.712178000	1.117080000

cAAC^{Me}-Si(F)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1138.9596543

6	-0.128703000	0.181069000	-0.144287000
7	0.679139000	-0.918655000	-0.274693000
6	2.108487000	-0.627359000	0.020974000
6	2.162682000	0.885390000	-0.273031000
6	0.724357000	1.448731000	-0.086988000
6	0.563712000	2.175439000	1.264097000
6	0.375483000	2.420946000	-1.229760000
6	3.036338000	-1.415143000	-0.908381000
6	2.418240000	-0.959770000	1.491751000
6	0.157261000	-2.267138000	-0.196254000
14	-1.922523000	0.112445000	0.023139000
15	-3.277128000	-1.510267000	0.020756000
9	-2.487683000	1.639528000	0.081706000
1	2.889638000	1.396950000	0.371498000
1	2.479122000	1.034136000	-1.315479000
1	-0.468524000	2.525719000	1.395758000
1	1.229431000	3.051344000	1.302811000
1	0.809780000	1.519134000	2.109034000
1	1.076348000	3.270032000	-1.232443000
1	0.441292000	1.914963000	-2.203018000
1	-0.641218000	2.818146000	-1.114380000
1	4.070931000	-1.071250000	-0.771136000
1	3.020554000	-2.493006000	-0.693452000

1	2.755977000	-1.260122000	-1.959063000
1	1.740274000	-0.424914000	2.169280000
1	2.312343000	-2.037370000	1.682209000
1	3.450908000	-0.674798000	1.736993000
1	0.921870000	-2.985914000	-0.512325000
1	-0.710201000	-2.360877000	-0.868195000
1	-0.178260000	-2.520561000	0.825395000

NHC^{Me}-Si(Cl)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1396.1949712

6	0.616312000	0.015938000	0.058672000
7	1.456424000	1.035580000	0.415755000
6	2.770633000	0.680287000	0.182919000
6	2.760891000	-0.587364000	-0.326382000
7	1.437627000	-0.983461000	-0.392791000
6	1.009121000	2.341569000	0.891126000
14	-1.271509000	0.125091000	-0.032586000
15	-2.168506000	1.689868000	-0.919316000
17	-1.830275000	-1.702156000	0.890844000
6	0.973149000	-2.263920000	-0.916249000
1	3.592669000	1.352488000	0.393647000
1	3.571715000	-1.229006000	-0.647456000
1	0.234854000	2.710882000	0.198548000
1	0.565137000	2.250547000	1.890402000
1	1.874058000	3.012488000	0.926110000
1	1.814138000	-2.764769000	-1.406893000
1	0.578258000	-2.888761000	-0.106294000
1	0.173568000	-2.090401000	-1.647729000

NHC^{Me}-Si(Cl)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1396.1640359

6	-0.641618000	0.071359000	0.080968000
7	-1.352186000	1.214328000	-0.185868000
6	-2.708624000	0.941623000	-0.248395000
6	-2.857320000	-0.397133000	-0.031931000
7	-1.593032000	-0.914825000	0.175124000
6	-0.780282000	2.541240000	-0.380589000
14	1.187978000	-0.166150000	0.600967000
15	2.432529000	1.594464000	0.252605000
17	1.764009000	-1.777806000	-0.702501000
6	-1.303180000	-2.298631000	0.527879000
1	-3.441434000	1.713340000	-0.447761000
1	-3.744237000	-1.017977000	-0.010649000
1	-0.746429000	3.092480000	0.568922000
1	0.248126000	2.423709000	-0.753543000
1	-1.391923000	3.089617000	-1.106559000
1	-2.233122000	-2.781493000	0.847123000
1	-0.863398000	-2.833720000	-0.321398000
1	-0.572688000	-2.301393000	1.351377000

NHC^{Me}-Si(F)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1035.8282735

6	0.479197000	0.018171000	0.121113000
7	0.926787000	1.311425000	0.187812000
6	2.285187000	1.363989000	-0.050317000
6	2.706562000	0.083574000	-0.272754000
7	1.596232000	-0.730939000	-0.155068000
6	0.078115000	2.472732000	0.439271000
14	-1.333142000	-0.531390000	0.164548000
15	-2.846964000	0.564189000	-0.565557000
9	-1.120856000	-2.034791000	0.803372000
6	1.598381000	-2.173095000	-0.387082000
1	2.833069000	2.297648000	-0.038074000
1	3.688930000	-0.310017000	-0.501724000
1	-0.854301000	2.343309000	-0.138688000
1	-0.184321000	2.529074000	1.503528000

1	0.625569000	3.372914000	0.139162000
1	2.637230000	-2.508421000	-0.470411000
1	1.100767000	-2.684900000	0.442573000
1	1.063418000	-2.405484000	-1.317631000

NHC^{Me}-Si(F)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1035.7948112

6	0.401038000	0.002071000	0.242729000
7	1.410103000	0.924336000	0.216238000
6	2.596025000	0.339596000	-0.197445000
6	2.328735000	-0.982052000	-0.412733000
7	0.984548000	-1.173592000	-0.139469000
6	1.218889000	2.338273000	0.512655000
14	-1.427021000	0.359400000	0.733055000
15	-2.040375000	0.818563000	-1.347163000
9	-1.886309000	-1.153844000	1.260239000
6	0.237112000	-2.405084000	-0.373193000
1	3.514638000	0.903687000	-0.298334000
1	2.973272000	-1.791755000	-0.731745000
1	0.977062000	2.895789000	-0.401484000
1	0.372747000	2.426379000	1.210394000
1	2.131121000	2.741596000	0.968128000
1	0.897243000	-3.126729000	-0.865453000
1	-0.137796000	-2.813452000	0.571535000
1	-0.620933000	-2.173000000	-1.019968000

PMe_3-Si(Cl)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1552.4372772

14	1.100462000	-0.023279000	-0.000054000
15	2.277910000	1.597363000	0.000004000
17	1.096824000	-2.148139000	0.000043000
15	-1.159835000	0.232956000	-0.000025000
6	-1.992850000	-0.492084000	-1.454641000
6	-1.540762000	2.007399000	-0.000382000
6	-1.992719000	-0.491307000	1.455055000
1	-1.579841000	-0.035614000	-2.363039000
1	-3.077817000	-0.323059000	-1.416886000
1	-1.785821000	-1.569413000	-1.478012000
1	-1.076427000	2.460719000	-0.884677000
1	-2.626409000	2.176994000	-0.000327000
1	-1.076220000	2.461054000	0.883635000
1	-3.077708000	-0.322424000	1.417164000
1	-1.785587000	-1.568598000	1.479123000
1	-1.579790000	-0.034204000	2.363171000

PMe_3-Si(Cl)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1552.4159913

14	-1.005531000	-0.097316000	-0.933233000
15	-1.499174000	-1.932078000	0.237402000
17	-1.701134000	1.632460000	0.192300000
15	1.105701000	0.031212000	-0.020743000
6	2.013967000	1.503446000	-0.611209000
6	2.115147000	-1.408661000	-0.504729000
6	1.184899000	0.131843000	1.798740000
1	2.091640000	1.463661000	-1.705159000
1	3.018099000	1.563135000	-0.169476000
1	1.436706000	2.395953000	-0.336080000
1	2.137547000	-1.483851000	-1.599495000
1	3.140610000	-1.316217000	-0.122621000
1	1.648932000	-2.316723000	-0.100947000
1	2.215306000	0.288042000	2.146602000
1	0.549619000	0.966750000	2.121331000
1	0.776272000	-0.796917000	2.215325000

PMe_3-Si(F)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1192.0680833

14	-1.142097000	0.585964000	0.000130000
15	-2.455193000	-0.919992000	-0.000023000
9	-0.929167000	2.210773000	-0.000026000
15	1.022392000	-0.127383000	0.000026000
6	2.406719000	1.074322000	0.001044000
6	1.286647000	-1.196823000	-1.451696000
6	1.286036000	-1.198660000	1.450489000
1	2.328020000	1.712811000	-0.887913000
1	3.380374000	0.564716000	0.000851000
1	2.327750000	1.711647000	0.890809000
1	1.237917000	-0.591255000	-2.365486000
1	2.260101000	-1.703413000	-1.392646000
1	0.468759000	-1.928077000	-1.471067000
1	2.259506000	-1.705188000	1.391170000
1	1.236952000	-0.594232000	2.365014000
1	0.468080000	-1.929869000	1.468616000

PMe_3-Si(F)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1192.0402322

14	1.130583000	0.690541000	-0.693203000
15	2.148699000	-1.100727000	0.154802000
9	1.183845000	1.984993000	0.359378000
15	-0.953150000	-0.093738000	-0.021841000
6	-2.341044000	0.985355000	-0.537548000
6	-1.177351000	-0.293952000	1.780316000
6	-1.298697000	-1.717089000	-0.777266000
1	-2.199472000	1.978867000	-0.091928000
1	-3.311849000	0.579022000	-0.221148000
1	-2.323722000	1.092460000	-1.629752000
1	-0.952588000	0.664630000	2.265933000
1	-2.201772000	-0.603555000	2.030172000
1	-0.453563000	-1.038295000	2.134359000
1	-2.315354000	-2.053406000	-0.532551000
1	-1.191346000	-1.638681000	-1.866777000
1	-0.563784000	-2.442466000	-0.405306000

aAAC^{Me}-Si(Cl)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1539.8491007

15	-0.792010000	-1.369531000	1.722288000
14	-1.720564000	0.104650000	0.670642000
17	-3.279756000	1.411817000	0.363609000
6	-0.138965000	-1.487663000	-1.286069000
6	-0.168266000	-0.478677000	-0.119012000
7	0.969422000	0.400085000	0.067830000
6	0.532405000	-2.818297000	-0.918442000
6	-1.537567000	-1.751619000	-1.855971000
6	2.137793000	-0.242128000	0.728380000
6	1.235939000	1.349403000	-1.032837000
6	3.313064000	-0.578953000	-0.201559000
6	2.583970000	0.532757000	1.977013000
6	2.080116000	2.539211000	-0.557261000
6	-0.058786000	1.895461000	-1.641842000
1	0.464594000	-1.006251000	-2.076739000
1	0.552648000	-3.494153000	-1.786145000
1	1.563236000	-2.686695000	-0.568786000
1	-0.036073000	-3.316119000	-0.116525000
1	-1.486547000	-2.393493000	-2.747562000
1	-2.038966000	-0.814312000	-2.144248000
1	-2.167715000	-2.261255000	-1.111358000
1	1.747662000	-1.201455000	1.104461000
1	1.795227000	0.844660000	-1.851383000
1	4.045102000	-1.195284000	0.339553000
1	2.986461000	-1.143225000	-1.085676000
1	3.838487000	0.319850000	-0.552771000
1	3.322524000	-0.055528000	2.542647000
1	1.716413000	0.716208000	2.623676000

1	3.040848000	1.499330000	1.731121000
1	2.216283000	3.247795000	-1.386805000
1	3.076488000	2.243804000	-0.211315000
1	1.569930000	3.057898000	0.267177000
1	0.195065000	2.617926000	-2.429628000
1	-0.686260000	1.116309000	-2.090779000
1	-0.655682000	2.423410000	-0.882801000

aAAC^{Me}-Si(Cl)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1539.8360979

15	-0.810135000	1.049717000	-1.744370000
14	-1.176863000	-0.963353000	-0.937003000
17	-3.143819000	-1.367308000	-0.208461000
6	-0.549447000	1.599065000	1.073847000
6	-0.237495000	0.583704000	-0.038693000
7	0.996568000	-0.165890000	0.067019000
6	0.130075000	2.950218000	0.784887000
6	-2.053705000	1.782262000	1.291342000
6	2.145486000	0.283028000	-0.779190000
6	1.276712000	-0.914311000	1.320643000
6	3.323733000	0.826412000	0.040308000
6	2.571655000	-0.746009000	-1.831544000
6	2.197471000	-2.117433000	1.072581000
6	0.005561000	-1.445361000	1.991621000
1	-0.108620000	1.209959000	2.006122000
1	-0.019755000	3.645111000	1.624454000
1	1.211405000	2.837466000	0.626735000
1	-0.297625000	3.409378000	-0.119037000
1	-2.241361000	2.523985000	2.080920000
1	-2.540046000	0.838913000	1.571523000
1	-2.534553000	2.136069000	0.367344000
1	1.721159000	1.130302000	-1.338375000
1	1.781945000	-0.227134000	2.027803000
1	4.029784000	1.318409000	-0.643446000
1	2.991250000	1.573874000	0.773313000
1	3.877902000	0.044273000	0.574785000
1	3.270245000	-0.274631000	-2.538187000
1	1.692360000	-1.089810000	-2.391988000
1	3.069580000	-1.620624000	-1.396946000
1	2.335422000	-2.660594000	2.017600000
1	3.190133000	-1.841335000	0.704255000
1	1.732915000	-2.799301000	0.346522000
1	0.287003000	-1.921212000	2.941352000
1	-0.745430000	-0.679980000	2.206258000
1	-0.466953000	-2.215913000	1.362479000

aAAC^{Me}-Si(F)P Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1179.5023282

15	-2.064378000	-1.542149000	-1.530776000
14	-1.758291000	-0.805945000	0.314021000
9	-2.343807000	-0.851977000	1.834852000
6	-0.796942000	1.917622000	-0.132345000
6	-0.409409000	0.473556000	0.143425000
7	0.892433000	0.124836000	0.173761000
6	-2.285623000	2.101777000	-0.444922000
6	-0.414551000	2.743247000	1.119765000
6	1.231959000	-1.236462000	0.674930000
6	1.886992000	0.929017000	-0.601181000
6	1.771291000	-2.178910000	-0.398702000
6	2.060696000	-1.208846000	1.962828000
6	1.799497000	0.600453000	-2.099361000
6	3.316508000	0.866451000	-0.067413000
1	-0.237456000	2.307142000	-0.997708000
1	-2.505750000	3.170880000	-0.578055000
1	-2.573789000	1.556952000	-1.351670000
1	-2.917221000	1.738118000	0.382251000

1	-0.651476000	3.804208000	0.958757000
1	0.653120000	2.657371000	1.363662000
1	-0.986362000	2.390702000	1.990063000
1	0.245579000	-1.653244000	0.955612000
1	1.566632000	1.968828000	-0.471119000
1	1.838977000	-3.189926000	0.026713000
1	1.078310000	-2.216548000	-1.249840000
1	2.772986000	-1.899030000	-0.748349000
1	2.017485000	-2.202560000	2.430384000
1	1.647802000	-0.480745000	2.673625000
1	3.116014000	-0.971306000	1.787469000
1	2.291220000	1.393405000	-2.680170000
1	0.750917000	0.525795000	-2.420277000
1	2.291226000	-0.350109000	-2.337723000
1	3.924720000	1.576449000	-0.644927000
1	3.370304000	1.159276000	0.988729000
1	3.773244000	-0.123686000	-0.184205000

aAAC^{Me}-Si(Cl)P Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1179.4775845

15	2.239261000	-2.496308000	0.146878000
14	1.826771000	-0.433174000	-0.038134000
9	3.110307000	0.562717000	-0.187629000
6	0.450902000	2.106262000	0.049776000
6	0.312515000	0.585015000	0.025208000
7	-0.947077000	0.011509000	0.020626000
6	1.329949000	2.597554000	1.217914000
6	0.927815000	2.671643000	-1.301044000
6	-1.032352000	-1.453557000	0.204996000
6	-2.155860000	0.830411000	-0.238649000
6	-2.045958000	-1.888181000	1.266600000
6	-1.164228000	-2.246270000	-1.104251000
6	-2.821059000	1.314202000	1.060717000
6	-3.170093000	0.181538000	-1.187276000
1	-0.543340000	2.529087000	0.245923000
1	1.298806000	3.696285000	1.269097000
1	0.963085000	2.199388000	2.174054000
1	2.377191000	2.296147000	1.098212000
1	0.953209000	3.771422000	-1.272846000
1	0.258760000	2.362973000	-2.117222000
1	1.937918000	2.313141000	-1.539106000
1	-0.044265000	-1.722485000	0.631994000
1	-1.794042000	1.716041000	-0.774849000
1	-1.916119000	-2.963406000	1.452550000
1	-1.881015000	-1.357161000	2.212833000
1	-3.086076000	-1.733399000	0.951062000
1	-0.850766000	-3.284262000	-0.926931000
1	-0.500191000	-1.832310000	-1.874161000
1	-2.192466000	-2.261490000	-1.485017000
1	-3.583372000	2.073076000	0.831092000
1	-2.080810000	1.762882000	1.736252000
1	-3.313078000	0.491883000	1.594467000
1	-3.958629000	0.917420000	-1.398965000
1	-2.705476000	-0.100415000	-2.139771000
1	-3.656055000	-0.702480000	-0.757624000