Supporting Information

EDA-NOCV and NICS Analysis of Bonding, Stability and Aromaticity of Functionalized Fulvenes: A Bonding Insight

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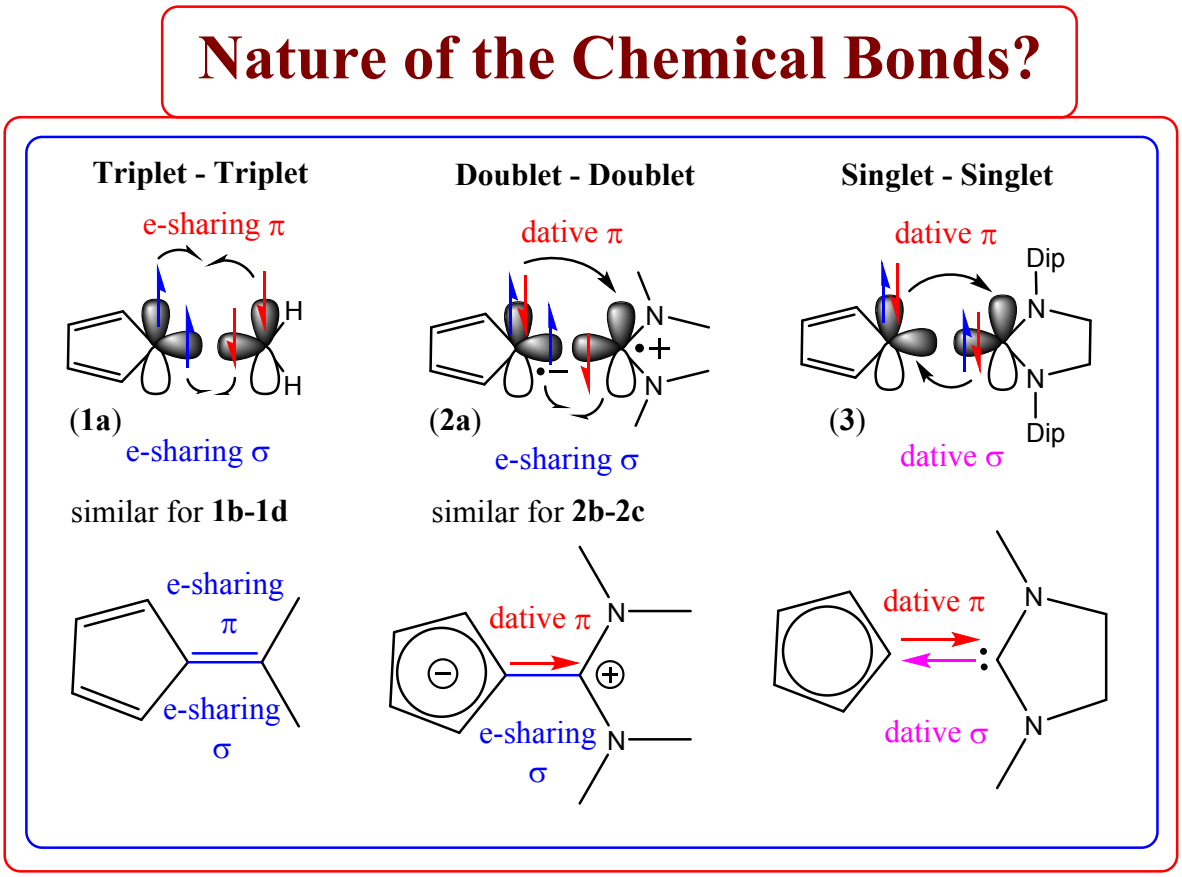


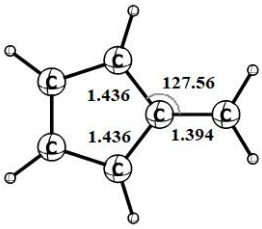
All that look same are not sometimes not similar!

Table S1. Dissociation energy (D_e), change in Gibbs free energy (ΔG^{298}) and HOMO-LUMO gap (Δ_{H-L}) of L−C_5H_4 complexes [L = H_2C (**1a**), aAAC (**1b**), $(CO_2Me)_2C$ (**1c**), Py (**1d**); aNHC (**2a**), NHC (**2b**), PPh_3 (**2c**); SNHC (**3**)].

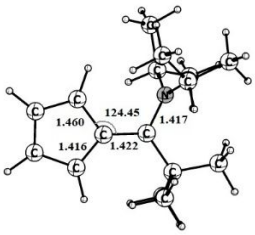
Complex	D_e (kcal/mol)	ΔG^{298} (kcal/mol)	Δ_{H-L} (kcal/mol)
CH_2-C_5H_4 (**1a**)	190.9	171.7	57.4
aAAC-C_5H_4 (**1b**)	129.4	110.3	53.9
$(CO_2Me)_2C$-C_5H_4 (**1c**)	156.9	138.7	47.0
Py-C_5H_4 (**1d**)	81.6	64.9	40.1
aNHC-C_5H_4 (**2a**)	128.3	111.1	63.5
NHC-C_5H_4 (**2b**)	128.0	108.6	60.0
PPh_3-C_5H_4 (**2c**)	92.2	75.2	40.6
SNHC-C_5H_4 (**3**)	132.7	111.9	63.2

Table S2. Aromaticity of L-C_5H_4 complexes [L = H_2C (**1a**), aAAC (**1b**), $(CO_2Me)_2C$ (**1c**), Py (**1d**); aNHC (**2a**), NHC (**2b**), PPh_3 (**2c**); SNHC (**3**)] at BP86-D3(BJ)/Def2-TZVPP level.

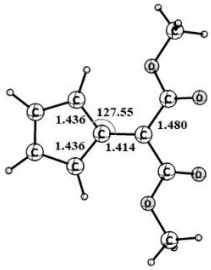
Complex	Sigma Aromaticity	Pi Aromaticity
CH_2-C_5H_4 (**1a**)	+1.518	-2.033
aAAC-C_5H_4 (**1b**)	-4.087	-5.940
$(CO_2Me)_2C$- C_5H_4 (**1c**)	+4.157	+0.345
Py-C_5H_4 (**1d**)	-0.670	-2.770
aNHC-C_5H_4 (**2a**)	-6.101	-6.351
NHC-C_5H_4 (**2b**)	-8.20	-7.639
PPh_3-C_5H_4 (**2c**)	-8.877	-8.076
SNHC-C_5H_4 (**3**)	-7.638	-7.585



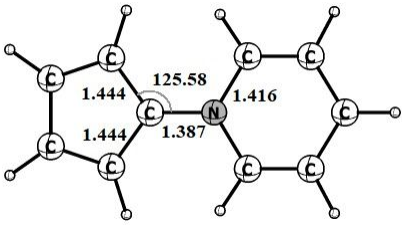
1a-T (36.5 kcal/mol)



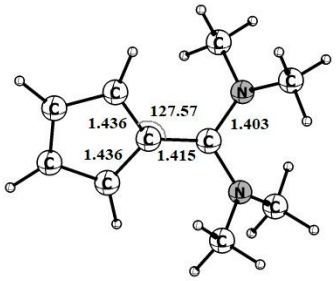
1b-T (37.8 kcal/mol)



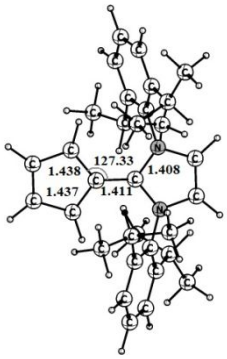
1c-T (28.1 kcal/mol)



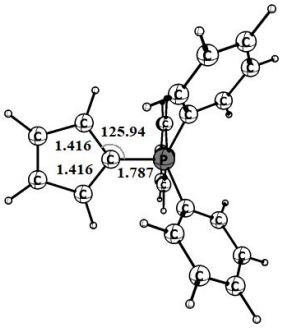
1d-T (35.0 kcal/mol)



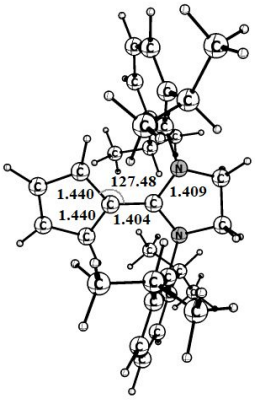
2a-T (50.3 kcal/mol)



2b-T (55.1 kcal/mol)

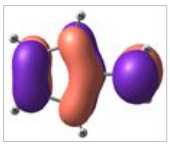


2c-T (52.4 kcal/mol)

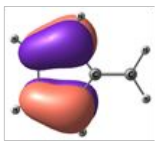


3-T (52.7 kcal/mol)

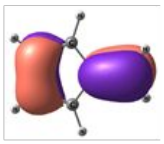
Figure S1. Optimized geometries of triplet state L-Cp [L = H_2C (**1a**), aAAC (**1b**), $(CO_2Me)_2C$ (**1c**), Py (**1d**); aNHC (**2a**), NHC (**2b**), PPh_3 (**2c**); SNHC (**3**)] complexes **1a-T** to **3-T** at BP86(D3BJ)/def2-TZVPP level.



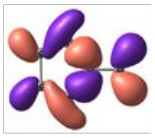
LUMO (-2.93)



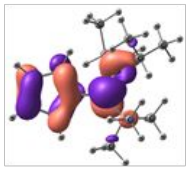
HOMO (-5.42)



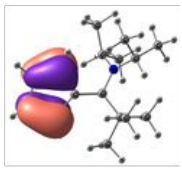
HOMO-1 (-6.58)



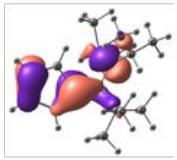
HOMO-2 (-8.39)



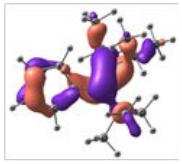
LUMO (-2.24)



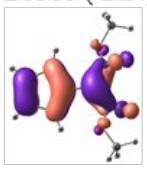
HOMO (-4.58)



HOMO-1 (-4.76)



HOMO-2 (-6.30)



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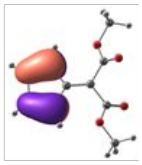

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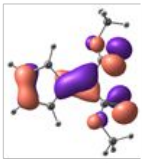
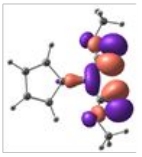


HOMO-1 (-6.58)



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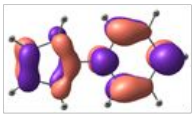
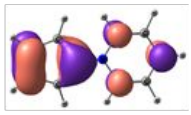


LUMO (-2.81)



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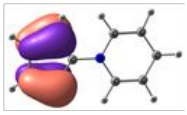

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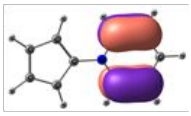
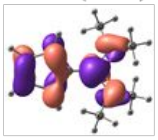


HOMO-2 (-7.39)



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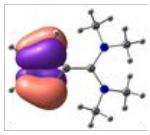

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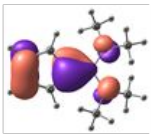
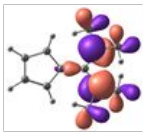


HOMO-1 (-4.55)



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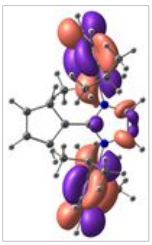
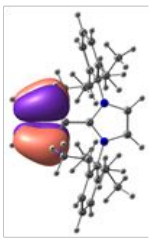


LUMO (-1.56)



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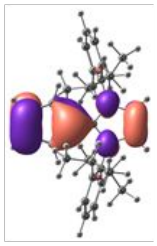

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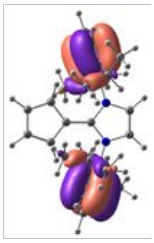

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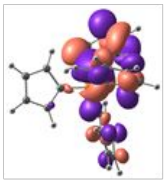

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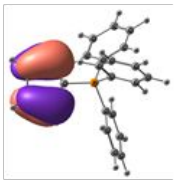

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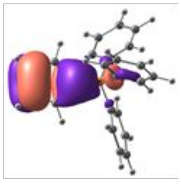

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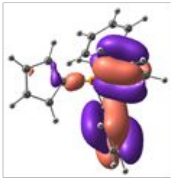
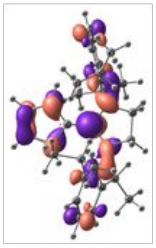
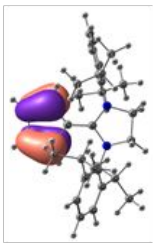


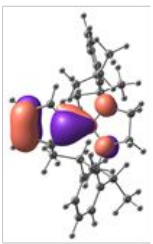
HOMO-2 (-6.70)



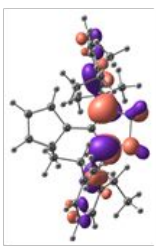
LUMO (-1.56)



HOMO (-4.30)



HOMO-1 (-4.59)



HOMO-2 (-5.81)

Figure S2. Molecular orbitals of L-Cp [L = H_2C (**1a**), aAAC (**1b**), $(CO_2Me)_2C$ (**1c**), Py (**1d**); aNHC (**2a**), NHC (**2b**), PPh_3 (**2c**); SNHC (**3**)] compounds **1a-T** to **3-T**, generated at BP86(D3BJ)/def2-TZVPP level.

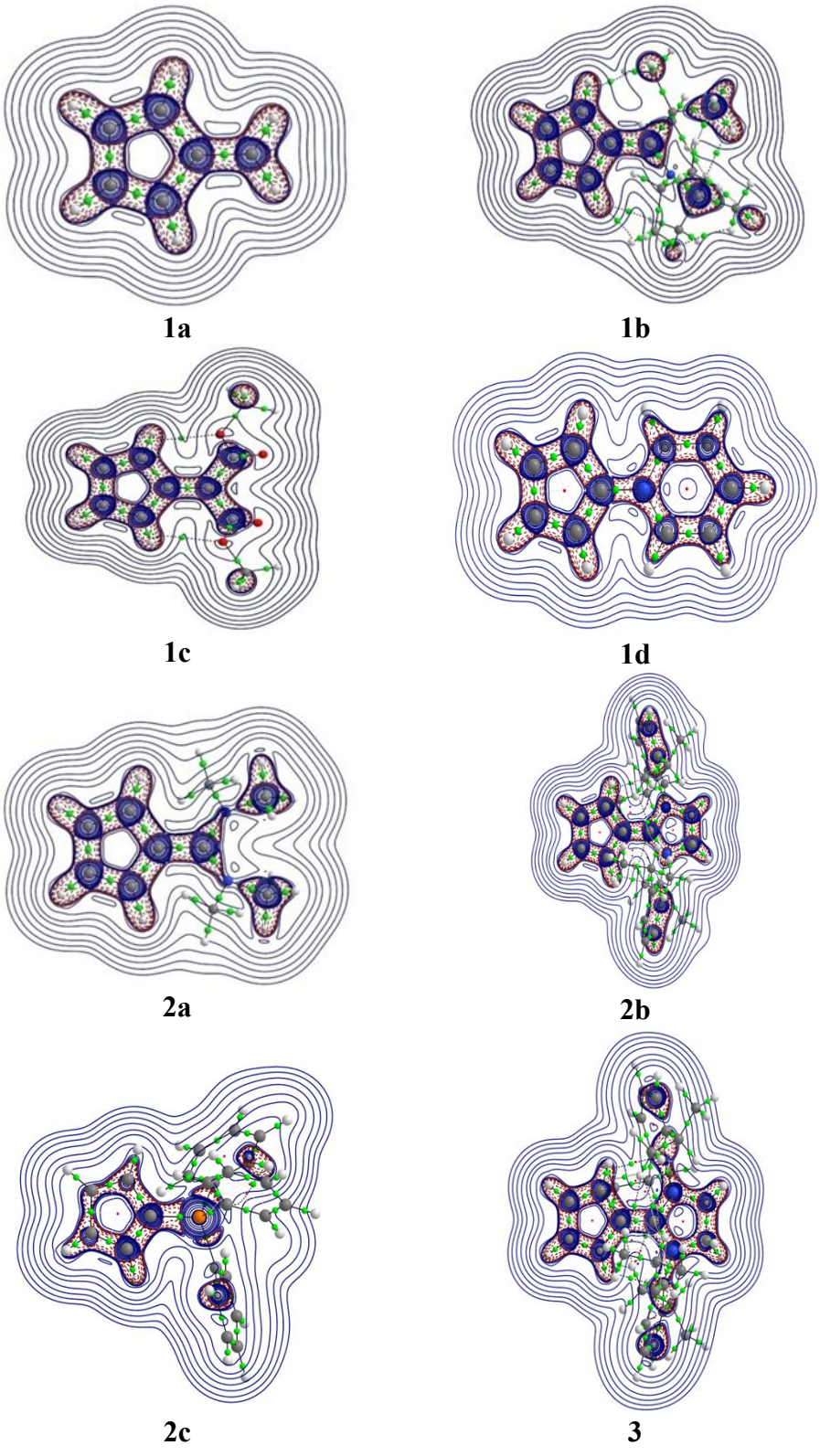
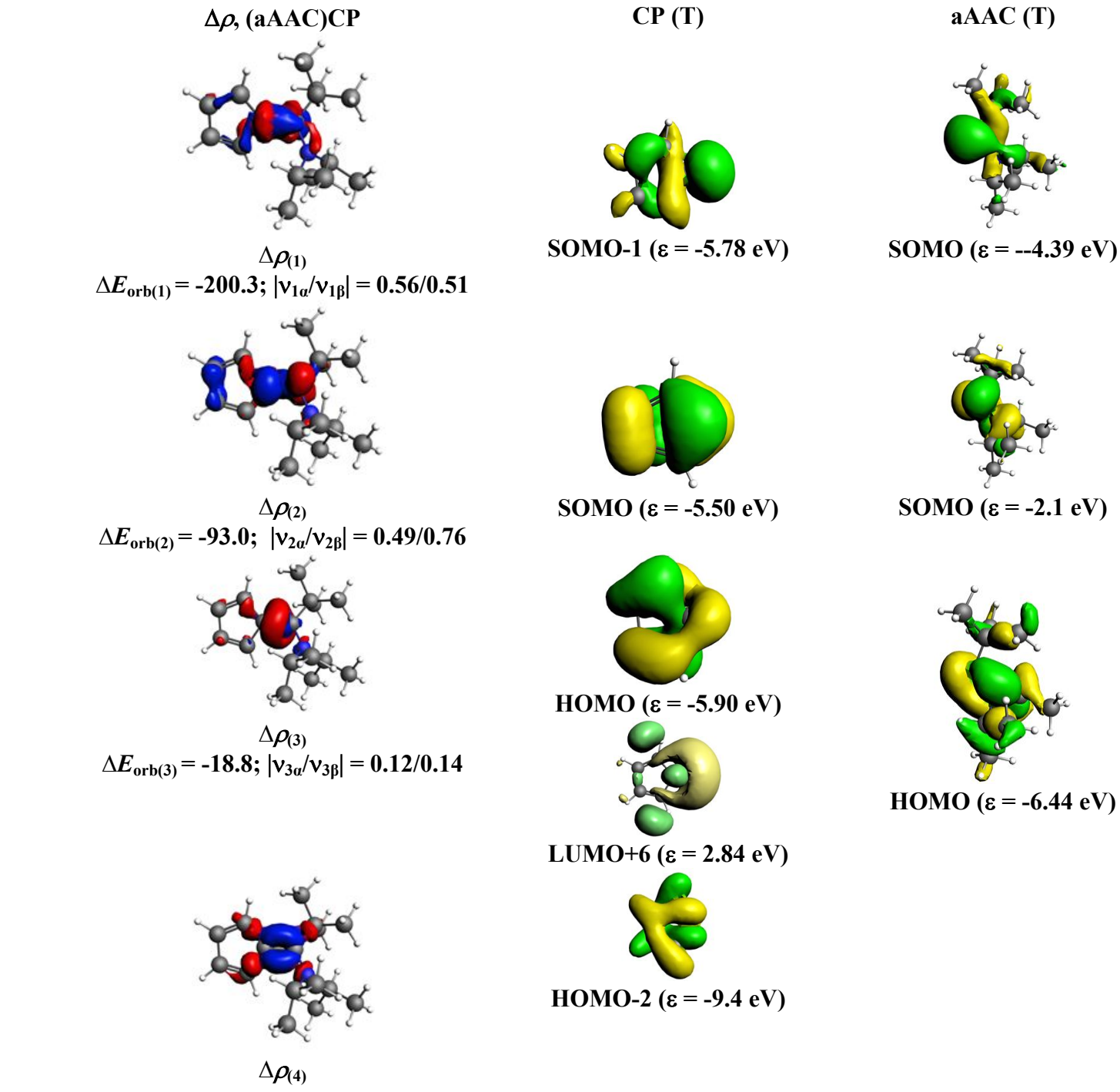
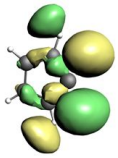


Figure S3. Electron density distribution in contour plot of L-C_5H_4 [L = H_2C (**1a**), aAAC (**1b**), $(CO_2Me)_2C$ (**1c**), Py (**1d**); aNHC (**2a**), NHC (**2b**), PPh_3 (**2c**); SNHC (**3**)] compounds **1a-T** to **3-T**. Contour plot of Laplacian distribution [$\nabla^2\boldsymbol{\rho}$ (r)] in the C_1-C_L-C_{Cp} plane. Solid blue lines indicate the areas of charge concentration ($\nabla^2\boldsymbol{\rho}$ (r) < 0) while dotted purple lines denotes charge depletion ($\nabla^2\boldsymbol{\rho}$ (r) > 0). Solid lines connecting atomic nuclei (black) are the bond paths and those thick solid blue lines separating the atomic basins indicates the zero-flux surface crossing the molecular plane.



$\Delta E_{orb(4)}$ = -8.2; $|\nu_{4\alpha}/\nu_{4\beta}|$ = 0.08/0.08



LUMO+11 (ε = 5.11 eV)

Figure S4. The shape of the deformation densities $\Delta\rho_{(1)-(4)}$ that correspond to $\Delta E_{orb(1)-(4)}$, and the associated MOs of aAAC-C_5H_4 (**1b**) and the fragments orbitals of aAAC and C_5H_4 in the triplet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)-(4)}$. 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.

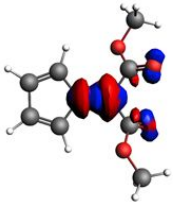
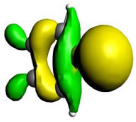
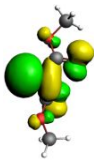
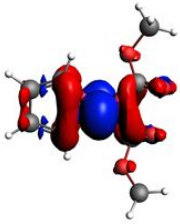
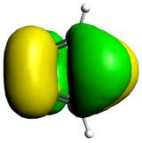
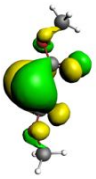
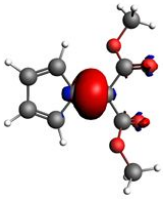
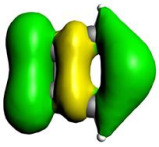
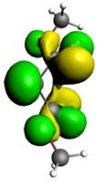
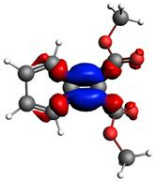
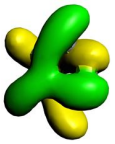
$\Delta\rho$, $(CO_2Me)_2C$-CP	CP (T)	$(CO_2Me)_2C$ (T)
 $\Delta\rho_{(1)}$ $\Delta E_{orb(1)}$ = -230.6; $\|\nu_{1\alpha}/\nu_{1\beta}\|$ = 0.55/0.50	 SOMO-1 (ε = -6.00 eV)	 SOMO-1 (ε = --6.14 eV)
 $\Delta\rho_{(2)}$ $\Delta E_{orb(2)}$ = -68.7; $\|\nu_{2\alpha}/\nu_{2\beta}\|$ = 0.65/0.64	 SOMO-1 (ε = -5.40 eV)	 SOMO-1 (ε = -5.30 eV)
 $\Delta\rho_{(3)}$ $\Delta E_{orb(3)}$ = -15.9; $\|\nu_{3\alpha}/\nu_{3\beta}\|$ = 0.13/0.08	 HOMO-3 (ε = -8.2 eV)	 HOMO-1 (ε = -12.4 eV)
 $\Delta\rho_{(4)}$ $\Delta E_{orb(4)}$ = -10.2; $\|\nu_{4\alpha}/\nu_{4\beta}\|$ = 0.08/0.08	 HOMO-1 (ε = -9.40 eV)	 LUMO+18 (ε = 5.16 eV)

Figure S5. The shape of the deformation densities $\Delta\rho_{(1)\text{-}(4)}$ that correspond to $\Delta E_{\text{orb}(1)\text{-}(4)}$, and the associated MOs of $(CO_2Me)_2C\text{-}C_5H_4$ (**1c**) and the fragments orbitals of $(CO_2Me)_2C$ and C_5H_4 in the triplet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au for $\Delta\rho_{(1)\text{-}(4)}$. 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.

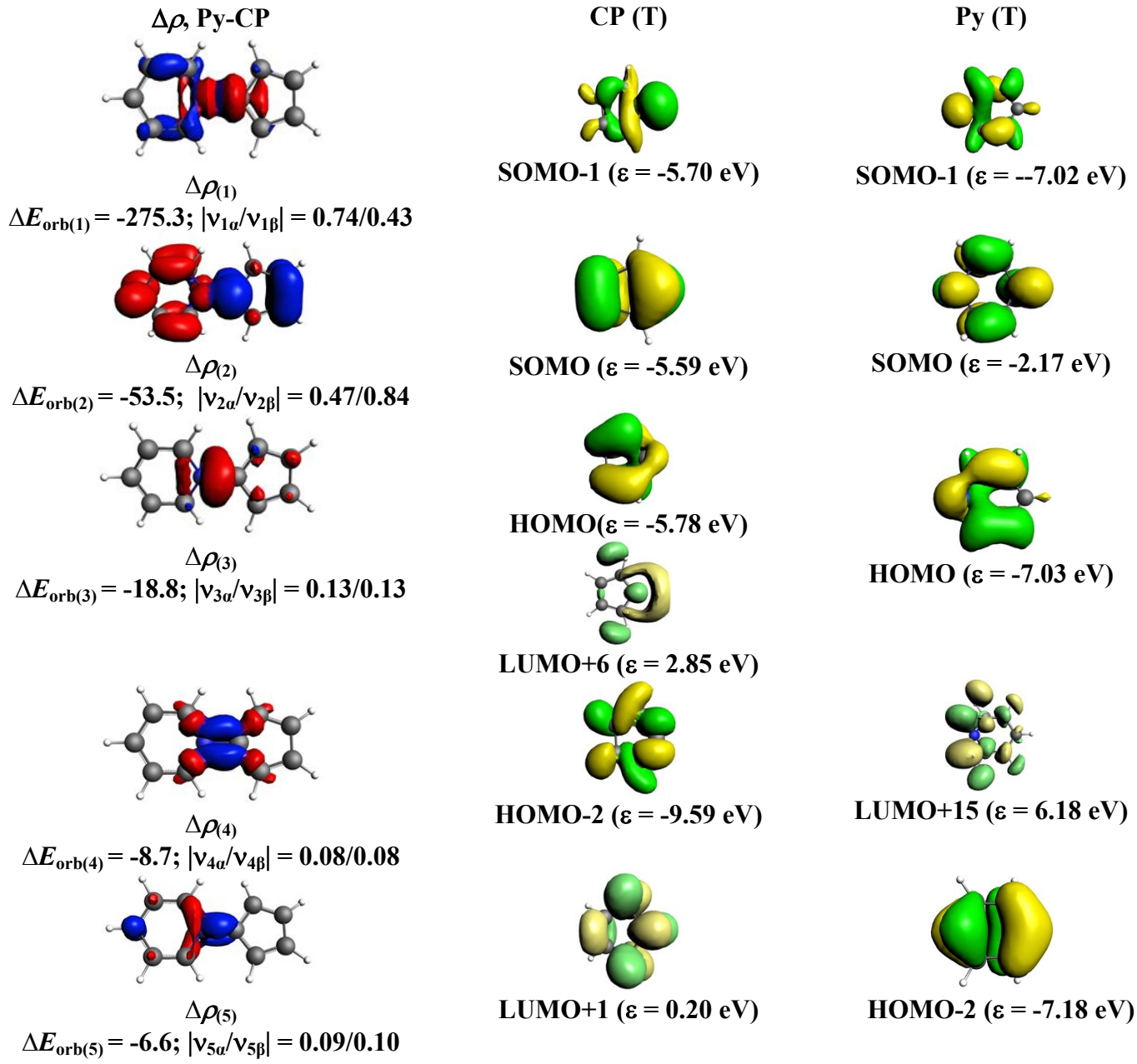
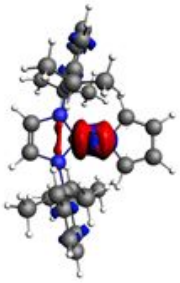
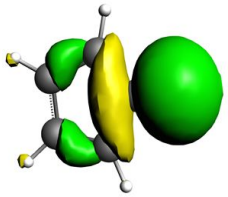
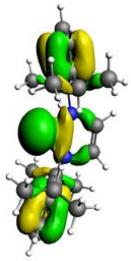
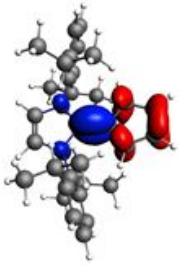
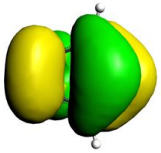
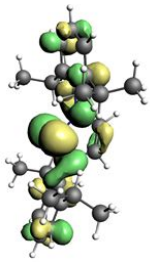
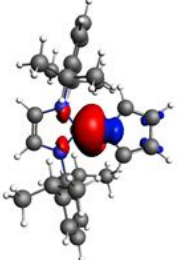
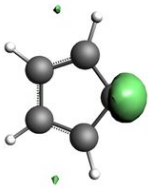
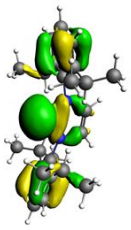
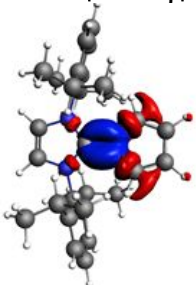
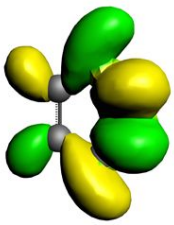
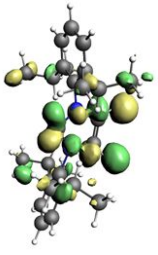
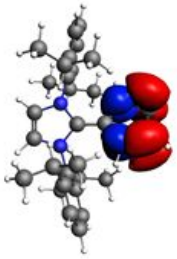


Figure S6. The shape of the deformation densities $\Delta\rho_{(1)\text{-}(5)}$ that correspond to $\Delta E_{\text{orb}(1)\text{-}(5)}$, and the associated MOs of Py- C_5H_4 (**1d**) and the fragments orbitals of Py and C_5H_4 in the triplet

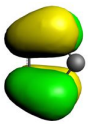
state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. The eigenvalues $|\nu_n|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is red→blue.

$\Delta\rho$, (NHC^{Dip})CP	CP (D)	NHC^{Dip} (D)
		
$\Delta\rho_{(1)}$ $\Delta E_{orb(1)}$ = -265.8; $\lvert\nu_{1\alpha}/\nu_{1\beta}\rvert$ = 0.70/0.43	SOMO (ε = 2.71 eV)	SOMO (ε = --9.52 eV)
		
$\Delta\rho_{(2)}$ $\Delta E_{orb(2)}$ = -69.5; $\lvert\nu_{2\alpha}/\nu_{2\beta}\rvert$ = 0.45/0.45	HOMO (ε = 2.04 eV)	LUMO+4 (ε = -4.51 eV)
		
$\Delta\rho_{(3)}$ $\Delta E_{orb(3)}$ = -33..4; $\lvert\nu_{3\alpha}/\nu_{3\beta}\rvert$ = 0.22/0.07	LUMO+6 (ε = 8.27 eV)	HOMO-1 (ε = -9.53 eV)
		
$\Delta\rho_{(4)}$ $\Delta E_{orb(4)}$ = -17.4; $\lvert\nu_{4\alpha}/\nu_{4\beta}\rvert$ = 0.11/0.11	HOMO-1 (ε = -1.78 eV)	LUMO+43 (ε = 0.46 eV)

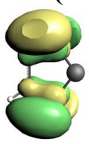


$\Delta\rho_{(5)}$

$\Delta E_{orb(5)}$ = -5.4; $|\nu_{5\alpha}/\nu_{5\beta}|$ = 0.09/0.09

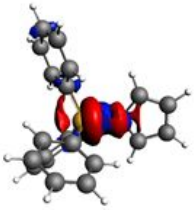
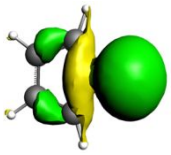
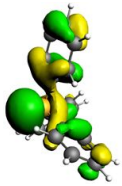
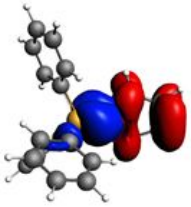
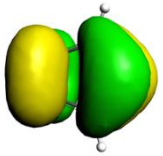
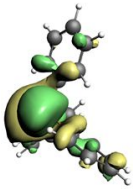
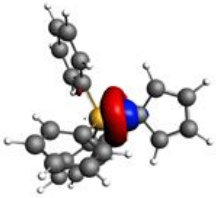
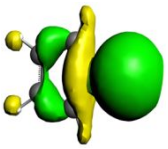
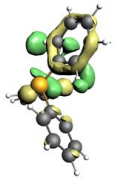
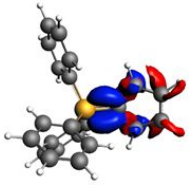
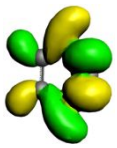
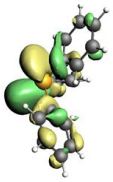


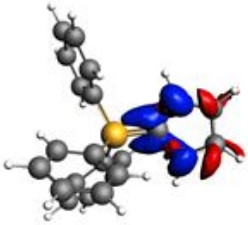
HOMO-2 (ε = 1.22 eV)



LUMO+12 (ε = 11.26 eV)

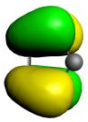
Figure S7. The shape of the deformation densities $\Delta\rho_{(1)-(5)}$ that correspond to $\Delta E_{orb(1)-(5)}$, and the associated MOs of NHC^{Dip}-C_5H_4 (**2b**) and the fragments orbitals of NHC^{Dip} and C_5H_4 in the triplet state at the BP86-D3(BJ)/TZ2P level. Isosurface values are 0.003 au. 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.

$\Delta\rho$, $(PPh_3)CP$	CP (D)	PPh_3 (D)
		
$\Delta\rho_{(1)}$ $\Delta E_{orb(1)}$ = -197.2; $\|\nu_{1\alpha}/\nu_{1\beta}\|$ = 0.67/0.50	SOMO (ε = 2.71 eV)	SOMO (ε = --9.52 eV)
		
$\Delta\rho_{(2)}$ $\Delta E_{orb(2)}$ = -53.9; $\|\nu_{2\alpha}/\nu_{2\beta}\|$ = 0.34/0.34	HOMO (ε = 1.95 eV)	LUMO+6 (ε = -3.59 eV)
		
$\Delta\rho_{(3)}$ $\Delta E_{orb(3)}$ = -18.8; $\|\nu_{3\alpha}/\nu_{3\beta}\|$ = 0.18/0.18	SOMO (ε = 2.71 eV)	LUMO+7 (ε = -3.14 eV)
		
$\Delta\rho_{(4)}$ $\Delta E_{orb(4)}$ = -15.0; $\|\nu_{4\alpha}/\nu_{4\beta}\|$ = 0.14/0.14	HOMO-1 (ε = 1.52 eV)	LUMO+18 (ε = -3.03 eV)

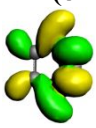


$\Delta\rho_{(5)}$

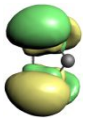
$\Delta E_{orb(5)}$ = **-11.4;** $|\nu_{5\alpha}/\nu_{5\beta}|$ = **0.11/0.11**



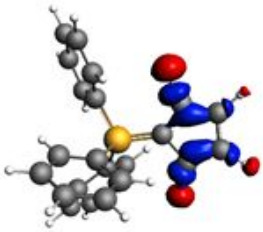
HOMO-2 (ε = -1.54 eV)



HOMO-1 (ε = 1.52 eV)

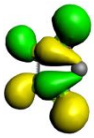


LUMO+12 (ε = 11.43 eV)

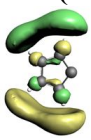


$\Delta\rho_{(6)}$

$\Delta E_{orb(5)}$ = **-5.8;** $|\nu_{5\alpha}/\nu_{5\beta}|$ = **0.07/0.07**



HOMO-5 (ε = -2.7 eV)



LUMO+1 (ε = 5.12 eV)

Figure S8. The shape of the deformation densities $\Delta\rho_{(1)-(6)}$ that correspond to $\Delta E_{orb(1)-(6)}$, and the associated MOs of PPh_3-C_5H_4 (**2c**) and the fragments orbitals of PPh_3 and C_5H_4 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.

Table S3. Optimized Coordinates of

1a Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -232.2891274

6	2.107690000	0.000001000	-0.000025000
6	0.759136000	0.000004000	-0.000017000
6	-0.123512000	-1.180775000	0.000054000
6	-1.409028000	-0.737772000	0.000210000
6	-1.409031000	0.737767000	-0.000242000
6	-0.123516000	1.180776000	0.000013000
1	0.224385000	-2.210765000	-0.000701000
1	-2.305265000	-1.355510000	0.000180000
1	-2.305270000	1.355503000	-0.000247000
1	0.224371000	2.210769000	0.000812000
1	2.675669000	-0.931605000	0.000256000
1	2.675678000	0.931601000	-0.000255000

Table S4. Optimized Coordinates of

1a Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -232.2309639

6	-2.174744000	0.000000000	0.000007000
6	-0.780399000	0.000000000	0.000003000
6	0.095152000	1.138472000	-0.000143000
6	1.484227000	0.685305000	-0.000039000

6	1.484227000	-0.685305000	0.000022000
6	0.095152000	-1.138472000	0.000150000
1	-0.229244000	2.177881000	-0.000254000
1	2.355005000	1.336242000	-0.000070000
1	2.355005000	-1.336242000	0.000041000
1	-0.229244000	-2.177881000	0.000269000
1	-2.736613000	0.932464000	-0.000107000
1	-2.736613000	-0.932464000	0.000123000

Table S5. Optimized Coordinates of

1b Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -680.9608212

6	-0.393934000	0.450084000	0.053457000
7	0.836422000	-0.195731000	0.076694000
6	-1.538360000	-0.350708000	-0.032892000
6	-2.907797000	-0.189029000	0.450839000
6	-3.633199000	-1.297073000	0.076045000
6	-2.779056000	-2.182118000	-0.690456000
6	-1.518138000	-1.640281000	-0.726638000
1	-3.274357000	0.596282000	1.099124000
1	-4.677744000	-1.482336000	0.320258000
1	-3.099877000	-3.093621000	-1.191440000
1	-0.668765000	-2.013821000	-1.290411000
6	0.993046000	-1.393273000	0.958029000
1	-0.033141000	-1.660381000	1.228941000
6	1.920549000	0.239638000	-0.832231000
1	1.681270000	1.275475000	-1.086512000
6	0.754351000	2.594705000	0.881290000
1	1.738983000	2.391753000	0.448766000
1	0.639921000	3.686912000	0.932717000
1	0.755919000	2.208437000	1.910202000
6	-1.704308000	2.528103000	0.771515000
1	-2.605731000	2.294379000	0.196261000
1	-1.815923000	2.129474000	1.788537000
1	-1.625304000	3.622565000	0.841489000
6	-0.426389000	1.998365000	0.084654000
6	-0.470932000	2.555492000	-1.362670000
1	0.440215000	2.351498000	-1.939628000
1	-1.318213000	2.115157000	-1.905401000
1	-0.608376000	3.646922000	-1.331966000
6	1.614415000	-2.636928000	0.317062000
1	2.665256000	-2.495205000	0.033506000
1	1.583508000	-3.455827000	1.049695000
1	1.053570000	-2.962839000	-0.566424000
6	1.716029000	-1.014294000	2.262864000
1	1.632968000	-1.846193000	2.977771000
1	2.782767000	-0.806127000	2.116131000
1	1.248765000	-0.129576000	2.715315000
6	1.874144000	-0.533128000	-2.163586000
1	2.544221000	-0.054793000	-2.893333000
1	2.190096000	-1.576925000	-2.049890000
1	0.855540000	-0.521870000	-2.574327000
6	3.327976000	0.258681000	-0.229590000
1	3.701624000	-0.744467000	0.007973000
1	4.018331000	0.698600000	-0.963170000
1	3.369141000	0.867233000	0.682802000

Table S6. Optimized Coordinates of

1b Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -680.9005729

6	-0.377566000	0.439855000	-0.016466000
7	0.893437000	-0.185892000	0.009679000
6	-1.522144000	-0.404712000	-0.016386000
6	-2.904065000	-0.095777000	0.004679000
6	-3.683632000	-1.336302000	-0.082476000
6	-2.810039000	-2.396117000	-0.153603000
6	-1.474380000	-1.860441000	-0.114268000
1	-3.353153000	0.890312000	0.064577000
1	-4.770526000	-1.386291000	-0.069546000
1	-3.064594000	-3.450300000	-0.223568000

1	-0.564071000	-2.448184000	-0.188859000
6	1.217428000	-1.012433000	1.184229000
1	0.235149000	-1.285466000	1.607572000
6	1.736961000	-0.067885000	-1.191399000
1	1.317554000	0.798662000	-1.722602000
6	0.872196000	2.684206000	0.067550000
1	1.429870000	2.594346000	-0.873305000
1	0.711673000	3.757202000	0.247523000
1	1.501408000	2.294109000	0.877553000
6	-1.232322000	2.392630000	1.322477000
1	-2.217529000	1.923408000	1.416996000
1	-0.642745000	2.098888000	2.203263000
1	-1.364906000	3.485767000	1.350836000
6	-0.494271000	1.975503000	0.021535000
6	-1.256331000	2.505838000	-1.214327000
1	-0.688840000	2.292957000	-2.132347000
1	-2.243733000	2.041896000	-1.324997000
1	-1.395531000	3.595820000	-1.144101000
6	1.955473000	-2.328004000	0.905184000
1	2.971020000	-2.169909000	0.520939000
1	2.046635000	-2.888780000	1.846015000
1	1.416664000	-2.961742000	0.189401000
6	1.948832000	-0.199798000	2.270430000
1	2.057662000	-0.794363000	3.190213000
1	2.951408000	0.100652000	1.935910000
1	1.380037000	0.706650000	2.516069000
6	1.582761000	-1.255426000	-2.164201000
1	2.053758000	-1.014776000	-3.129634000
1	2.055993000	-2.168181000	-1.780913000
1	0.518479000	-1.459073000	-2.342377000
6	3.212123000	0.249840000	-0.912761000
1	3.735232000	-0.584998000	-0.429300000
1	3.729805000	0.451577000	-1.861578000
1	3.313083000	1.135193000	-0.272684000

Table S7. Optimized Coordinates of

1c Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -688.2526116

6	-0.000056000	-0.206859000	0.000420000
6	-0.000776000	1.154053000	0.000166000
6	-1.170425000	2.037450000	-0.180048000
6	-0.731238000	3.320520000	-0.116221000
6	0.728289000	3.321049000	0.115881000
6	1.168302000	2.038286000	0.180063000
1	-2.187232000	1.691970000	-0.327416000
1	-1.342580000	4.215100000	-0.217424000
1	1.339037000	4.216066000	0.216802000
1	2.185357000	1.693529000	0.327511000
6	-1.213583000	-1.045420000	-0.260184000
8	-1.202681000	-1.973369000	-1.047372000
6	1.214896000	-1.043383000	0.261359000
8	1.206530000	-1.968821000	1.051487000
8	-2.294929000	-0.661120000	0.455736000
8	2.294312000	-0.660168000	-0.458012000
6	-3.485393000	-1.449167000	0.209506000
1	-4.246600000	-1.037542000	0.878417000
1	-3.793391000	-1.357334000	-0.839866000
1	-3.292745000	-2.505087000	0.436622000
6	3.486089000	-1.446325000	-0.212012000
1	3.293959000	-2.503106000	-0.435530000
1	4.245433000	-1.035978000	-0.883817000
1	3.796280000	-1.351028000	0.836405000

Table S8. Optimized Coordinates of

1c Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -688.2078704

6	-0.000657000	-0.305745000	0.000642000
6	0.000668000	1.108471000	0.000441000
6	-1.114123000	1.984711000	-0.227082000

6	-0.670292000	3.363558000	-0.137623000
6	0.677338000	3.361882000	0.138345000
6	1.117652000	1.981930000	0.227879000
1	-2.128563000	1.660870000	-0.434855000
1	-1.308834000	4.233245000	-0.270036000
1	1.318078000	4.229965000	0.270667000
1	2.131312000	1.655600000	0.435675000
6	-1.226965000	-1.114941000	-0.176648000
8	-1.270972000	-2.189577000	-0.749451000
6	1.225161000	-1.115925000	0.178500000
8	1.269402000	-2.187590000	0.756684000
8	-2.340623000	-0.518952000	0.360512000
8	2.337753000	-0.524240000	-0.365436000
6	-3.558600000	-1.271365000	0.174530000
1	-4.343569000	-0.678079000	0.654479000
1	-3.770479000	-1.408615000	-0.894159000
1	-3.474261000	-2.258349000	0.647229000
6	3.555399000	-1.277297000	-0.179677000
1	3.468109000	-2.266622000	-0.646908000
1	4.339488000	-0.687574000	-0.665409000
1	3.770742000	-1.409241000	0.888991000

Table S9. Optimized Coordinates of

1d Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -441.3631478

6	0.993445000	-0.000003000	0.000000000
6	1.828713000	-1.160007000	0.127734000
6	3.143183000	-0.714653000	0.084046000
6	3.143179000	0.714657000	-0.084041000
6	1.828708000	1.160004000	-0.127743000
1	1.508999000	-2.185230000	0.291573000
1	4.026986000	-1.341841000	0.175787000
1	4.026980000	1.341851000	-0.175775000
1	1.508988000	2.185226000	-0.291586000
6	-1.113401000	1.177732000	0.098426000
6	-1.113406000	-1.177735000	-0.098424000
6	-2.492369000	1.190399000	0.089134000
1	-0.515402000	2.075925000	0.205571000
6	-2.492373000	-1.190396000	-0.089133000
1	-0.515412000	-2.075930000	-0.205572000
6	-3.224593000	0.000003000	0.000001000
1	-2.992164000	2.155394000	0.168685000
1	-2.992172000	-2.155390000	-0.168687000
1	-4.312495000	0.000005000	-0.000001000
7	-0.392974000	-0.000003000	0.000002000

Table S10. Optimized Coordinates of

1d Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -441.3073625

6	0.992439000	0.000001000	0.000001000
6	1.832991000	1.171991000	-0.080406000
6	3.142155000	0.728861000	-0.051670000
6	3.142154000	-0.728861000	0.051678000
6	1.832990000	-1.171991000	0.080393000
1	1.505929000	2.201389000	-0.174793000
1	4.030022000	1.354323000	-0.104448000
1	4.030020000	-1.354324000	0.104463000
1	1.505926000	-2.201390000	0.174770000
6	-1.121001000	-1.213941000	-0.055040000
6	-1.121002000	1.213942000	0.055041000
6	-2.484871000	-1.212739000	-0.059017000
1	-0.522380000	-2.114930000	-0.116394000
6	-2.484872000	1.212738000	0.059018000
1	-0.522382000	2.114932000	0.116395000
6	-3.224600000	-0.000001000	0.000001000
1	-2.996184000	-2.173796000	-0.110898000
1	-2.996186000	2.173795000	0.110899000
1	-4.311603000	-0.000001000	0.000001000
7	-0.394494000	0.000001000	0.000001000

Table S11. Optimized Coordinates of

2a Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -500.3700721

7	1.179850000	1.162638000	-0.044116000
6	0.440465000	-0.000073000	0.000020000
7	1.180302000	-1.162522000	0.044223000
6	-0.957361000	-0.000211000	0.000018000
6	-1.821388000	1.044810000	0.514867000
6	-3.129804000	0.643817000	0.327795000
6	-3.129875000	-0.644022000	-0.327635000
6	-1.821515000	-1.045145000	-0.514825000
1	-1.488360000	1.948760000	1.019181000
1	-4.016630000	1.195272000	0.634928000
1	-4.016776000	-1.195409000	-0.634679000
1	-1.488655000	-1.949135000	-1.019163000
6	0.695656000	-2.366340000	0.700828000
1	-0.176945000	-2.120192000	1.313261000
1	0.404235000	-3.143047000	-0.025792000
1	1.495416000	-2.779741000	1.338848000
6	2.406138000	-1.326047000	-0.722242000
1	2.587136000	-0.432055000	-1.327743000
1	3.281393000	-1.501233000	-0.073251000
1	2.307478000	-2.192030000	-1.398548000
6	2.405538000	1.326819000	0.722456000
1	2.587359000	0.432603000	1.327352000
1	3.280524000	1.503224000	0.073459000
1	2.306112000	2.192261000	1.399341000
6	0.694891000	2.366078000	-0.701267000
1	-0.177194000	2.119249000	-1.314154000
1	0.402510000	3.142787000	0.024963000
1	1.494854000	2.779758000	-1.338834000

Table S12. Optimized Coordinates of

2a Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -500.2898237

7	1.270784000	-1.170001000	0.094889000
6	0.502356000	-0.000002000	0.000003000
7	1.270703000	1.170045000	-0.094880000
6	-0.912774000	-0.000027000	0.000006000
6	-1.788114000	-1.053750000	-0.429845000
6	-3.184568000	-0.633967000	-0.252308000
6	-3.184577000	0.633880000	0.252324000
6	-1.788130000	1.053691000	0.429838000
1	-1.475522000	-2.005066000	-0.853872000
1	-4.052737000	-1.241657000	-0.495532000
1	-4.052754000	1.241557000	0.495548000
1	-1.475547000	2.005020000	0.853845000
6	0.778095000	2.320278000	-0.821929000
1	0.089700000	1.989600000	-1.608653000
1	0.244679000	3.053542000	-0.183311000
1	1.624485000	2.850294000	-1.290082000
6	2.253421000	1.466005000	0.938364000
1	2.595951000	0.524045000	1.382629000
1	3.121515000	1.988946000	0.505891000
1	1.834124000	2.105986000	1.741848000
6	2.253455000	-1.465924000	-0.938413000
1	2.595958000	-0.523948000	-1.382667000
1	3.121572000	-1.988870000	-0.505993000
1	1.834126000	-2.105883000	-1.741898000
6	0.778266000	-2.320261000	0.821962000
1	0.089911000	-1.989617000	1.608734000
1	0.244838000	-3.053547000	0.183379000
1	1.624710000	-2.850242000	1.290054000

Table S13. Optimized Coordinates of

2b Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -1353.6097367

6	0.677250000	0.019381000	-2.261194000
6	-0.677667000	-0.019118000	-2.261087000
7	-1.094621000	-0.028924000	-0.929097000

6	-0.000037000	0.000153000	-0.078644000	1	-6.109253000	-0.568573000	0.652540000
7	1.094408000	0.029239000	-0.929271000	1	-5.312039000	1.623406000	-0.171634000
6	2.461036000	0.183236000	-0.526417000	1	-1.968612000	2.120397000	-1.751692000
6	0.000047000	0.000191000	1.323532000	1	-4.317188000	2.628796000	-2.544765000
6	-2.461153000	-0.183230000	-0.526033000	1	-3.365078000	4.073924000	-2.123413000
6	-2.890203000	-1.446579000	-0.082161000	1	-4.615943000	3.491229000	-1.017415000
6	-4.220895000	-1.559707000	0.341835000	1	-1.354603000	2.465836000	0.653179000
6	-5.077783000	-0.461368000	0.313421000	1	-1.719073000	4.008830000	-0.167123000
6	-4.627057000	0.776069000	-0.150764000	1	-2.909164000	3.266583000	0.931542000
6	-3.304718000	0.944390000	-0.579047000	1	-0.982395000	-2.335794000	-0.422918000
6	-2.773055000	2.300487000	-1.022101000	1	-1.374502000	-2.362984000	2.036501000
6	-3.832299000	3.165767000	-1.717171000	1	-2.708621000	-3.524933000	1.817255000
6	-2.146110000	3.052266000	0.168522000	1	-1.047550000	-3.997296000	1.395973000
6	-1.965394000	-2.651415000	-0.046814000	1	-1.774313000	-4.610090000	-0.981625000
6	-1.761983000	-3.161471000	1.389687000	1	-2.591549000	-3.404353000	-2.008913000
6	-2.477732000	-3.764832000	-0.976505000	1	-3.454739000	-4.144718000	-0.643091000
6	3.304286000	-0.944616000	-0.579394000	1	5.311459000	-1.624140000	-0.172095000
6	4.626716000	-0.776605000	-0.151266000	1	6.109380000	0.567737000	0.651666000
6	5.077838000	0.460768000	0.312690000	1	4.586942000	2.521729000	0.701823000
6	4.221259000	1.559355000	0.341046000	1	1.967246000	-2.120429000	-1.751169000
6	2.890483000	1.446534000	-0.082757000	1	0.982890000	2.336211000	-0.423478000
6	2.772256000	-2.300632000	-1.022238000	1	4.315168000	-2.628674000	-2.546187000
6	1.965986000	2.651613000	-0.047446000	1	4.615204000	-3.491295000	-1.019200000
6	3.830975000	-3.165784000	-1.718276000	1	3.363472000	-4.073912000	-2.124260000
6	2.146245000	-3.052565000	0.168776000	1	2.909883000	-3.266954000	0.931194000
6	1.762788000	3.161808000	1.389039000	1	1.355097000	-2.466181000	0.654079000
6	2.478553000	3.764848000	-0.977226000	1	1.718967000	-4.009100000	-0.166646000
6	-1.138004000	0.242186000	2.188510000	1	1.375163000	2.363456000	2.035932000
6	-0.700611000	0.155580000	3.501437000	1	2.709545000	3.525068000	1.816518000
6	0.700849000	-0.155256000	3.501386000	1	1.048556000	3.997805000	1.395322000
6	1.138176000	-0.241744000	2.188428000	1	2.592217000	3.404285000	-2.009622000
1	1.394525000	0.055741000	-3.070348000	1	1.775351000	4.610287000	-0.982350000
1	-1.395062000	-0.055519000	-3.070132000	1	3.455676000	4.144504000	-0.643890000
1	-4.586260000	-2.522130000	0.702804000	1	-2.150331000	0.467152000	1.873157000

1	-1.320636000	0.301723000	4.383760000
1	1.320927000	-0.301445000	4.383664000
1	2.150494000	-0.466651000	1.873013000

Table S14. Optimized Coordinates of

2b Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -1353.5218215

6	-0.676784000	-0.021226000	-2.199890000
6	0.677470000	0.020735000	-2.199638000
7	1.116135000	0.036307000	-0.872168000
6	-0.000070000	0.000256000	-0.015317000
7	-1.115959000	-0.036201000	-0.872604000
6	-2.470025000	-0.250332000	-0.484216000
6	-0.000341000	0.000276000	1.395673000
6	2.470158000	0.250259000	-0.483547000
6	2.832943000	1.478382000	0.121098000
6	4.160089000	1.622672000	0.543848000
6	5.096542000	0.607366000	0.345081000
6	4.717438000	-0.589536000	-0.271688000
6	3.396353000	-0.798464000	-0.682054000
6	2.927287000	-2.146297000	-1.213217000
6	4.041794000	-2.978786000	-1.856896000
6	2.237836000	-2.937297000	-0.083745000
6	1.826574000	2.609871000	0.237903000
6	2.151530000	3.614667000	1.347461000
6	1.661546000	3.321449000	-1.119102000
6	-3.396274000	0.798311000	-0.682814000
6	-4.717326000	0.589385000	-0.272350000
6	-5.096337000	-0.607479000	0.344567000
6	-4.159855000	-1.622749000	0.543332000
6	-2.832728000	-1.478438000	0.120512000
6	-2.927276000	2.146036000	-1.214317000
6	-1.826283000	-2.609859000	0.237326000
6	-4.041834000	2.978297000	-1.858222000
6	-2.237848000	2.937397000	-0.085082000
6	-2.151092000	-3.614627000	1.346964000
6	-1.661287000	-3.321556000	-1.119606000
6	1.130144000	-0.167203000	2.267632000
6	0.673869000	-0.095876000	3.661922000
6	-0.675421000	0.096571000	3.661675000
6	-1.131172000	0.167841000	2.267197000
1	-1.381345000	-0.073802000	-3.019685000
1	1.382343000	0.073314000	-3.019160000
1	4.470679000	2.550577000	1.023784000
1	6.127165000	0.746078000	0.674763000
1	5.455815000	-1.379278000	-0.408599000
1	2.166763000	-1.963588000	-1.987954000
1	4.569475000	-2.415759000	-2.639766000
1	3.616144000	-3.883387000	-2.313634000
1	4.784836000	-3.308987000	-1.115781000
1	1.396368000	-2.376857000	0.345103000
1	1.853283000	-3.895875000	-0.462072000
1	2.951444000	-3.148207000	0.726683000
1	0.853885000	2.159854000	0.489591000
1	2.290675000	3.110231000	2.313757000
1	3.058661000	4.197330000	1.126396000
1	1.323676000	4.329686000	1.454005000
1	0.901421000	4.113400000	-1.045535000
1	1.343596000	2.621432000	-1.903482000
1	2.609804000	3.782598000	-1.433902000
1	-5.455764000	1.379055000	-0.409329000
1	-6.126931000	-0.746184000	0.674340000
1	-4.470387000	-2.550632000	1.023347000
1	-2.166756000	1.963139000	-1.989012000
1	-0.853626000	-2.159734000	0.488947000
1	-4.569521000	2.415010000	-2.640901000
1	-4.784858000	3.308695000	-1.117180000
1	-3.616227000	3.882772000	-2.315246000
1	-2.951427000	3.148394000	0.725348000

1	-1.396250000	2.377189000	0.343819000
1	-1.853470000	3.895944000	-0.463667000
1	-2.290202000	-3.110173000	2.313253000
1	-3.058195000	-4.197356000	1.125966000
1	-1.323176000	-4.329581000	1.453466000
1	-1.343486000	-2.621625000	-1.904120000
1	-0.901069000	-4.113417000	-1.046014000
1	-2.609520000	-3.782863000	-1.434258000
1	2.155880000	-0.345054000	1.961742000
1	1.324866000	-0.188307000	4.527509000
1	-1.326741000	0.189099000	4.527006000
1	-2.156772000	0.345844000	1.960938000

Table S15. Optimized Coordinates of

2c Singlet
BP86(D3BJ)/def2-TZVPP
Energy: -1229.6538457

6	0.011357000	-0.251104000	1.962639000
6	0.661769000	-1.343009000	2.643890000
6	0.165510000	-1.362896000	3.948345000
6	-0.794671000	-0.314713000	4.093782000
6	-0.907271000	0.366312000	2.881904000
1	1.407792000	-2.006662000	2.211996000
1	0.478751000	-2.050679000	4.732103000
1	-1.327728000	-0.065705000	5.009681000
1	-1.539538000	1.224059000	2.666401000
15	0.027999000	-0.024757000	0.266306000
6	-0.532147000	1.638364000	-0.183738000
6	0.380322000	2.634719000	-0.556452000
6	-1.901928000	1.937944000	-0.096955000
6	-0.074394000	3.925135000	-0.836391000
1	1.442612000	2.399397000	-0.628510000
6	-2.348414000	3.231848000	-0.368884000
1	-2.611594000	1.159051000	0.184217000
6	-1.436362000	4.225158000	-0.739818000
1	0.637324000	4.697739000	-1.129679000
1	-3.411341000	3.464252000	-0.293720000
1	-1.788737000	5.234424000	-0.956617000
6	1.704290000	-0.260488000	-0.387566000
6	1.941697000	-0.781827000	-1.667854000
6	2.783898000	0.126666000	0.424118000
6	3.250639000	-0.905338000	-2.137191000
1	1.106368000	-1.104859000	-2.289380000
6	4.090341000	-0.001223000	-0.051713000
1	2.583153000	0.504780000	1.427297000
6	4.324518000	-0.513207000	-1.331527000
1	3.433054000	-1.316166000	-3.130959000
1	4.927335000	0.293539000	0.582390000
1	5.346466000	-0.615129000	-1.699416000
6	-1.057567000	-1.152007000	-0.668659000
6	-1.464521000	-2.336269000	-0.038069000
6	-1.494462000	-0.860046000	-1.970888000
6	-2.289026000	-3.234720000	-0.718709000
1	-1.138541000	-2.527352000	0.987434000
6	-2.320756000	-1.761651000	-2.644751000
1	-1.202458000	0.076963000	-2.448225000
6	-2.714060000	-2.950374000	-2.020497000
1	-2.608435000	-4.154678000	-0.227513000
1	-2.664140000	-1.533774000	-3.654820000
1	-3.362901000	-3.651489000	-2.547362000

Table S16. Optimized Coordinates of

2c Triplet
BP86(D3BJ)/def2-TZVPP
Energy: -1229.5703488

6	0.179003000	0.000263000	1.913996000
6	0.428543000	-1.132607000	2.726656000
6	0.777870000	-0.683608000	4.075699000
6	0.777965000	0.684902000	4.075421000
6	0.428744000	1.133418000	2.726150000
1	0.385723000	-2.168270000	2.395324000
1	0.995393000	-1.340708000	4.913753000

1	0.995541000	1.342321000	4.913210000
1	0.386140000	2.168967000	2.394441000
15	0.021299000	-0.000040000	0.134087000
6	-0.832560000	1.511976000	-0.309355000
6	-0.739603000	2.014423000	-1.633302000
6	-1.851799000	2.026866000	0.533067000
6	-1.576038000	3.037866000	-2.061264000
1	-0.002551000	1.593417000	-2.318287000
6	-2.686177000	3.048503000	0.090636000
1	-1.985170000	1.613438000	1.533583000
6	-2.553126000	3.572256000	-1.203946000
1	-1.472466000	3.423678000	-3.076857000
1	-3.453103000	3.440560000	0.761003000
1	-3.212054000	4.369704000	-1.547323000
6	1.625334000	-0.000657000	-0.677157000
6	2.322476000	-1.217059000	-0.867517000
6	2.323565000	1.215234000	-0.866870000
6	3.643653000	-1.211863000	-1.304518000
1	1.816755000	-2.163414000	-0.673307000
6	3.644743000	1.209092000	-1.303869000
1	1.818672000	2.161933000	-0.672161000
6	4.314889000	-0.001618000	-1.534335000
1	4.159110000	-2.160482000	-1.463279000
1	4.161057000	2.157333000	-1.462111000
1	5.352058000	-0.001988000	-1.870091000
6	-0.833538000	-1.511576000	-0.308900000
6	-1.852642000	-2.025991000	0.533986000
6	-0.741400000	-2.014116000	-1.632883000
6	-2.687662000	-3.047278000	0.091970000
1	-1.985401000	-1.612472000	1.534544000
6	-1.578472000	-3.037210000	-2.060420000
1	-0.004496000	-1.593438000	-2.318228000
6	-2.555412000	-3.571148000	-1.202653000
1	-3.454460000	-3.438969000	0.762697000
1	-1.475533000	-3.423096000	-3.076050000
1	-3.214843000	-4.368313000	-1.545717000

Table S17. Optimized Coordinates of 3 Singlet

BP86(D3BJ)/def2-TZVPP
Energy: -1354.8196961

6	0.741329000	0.176128000	-2.298057000
6	-0.741288000	-0.176155000	-2.298091000
7	-1.111152000	0.071396000	-0.897393000
6	-0.000052000	0.000052000	-0.079890000
7	1.111090000	-0.071308000	-0.897300000
6	2.443579000	0.247911000	-0.483334000
6	-0.000117000	0.000080000	1.315945000
6	-2.443618000	-0.247916000	-0.483418000
6	-2.757113000	-1.554973000	-0.061649000
6	-4.071331000	-1.803842000	0.356690000
6	-5.033733000	-0.796702000	0.339578000
6	-4.705782000	0.483912000	-0.110539000
6	-3.404954000	0.783211000	-0.531264000
6	-3.007313000	2.185609000	-0.970063000
6	-4.150801000	2.959334000	-1.638263000
6	-2.424123000	2.982366000	0.212788000
6	-1.729196000	-2.674983000	-0.040574000
6	-1.491140000	-3.197695000	1.385908000
6	-2.133272000	-3.811896000	-0.995572000
6	3.404851000	-0.783302000	-0.531159000
6	4.705709000	-0.484065000	-0.110514000
6	5.033777000	0.796555000	0.339512000
6	4.071450000	1.803758000	0.356627000
6	2.757177000	1.554954000	-0.061607000
6	3.007134000	-2.185711000	-0.969858000
6	1.729360000	2.675063000	-0.040575000
6	4.150442000	-2.959275000	-1.638568000
6	2.424482000	-2.982564000	0.213183000
6	1.491341000	3.197817000	1.385905000

6	2.133541000	3.811930000	-0.995575000
6	-1.140330000	0.239636000	2.185963000
6	-0.703362000	0.155533000	3.494200000
6	0.703127000	-0.155350000	3.494211000
6	1.140093000	-0.239503000	2.185977000
1	0.913265000	1.236954000	-2.554767000
1	-0.913180000	-1.237004000	-2.554744000
1	-4.340883000	-2.802289000	0.704750000
1	-6.050113000	-1.010070000	0.674169000
1	-5.471624000	1.259231000	-0.126820000
1	-2.200370000	2.078868000	-1.711644000
1	-4.603126000	2.387274000	-2.460810000
1	-3.774005000	3.908387000	-2.045321000
1	-4.946344000	3.209359000	-0.920996000
1	-1.567813000	2.467036000	0.666166000
1	-2.097478000	3.978759000	-0.120334000
1	-3.183792000	3.116470000	0.997266000
1	-0.771532000	-2.270160000	-0.396121000
1	-1.173353000	-2.384726000	2.051864000
1	-2.407038000	-3.646003000	1.799258000
1	-0.710477000	-3.972022000	1.380007000
1	-1.354807000	-4.588453000	-1.015900000
1	-2.281261000	-3.443404000	-2.021300000
1	-3.071963000	-4.286865000	-0.674552000
1	5.471499000	-1.259438000	-0.126790000
1	6.050193000	1.009869000	0.674026000
1	4.341086000	2.802210000	0.704606000
1	2.199896000	-2.079013000	-1.711117000
1	0.771668000	2.270324000	-0.396148000
1	4.602312000	-2.387118000	-2.461296000
1	4.946335000	-3.209190000	-0.921656000
1	3.773601000	-3.908373000	-2.045479000
1	3.184439000	-3.116621000	0.997391000
1	1.568272000	-2.467332000	0.666871000
1	2.097803000	-3.978978000	-0.119845000
1	1.173512000	2.384882000	2.051882000
1	2.407277000	3.646068000	1.799229000
1	0.710724000	3.972192000	1.380009000
1	2.281518000	3.443406000	-2.021293000
1	1.355121000	4.588531000	-1.015928000
1	3.072252000	4.286856000	-0.674550000
1	-2.154430000	0.455745000	1.871968000
1	-1.322323000	0.300012000	4.377540000
1	1.322071000	-0.299830000	4.377563000
1	2.154201000	-0.455573000	1.871985000
1	-1.338535000	0.446822000	-2.976967000
1	1.338629000	-0.446913000	-2.976828000

Table S18. Optimized Coordinates of 3 Triplet

BP86(D3BJ)/def2-TZVPP
Energy: -1354.7357274

6	0.740563000	0.181054000	-2.301243000
6	-0.740586000	-0.181112000	-2.301232000
7	-1.130663000	0.125721000	-0.917968000
6	0.000001000	-0.000008000	-0.086031000
7	1.130658000	-0.125747000	-0.917978000
6	2.434277000	0.287541000	-0.496216000
6	0.000001000	0.000001000	1.317904000
6	-2.434280000	-0.287550000	-0.496181000
6	-2.673418000	-1.591947000	-0.010531000
6	-3.961499000	-1.894030000	0.454931000
6	-4.983720000	-0.948784000	0.415146000
6	-4.736714000	0.327506000	-0.099134000
6	-3.463213000	0.680711000	-0.556811000
6	-3.148868000	2.090502000	-1.038499000
6	-4.354865000	2.812435000	-1.651034000
6	-2.537056000	2.921709000	0.105505000
6	-1.603426000	-2.673048000	-0.018305000
6	-1.372236000	-3.272729000	1.377525000

6	-1.951275000	-3.769759000	-1.041110000	1	-2.880484000	-4.290090000	-0.764737000
6	3.463219000	-0.680710000	-0.556847000	1	5.545400000	-1.057814000	-0.131100000
6	4.736726000	-0.327480000	-0.099205000	1	5.979329000	1.205458000	0.780235000
6	4.983729000	0.948823000	0.415043000	1	4.166890000	2.892686000	0.844656000
6	3.961499000	1.894059000	0.454828000	1	2.377092000	-2.004696000	-1.818293000
6	2.673411000	1.591952000	-0.010602000	1	0.656360000	2.213047000	-0.330530000
6	3.148883000	-2.090513000	-1.038506000	1	4.826299000	-2.214337000	-2.443801000
6	1.603407000	2.673041000	-0.018380000	1	5.122079000	-3.039439000	-0.895776000
6	4.354873000	-2.812435000	-1.651066000	1	4.037481000	-3.770712000	-2.086464000
6	2.537119000	-2.921715000	0.105526000	1	3.257450000	-3.030143000	0.930395000
6	1.372257000	3.272773000	1.377435000	1	1.632628000	-2.444847000	0.504372000
6	1.951211000	3.769718000	-1.041237000	1	2.268958000	-3.928641000	-0.247820000
6	-1.119920000	0.227038000	2.193971000	1	1.101387000	2.492548000	2.100338000
6	-0.668491000	0.133953000	3.588260000	1	2.271853000	3.787012000	1.747214000
6	0.668477000	-0.133932000	3.588266000	1	0.556769000	4.009842000	1.344434000
6	1.119915000	-0.227032000	2.193981000	1	2.093463000	3.348975000	-2.047145000
1	0.887300000	1.254059000	-2.526541000	1	1.146269000	4.517898000	-1.090563000
1	-0.887326000	-1.254121000	-2.526504000	1	2.880424000	4.290071000	-0.764912000
1	-4.166893000	-2.892646000	0.844786000	1	-2.139832000	0.439184000	1.890659000
1	-5.979316000	-1.205400000	0.780364000	1	-1.312884000	0.262347000	4.454263000
1	-5.545380000	1.057848000	-0.131026000	1	1.312863000	-0.262320000	4.454274000
1	-2.377101000	2.004662000	-1.818306000	1	2.139829000	-0.439182000	1.890679000
1	-4.826324000	2.214335000	-2.443746000	1	-1.332039000	0.407224000	-3.016834000
1	-4.037469000	3.770701000	-2.086454000	1	1.332010000	-0.407297000	-3.016839000
1	-5.122045000	3.039463000	-0.895724000				
1	-1.632560000	2.444831000	0.504329000				
1	-2.268891000	3.928626000	-0.247861000				
1	-3.257360000	3.030158000	0.930394000				
1	-0.656384000	-2.213075000	-0.330503000				
1	-1.101334000	-2.492478000	2.100389000				
1	-2.271825000	-3.786944000	1.747354000				
1	-0.556756000	-4.009807000	1.344526000				
1	-1.146343000	-4.517949000	-1.090435000				
1	-2.093554000	-3.349051000	-2.047030000				