Supplementary Information

Redox Active Tin(II) Complexes with Sterically Demanding *o*-Phenylenediamido Ligands and their Reactivity with Organic Azides

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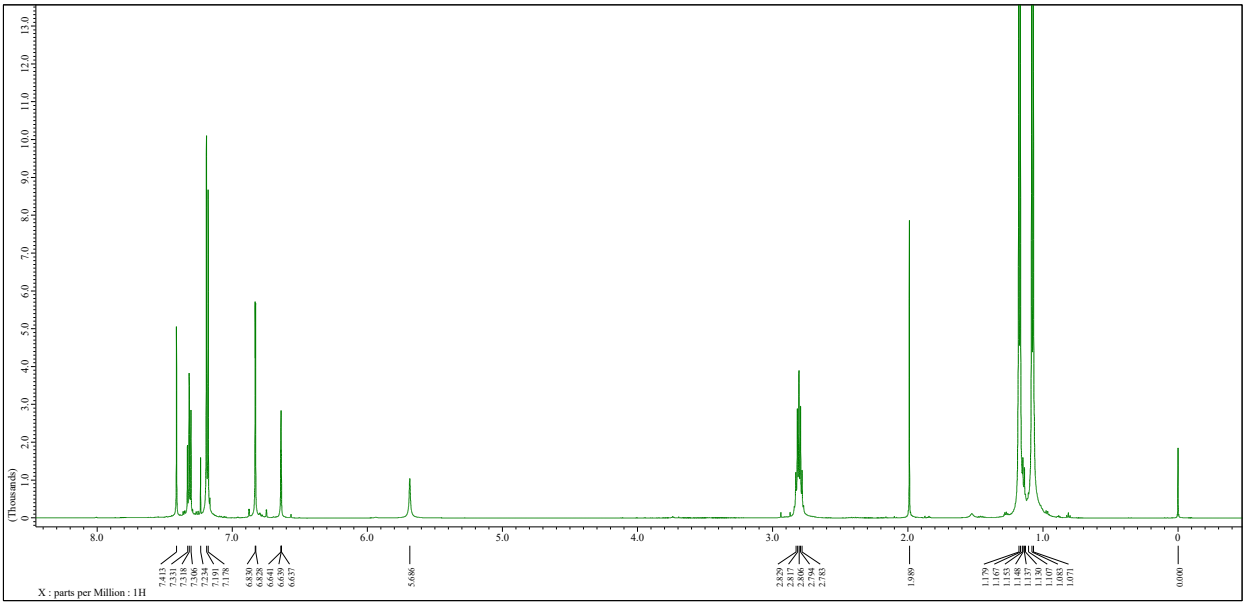


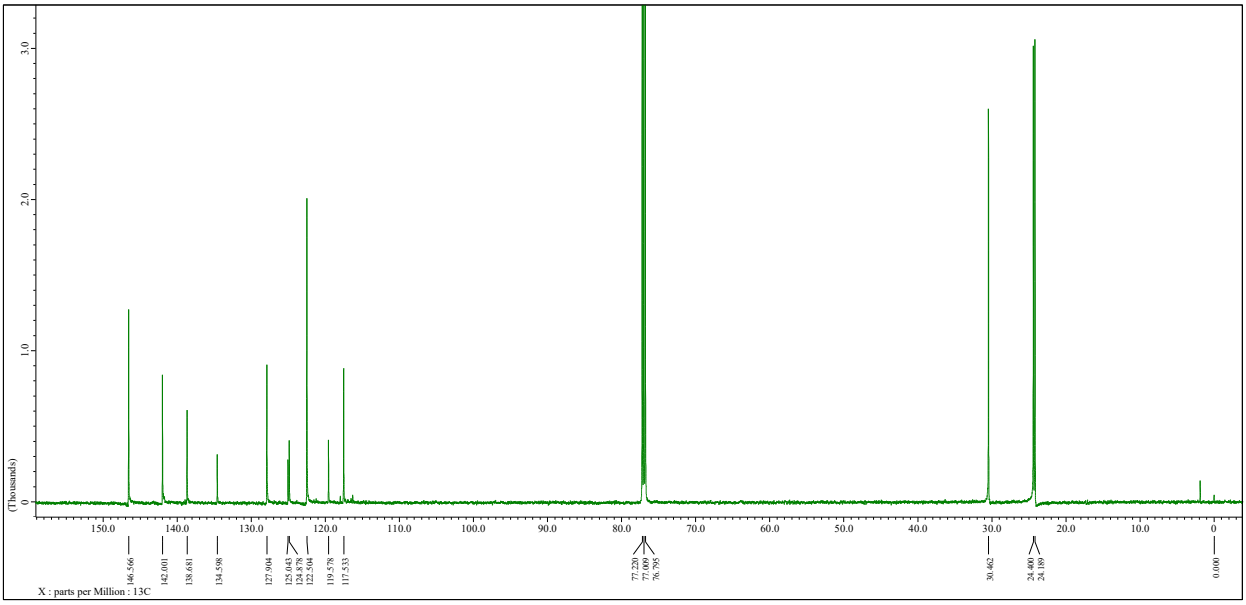


Figure S1. ^{1}H and ^{13}C NMR spectra of $^{Cl}LH_2$.

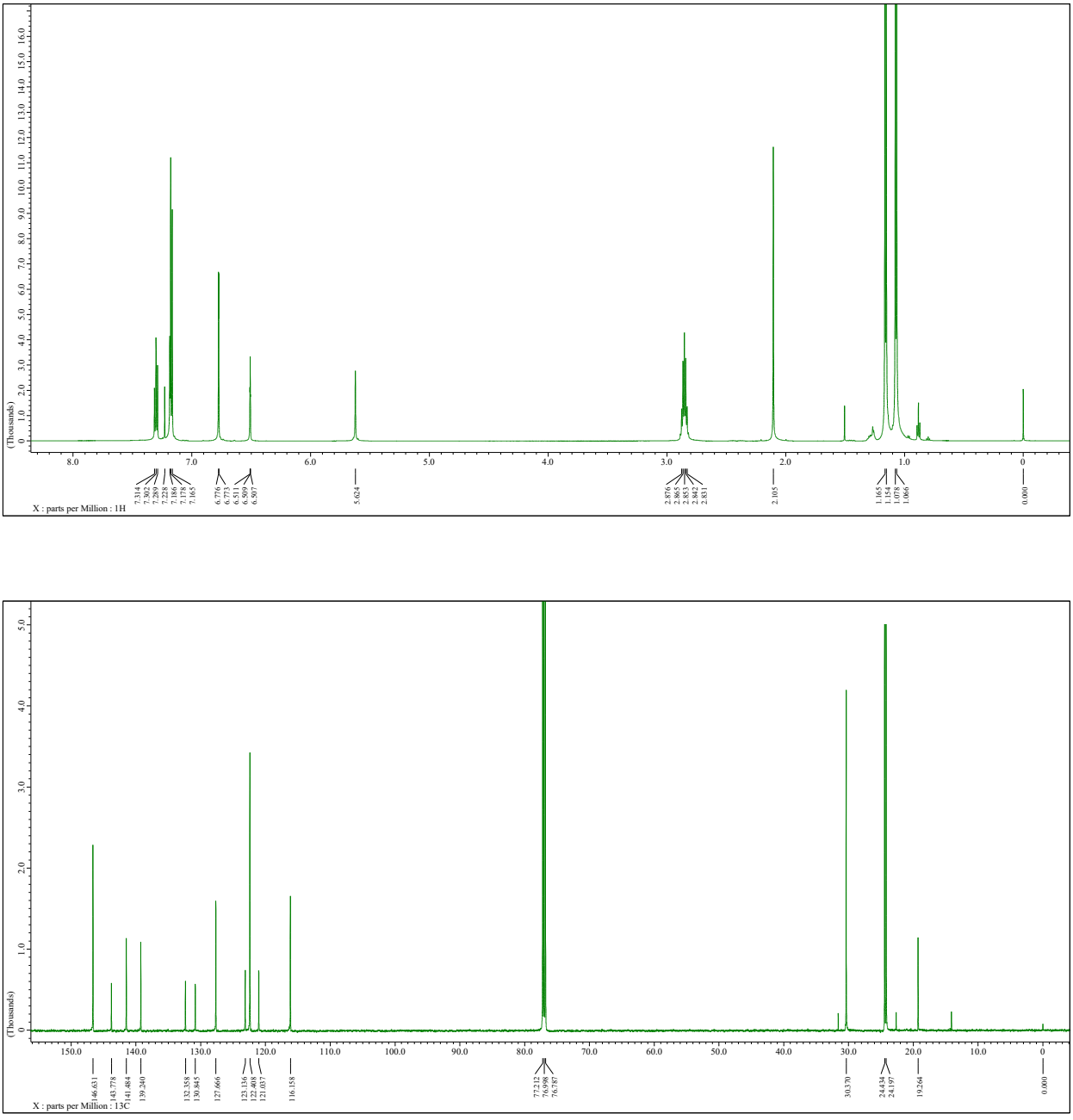
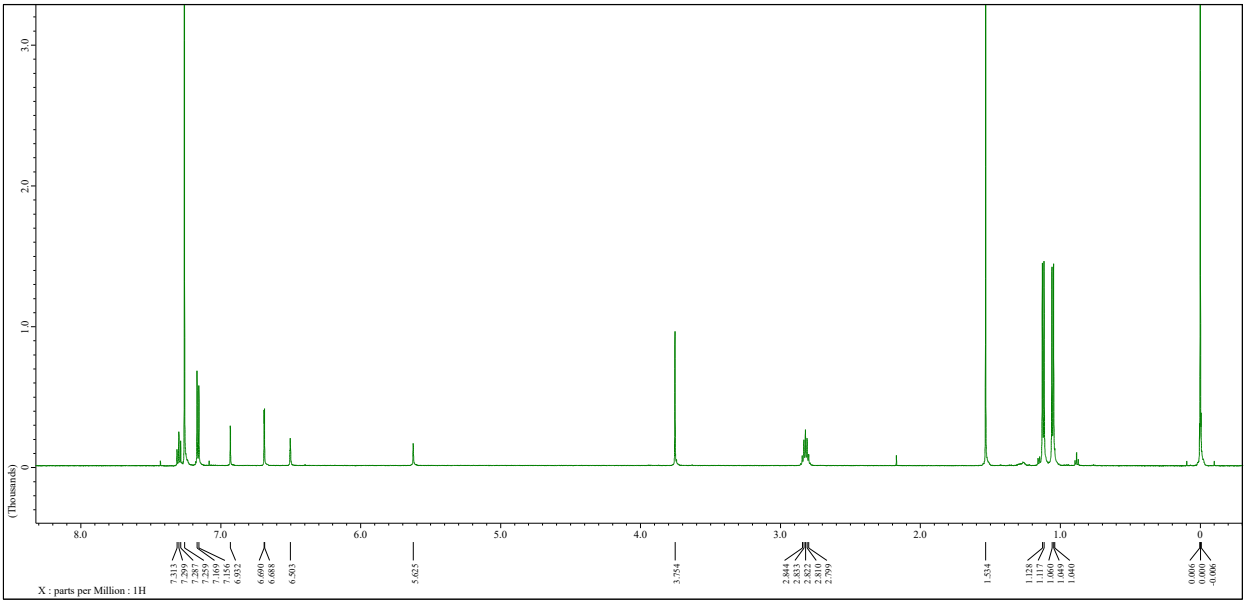


Figure S2. ^{1}H and ^{13}C NMR spectra of $^{Me}LH_2$.



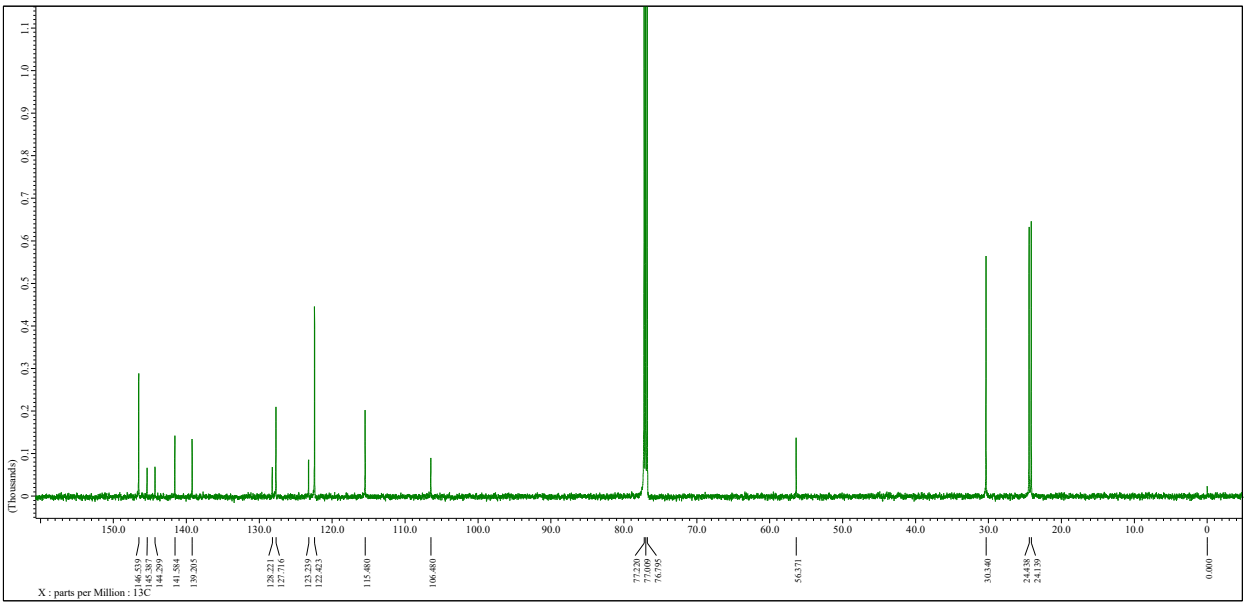
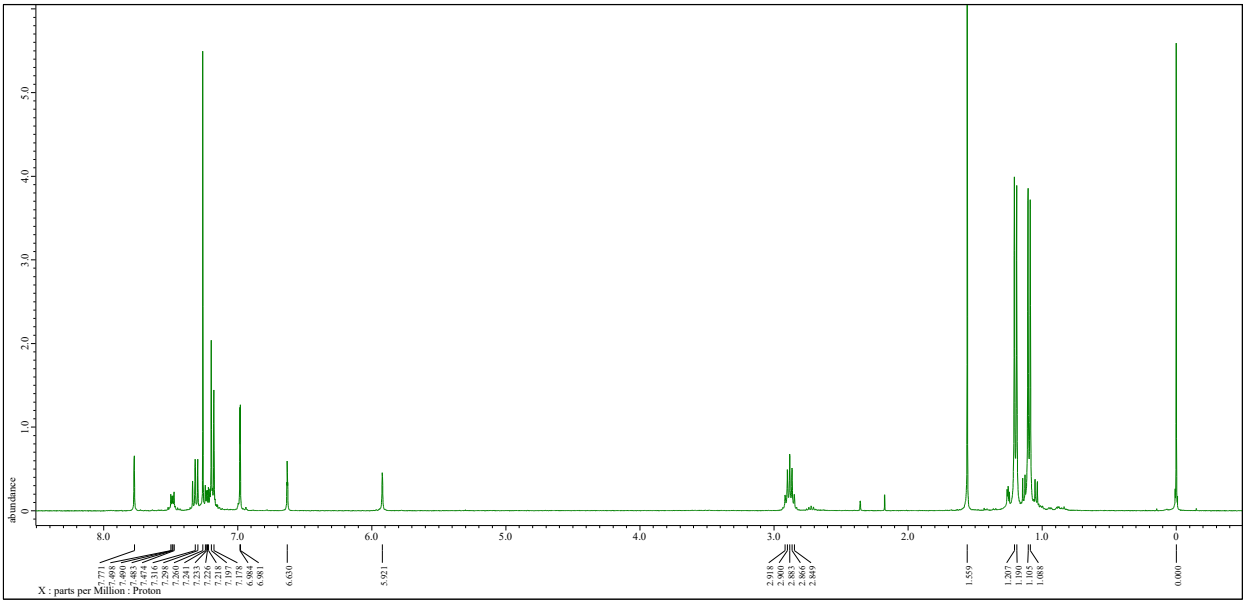


Figure S3. ^{1}H and ^{13}C NMR spectra of $^{OMe}LH_2$.



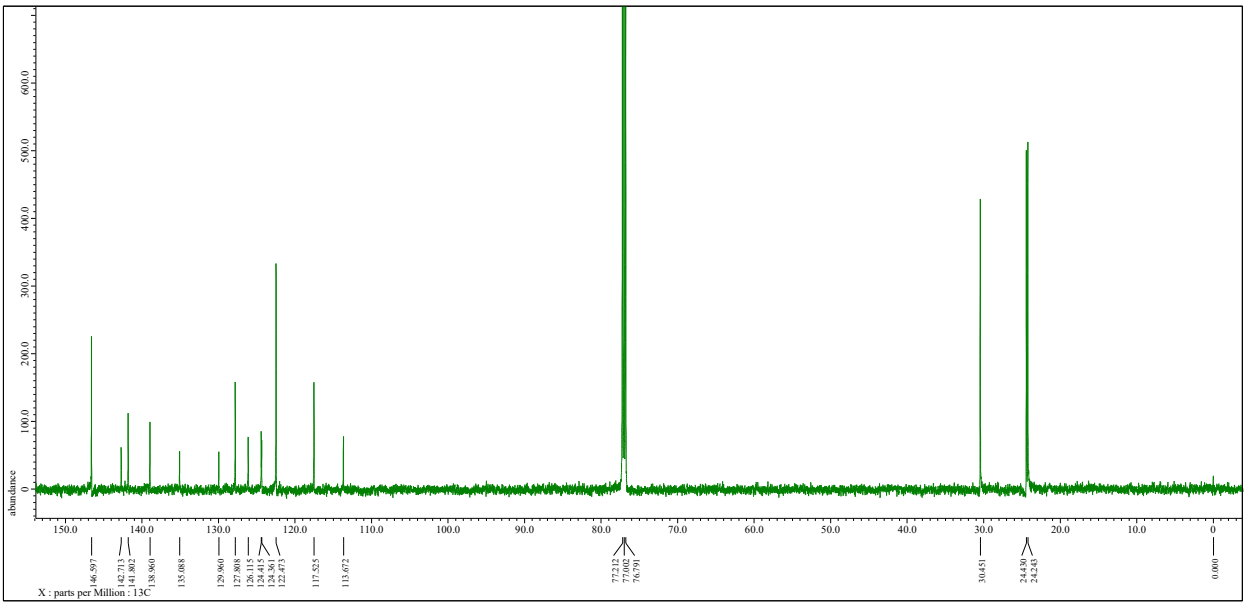


Figure S4. ^{1}H and ^{13}C NMR spectra of $^{naph}LH_2$.

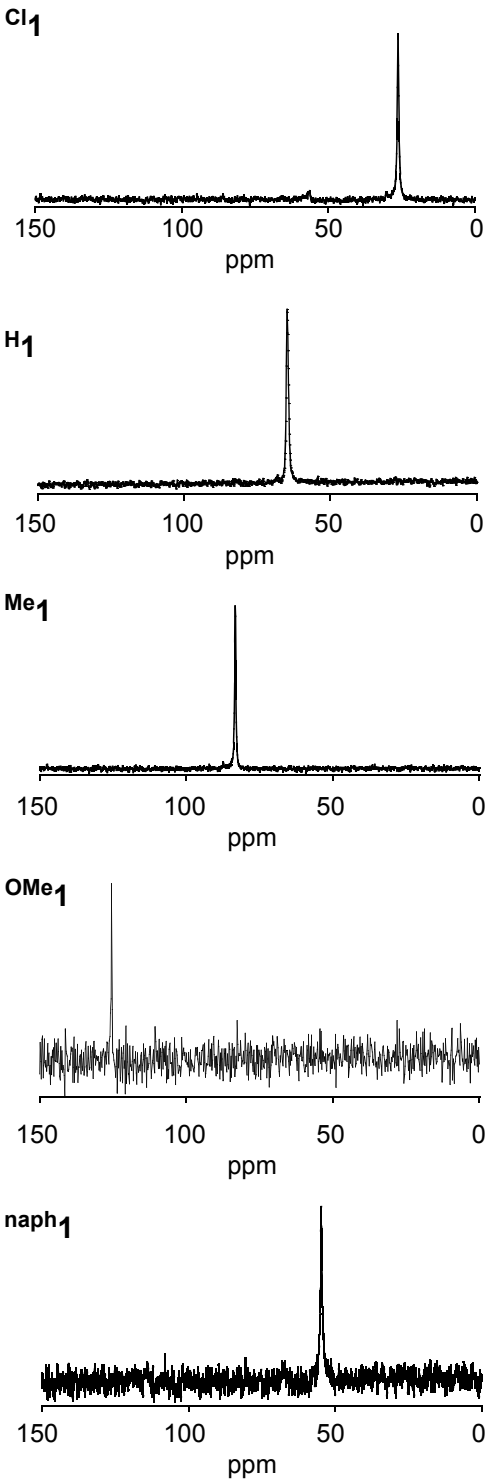


Figure S5. ^{119}Sn-NMR spectra of ^{R}**1** in C_6D_6.

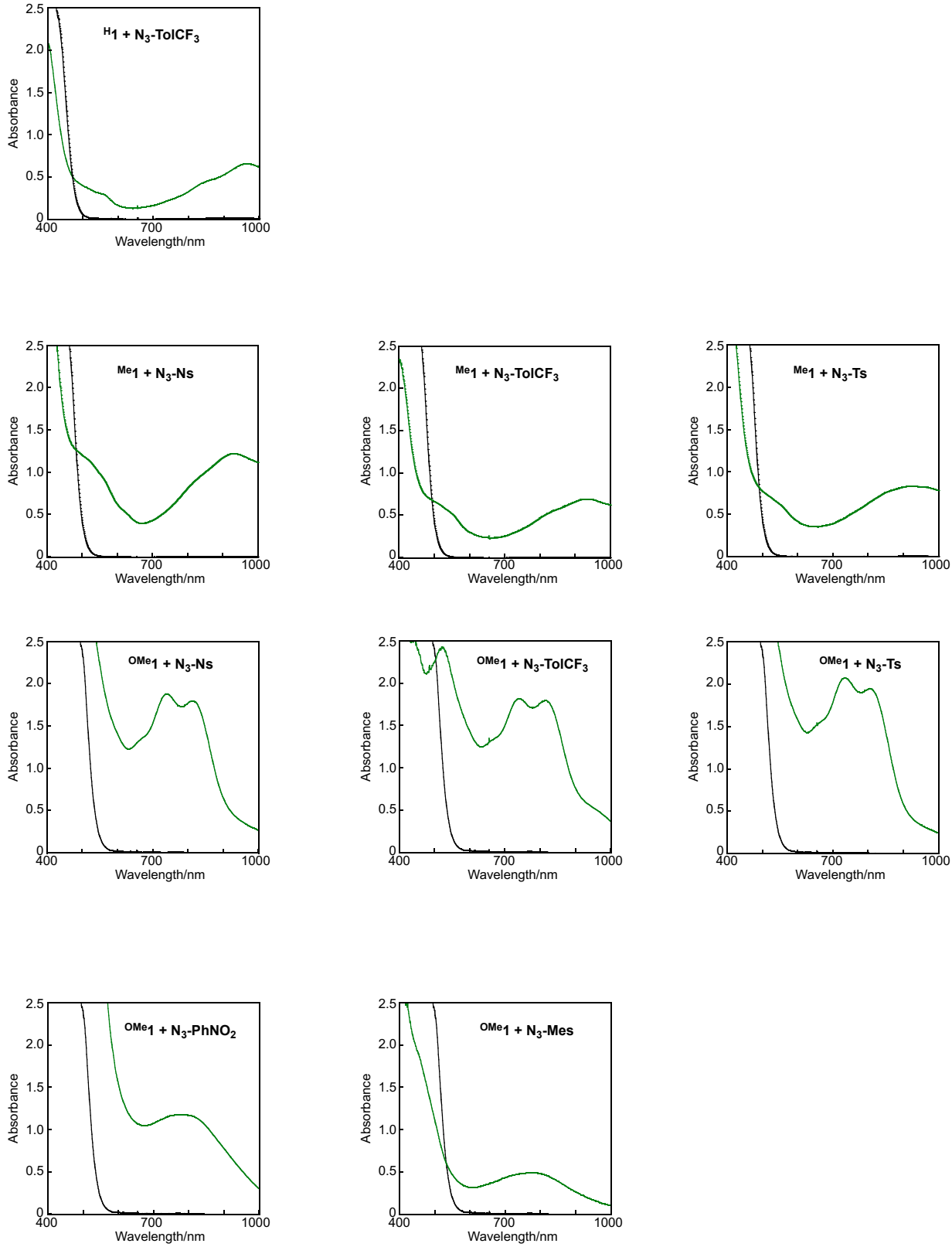


Figure S6. Absorption spectral changes of ^{R}**1** (1.0 mM) by the reactions with one equivalent of N_3-R' in toluene at −30 ºC.

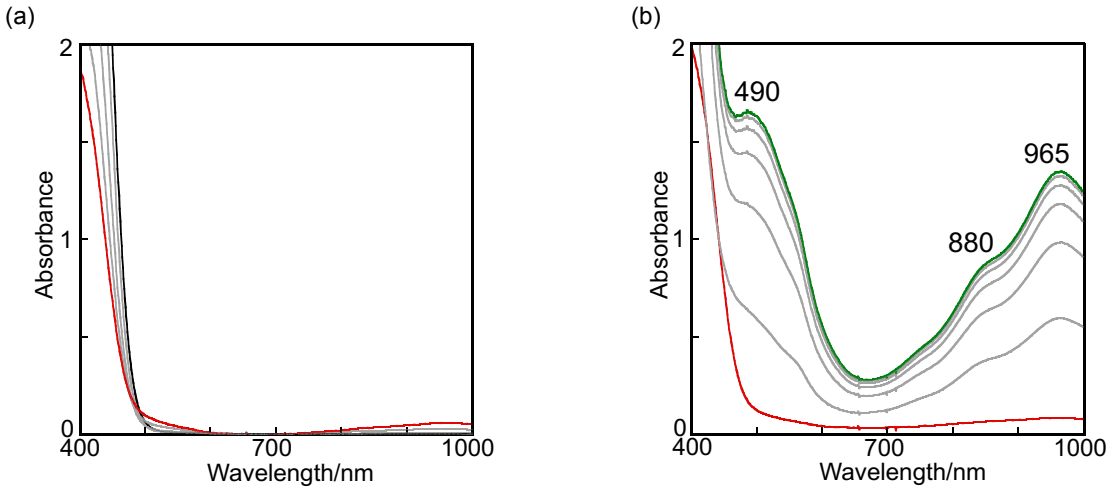


Figure S7. Time dependent spectral changes from $^{H}\mathbf{1}$ (1.0 mM) to $^{H}\mathbf{1}^{N3\text{-}TolCF3}$ (black to red, a) and those from $^{H}\mathbf{1}^{N3\text{-}TolCF3}$ to $^{H}\mathbf{2}^{TolCF3\text{-}N\bullet}$ (red to green, b) in the presence of 20.0 mM of N_3-TolCF_3 in toluene at –40 ºC.

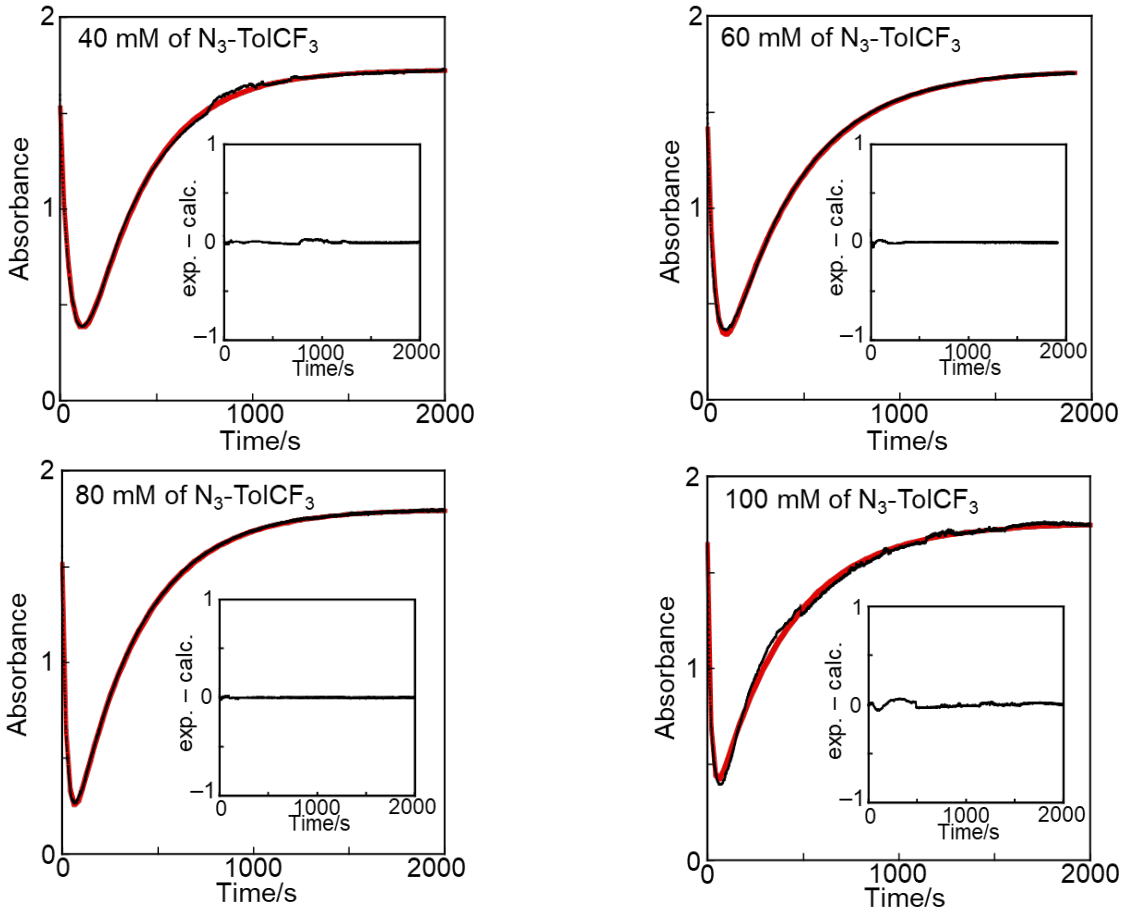


Figure S8. Time course plots of the absorbance change at 455 nm in the presence of various amounts of N_3-TolCF_3.

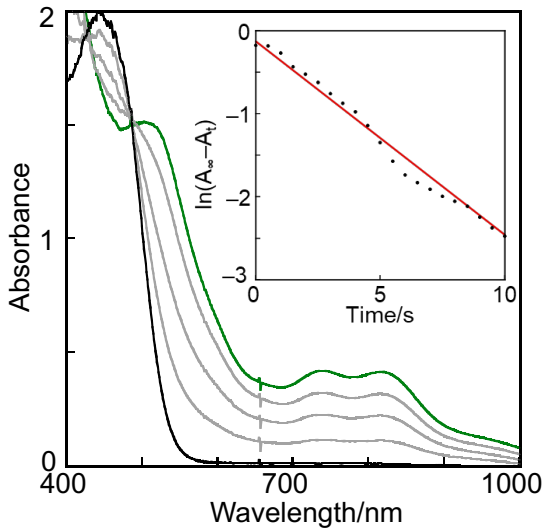


Figure S9. Absorption spectral changes of ^{OMe}**1** upon a treatment with 20 equiv. of N_3-TolCF_3 in toluene at –40 ºC. inset: first-order plot based on absorbance change at 590 nm.

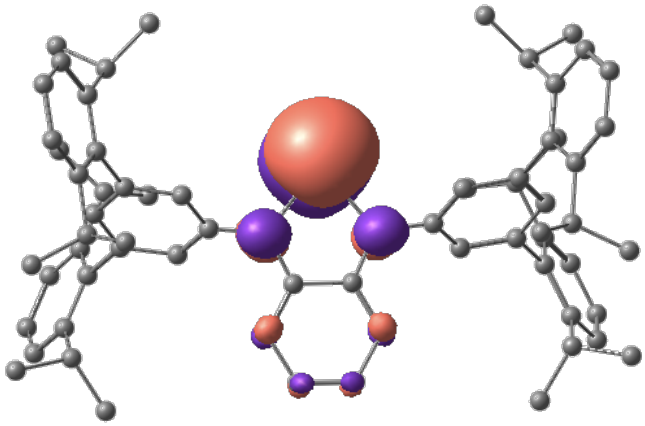


Figure S10. LUMO of ^{H}**1**.

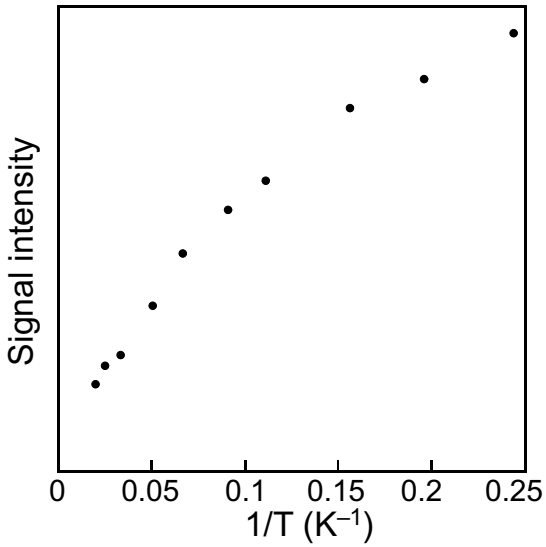


Figure S11. Temperature dependence of signal intensity at $g = 4.002$.

Table S1. Crystallographic Data for [Sn(^{Cl}L)(THF)$_2$]•CH_3CN (^{Cl}1•CH_3CN) and [Sn(^{Me}L)(THF)(CH_3CN]•CH_3CN (^{Me}1•CH_3CN)

	^{Cl}**1**•CH_3CN	^{Me}**1**•CH_3CN
formula	$C_{76}H_{87}Cl_2N_3O_2Sn$	$C_{76}H_{96}N_4OSn$
formula weight	1264.07	1200.25
crystal system	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$
a, Å	17.3591(7)	17.0941(9)
b, Å	18.5527(9)	18.8683(11)
c, Å	22.2644(9)	22.2358(12)
α, deg	90	90
β, deg	106.469(7)	106.608(7)
γ, deg	90	90
V, Å^3	6875.3(6)	6872.7(7)
Z	4	4
ρ calc, g/cm^3	1.221	1.160
μ/cm^{-1}	4.96	4.16
F(000)	2656.0	2552.0
Mo$K\alpha$, cm^{-1}	0.71075	0.71075
T, K	115	115
$2\theta_{max}$, deg	54.952	54.97
no. of refins obsd	15717	15678
no. of variables	753	759
R^a	0.0450	0.0534
wR^b	0.1116	0.1424
GOF	1.083	1.096
max./min. Δρ, e Å^{-3}	1.67/ –0.88	1.65/ –1.33

^{a} $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$. ^{b} $wR2 = (\Sigma(w(F_o^2 - F_c^2)^2)/ \Sigma w(F_o^2)^2)^{1/2}$.

Table S2. Crystallographic Data for [Sn(^{OMe}L)(THF)(CH_3CN)]•CH_3CN (^{OMe}1•CH_3CN), [Sn(^{naph}L)(THF)$_2$]•CH_3CN (^{naph}1•CH_3CN), and [Sn(L^{Bu2Ph})(THF)] (SnL^{Bu2Ph})

	^{OMe}1•CH_3CN	^{naph}1•CH_3CN	SnL^{Bu2Ph}
formula	$C_{75.42}H_{93}N_{3.98}O_3Sn$	$C_{80}H_{99}N_3O_2Sn$	$C_{38}H_{46}N_2OSn$
formula weight	1222.11	1253.31	665.51
crystal system	monoclinic	monoclinic	orthorhombic
space group	$P2_1/c$	$P2_1/c$	*P*nma
a, Å	16.8998(13)	17.3796(8)	9.5302(8)
b, Å	18.8654(16)	18.5286(10)	31.242(2)
c, Å	22.6765(19)	22.9413(10)	11.5295(10)
α, deg	90	90	90
β, deg	109.078(8)	101.332(7)	90
γ, deg	90	90	90
V, Å^3	6832.7(10)	7243.5(6)	3432.8(5)
Z	4	4	4
ρ calc, g/cm^3	1.188	1.149	1.2876
μ/cm^{-1}	4.22	3.98	7.75
F(000)	2590.0	2664.0	1382.0
Mo*K*α, cm^{-1}	0.71075	0.71075	0.71075
T, K	115	115	158
2θmax, deg	50.696	54.972	54.965
no. of refins obsd	12475	16473	30040
no. of variables	763	791	204
R^a	0.0611	0.0640	0.0578
wR^b	0.1252	0.1233	0.1315
GOF	0.933	1.186	1.039
max./min. Δρ, e Å^{-3}	1.85/ –0.71	0.85/ –0.66	1.50/-2.53

^{a} $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$. ^{b} $wR2 = (\Sigma(w(F_o^2 - F_c^2)^2)/ \Sigma w(F_o^2)^2)^{1/2}$.

Table S3. Combination of ^{R}1 and N_3-R' that generates tin(II) nitrene radical complex

	N_3-Ns	N_3-TolCF_3	N_3-Ts	N_3-PhNO_2	N_3-Mes
	(2131)[a]	(2130)[a]	(2126)[a]	(2123)[a]	(2121)[a]
^{OMe}**1**	^{OMe}**2**$^{N•}$-Ns (820, 742)[b]	^{OMe}**2**$^{N•}$-TolCF3 (820, 742)[b]	^{OMe}**2**$^{N•}$-Ts (814, 736)[b]	^{OMe}**2**$^{N•}$-PhNO2 (790)[b]	^{OMe}**2**$^{N•}$-Mes (790)[b]
^{Me}**1**	^{Me}**2**$^{N•}$-Ns (934)[b]	^{Me}**2**$^{N•}$-TolCF3 (946)[b]	^{Me}**2**$^{N•}$-Ts (928)[b]	_ [c]	_ [c]
^{H}**1**	^{H}**2**$^{N•}$-Ns (960)[b]	^{H}**2**$^{N•}$-TolCF3 (965)[b]	_ [c]	_ [c]	_ [c]
^{Cl}**1**	_ [c]	_ [c]	_ [c]	_ [c]	_ [c]
^{naph}**1**	_ [c]	_ [c]	_ [c]	_ [c]	_ [c]

[a] ν(N≡N) stretch (cm^{-1}) of azides. [b] λ_{max} of near-IR absorption bands of ^{R}**2**$^{R'-N•}$. [c] ^{R}**2**$^{R'-N•}$ was not formed.

Table S4. Optimized structure of ^{H}1 in the closed shell singlet

Sn	**0.000034**	**0.940639**	**0.769304**
N	**-1.321758**	**-0.047116**	**-0.543855**
N	**1.321800**	**-0.047155**	**-0.543833**
C	**4.824253**	**-1.201039**	**0.147455**
C	**-2.733863**	**-0.040265**	**-0.360298**
C	**-3.424376**	**1.184760**	**-0.355194**
H	**-2.881959**	**2.101421**	**-0.578125**
C	**5.691042**	**3.267441**	**1.122211**
C	**-3.445523**	**-1.229467**	**-0.105044**
H	**-2.911286**	**-2.176578**	**-0.089361**
C	**2.733916**	**-0.040312**	**-0.360316**
C	**6.368477**	**4.498276**	**1.100454**
H	**6.499662**	**5.056038**	**2.025682**
C	**4.804862**	**1.235802**	**-0.093047**
C	**5.571209**	**-2.477324**	**0.421763**
C	**0.716789**	**-0.803540**	**-1.548551**
C	**-5.528703**	**2.553887**	**-0.091432**
C	**-4.804746**	**1.235897**	**-0.092682**
C	**-5.571236**	**-2.477314**	**0.421342**
C	**-1.406255**	**-1.493842**	**-2.570455**
H	**-2.491530**	**-1.474970**	**-2.588155**
C	**3.445524**	**-1.229501**	**-0.104862**
H	**2.911228**	**-2.176576**	**-0.088988**
C	**1.406299**	**-1.493897**	**-2.570415**
H	**2.491576**	**-1.475071**	**-2.588077**
C	**-6.174832**	**-3.182221**	**-0.650408**
C	**5.528904**	**2.553745**	**-0.092043**
C	**5.493486**	**0.037604**	**0.153110**
H	**6.562923**	**0.065994**	**0.351620**
C	**0.703959**	**-2.177088**	**-3.563851**
H	**1.250894**	**-2.700723**	**-4.344933**
C	**-4.824244**	**-1.200985**	**0.147328**

C	**-0.703913**	**-2.177056**	**-3.563874**
H	**-1.250845**	**-2.700666**	**-4.344973**
C	**-5.660988**	**-2.970877**	**1.747271**
C	**3.424473**	**1.184684**	**-0.355462**
H	**2.882074**	**2.101329**	**-0.578509**
C	**-6.354427**	**-4.170919**	**1.978639**
H	**-6.429374**	**-4.561688**	**2.991549**
C	**-0.716750**	**-0.803518**	**-1.548564**
C	**5.150357**	**2.744040**	**2.452128**
H	**4.662594**	**1.782944**	**2.263799**
C	**-5.690240**	**3.267705**	**1.122828**
C	**6.859327**	**-4.378339**	**-0.374748**
H	**7.325422**	**-4.930354**	**-1.188607**
C	**-6.712062**	**4.310592**	**-1.283347**
H	**-7.110839**	**4.722220**	**-2.208468**
C	**6.175071**	**-3.182328**	**-0.649772**
C	**5.891268**	**2.339568**	**-2.637288**
H	**5.358868**	**1.402846**	**-2.447880**
C	**6.876709**	**5.020598**	**-0.092043**
H	**7.398585**	**5.975793**	**-0.092124**
C	**6.041818**	**3.075496**	**-1.306542**
C	**-5.493417**	**0.037686**	**0.153277**
H	**-6.562842**	**0.066085**	**0.351847**
C	**-6.042127**	**3.075568**	**-1.305747**
C	**-5.149055**	**2.744345**	**2.452555**
H	**-4.661223**	**1.783315**	**2.264048**
C	**-6.950602**	**-4.873539**	**0.927974**
H	**-7.483543**	**-5.802125**	**1.124036**
C	**-5.021064**	**-2.246069**	**2.930548**
H	**-4.569298**	**-1.322296**	**2.556802**
C	**6.095753**	**-2.690010**	**-2.094185**
H	**5.566064**	**-1.732575**	**-2.096142**
C	**6.711831**	**4.310481**	**-1.284339**
H	**7.110215**	**4.722166**	**-2.209604**

C	**-6.859089**	**-4.378298**	**-0.375673**
H	**-7.324970**	**-4.930249**	**-1.189698**
C	**-5.892324**	**2.339466**	**-2.636475**
H	**-5.359451**	**1.402965**	**-2.447312**
C	**6.285113**	**2.487973**	**3.465789**
H	**7.025307**	**1.787987**	**3.061498**
H	**5.883346**	**2.061533**	**4.393339**
H	**6.810205**	**3.415002**	**3.725136**
C	**-6.095233**	**-2.689737**	**-2.094754**
H	**-5.565529**	**-1.732310**	**-2.096497**
C	**-6.067061**	**-1.844831**	**3.991130**
H	**-6.854638**	**-1.220712**	**3.553501**
H	**-5.592926**	**-1.277329**	**4.801573**
H	**-6.547447**	**-2.723239**	**4.438140**
C	**6.950565**	**-4.873431**	**0.928975**
H	**7.483513**	**-5.801966**	**1.125260**
C	**5.660681**	**-2.970737**	**1.747769**
C	**-6.876339**	**5.020835**	**-0.091042**
H	**-7.398150**	**5.976066**	**-0.090975**
C	**-3.888970**	**-3.086051**	**3.558917**
H	**-4.270339**	**-4.027763**	**3.971575**
H	**-3.406992**	**-2.534200**	**4.375599**
H	**-3.122519**	**-3.335119**	**2.816001**
C	**5.020422**	**-2.245846**	**2.930814**
H	**4.569241**	**-1.321824**	**2.556976**
C	**-6.367588**	**4.498593**	**1.101268**
H	**-6.498305**	**5.056445**	**2.026507**
C	**5.044041**	**3.150172**	**-3.640476**
H	**4.053940**	**3.377551**	**-3.229065**
H	**4.904263**	**2.585240**	**-4.570345**
H	**5.525220**	**4.101667**	**-3.896764**
C	**4.083317**	**3.689564**	**3.042479**
H	**4.504470**	**4.673711**	**3.280092**
H	**3.669199**	**3.271954**	**3.968662**

H	**3.257480**	**3.842991**	**2.338051**
C	**7.495396**	**-2.435549**	**-2.691020**
H	**8.061634**	**-1.722117**	**-2.081282**
H	**7.410968**	**-2.025905**	**-3.705195**
H	**8.082213**	**-3.359605**	**-2.753880**
C	**6.354114**	**-4.170726**	**1.979427**
H	**6.428856**	**-4.561372**	**2.992399**
C	**-5.046195**	**3.150136**	**-3.640532**
H	**-5.528014**	**4.101299**	**-3.896854**
H	**-4.906801**	**2.584930**	**-4.570291**
H	**-4.055918**	**3.378147**	**-3.229901**
C	**5.285114**	**-3.663052**	**-2.976265**
H	**5.765781**	**-4.647049**	**-3.033121**
H	**5.197854**	**-3.274519**	**-3.998708**
H	**4.274320**	**-3.809829**	**-2.578296**
C	**7.262456**	**1.970572**	**-3.240994**
H	**7.850625**	**2.863991**	**-3.482362**
H	**7.131989**	**1.397570**	**-4.167404**
H	**7.850592**	**1.362574**	**-2.543923**
C	**-6.283471**	**2.488116**	**3.466559**
H	**-6.808633**	**3.415075**	**3.726008**
H	**-5.881362**	**2.061781**	**4.394012**
H	**-7.023667**	**1.787991**	**3.062519**
C	**-5.284453**	**-3.662693**	**-2.976796**
H	**-4.273747**	**-3.809564**	**-2.578642**
H	**-5.196973**	**-3.274034**	**-3.999171**
H	**-5.765147**	**-4.646665**	**-3.033878**
C	**-4.081959**	**3.689977**	**3.042646**
H	**-3.256372**	**3.843600**	**2.337974**
H	**-3.667490**	**3.272335**	**3.968657**
H	**-4.503185**	**4.674038**	**3.280500**
C	**-7.494761**	**-2.435175**	**-2.691807**
H	**-8.081664**	**-3.359170**	**-2.754704**
H	**-7.410149**	**-2.025585**	**-3.705990**

H	**-8.061014**	**-1.721650**	**-2.082185**
C	**-7.263889**	**1.969884**	**-3.238987**
H	**-7.851218**	**1.361762**	**-2.541345**
H	**-7.134006**	**1.396816**	**-4.165439**
H	**-7.852571**	**2.863079**	**-3.479942**
C	**6.065944**	**-1.845208**	**3.992088**
H	**6.545533**	**-2.723876**	**4.439442**
H	**5.591571**	**-1.277452**	**4.802213**
H	**6.854160**	**-1.221520**	**3.554996**
C	**3.887636**	**-3.085494**	**3.558382**
H	**3.121492**	**-3.334098**	**2.814992**
H	**3.405426**	**-2.533626**	**4.374917**
H	**4.268415**	**-4.027446**	**3.971037**

Table S5. Optimized structure of $^{H}1^{N3\text{-}TolCF3}$ in the closed shell singlet

C	**-0.076334**	**-3.233361**	**0.345130**
C	**0.266643**	**-3.963381**	**-0.799602**
C	**1.204049**	**-5.002855**	**-0.776097**
C	**1.823923**	**-5.312715**	**0.439986**
C	**1.498596**	**-4.584829**	**1.592776**
C	**0.555121**	**-3.547160**	**1.552454**
S	**-0.548322**	**-3.568893**	**-2.348805**
O	**-0.335868**	**-4.658668**	**-3.312280**
C	**2.198487**	**-4.889554**	**2.900469**
N	**0.399454**	**-2.153176**	**-2.884934**
N	**1.128801**	**-2.403638**	**-3.873686**
N	**1.815089**	**-2.539547**	**-4.779482**
O	**-1.872910**	**-3.008987**	**-2.067129**
C	**-3.577886**	**-0.256644**	**-0.662022**
C	**-4.971721**	**-0.152669**	**-0.824988**
C	**-5.704092**	**0.650740**	**0.062911**
C	**-5.067731**	**1.357329**	**1.100730**
C	**-3.676603**	**1.256229**	**1.237622**

C	**-2.922275**	**0.448863**	**0.362641**
C	**-5.671392**	**-0.894118**	**-1.930827**
C	**-6.139938**	**-2.213318**	**-1.709796**
C	**-6.803442**	**-2.880630**	**-2.753146**
C	**-7.001268**	**-2.266020**	**-3.992358**
C	**-6.531623**	**-0.966761**	**-4.202965**
C	**-5.864413**	**-0.263760**	**-3.185806**
N	**-1.496900**	**0.410477**	**0.446036**
C	**-0.840985**	**0.083874**	**1.634559**
C	**-1.467476**	**-0.448621**	**2.783531**
C	**-0.724448**	**-0.741278**	**3.930161**
C	**0.662142**	**-0.501450**	**3.952379**
C	**1.306305**	**0.000209**	**2.819000**
C	**0.580404**	**0.278380**	**1.639386**
C	**-5.860878**	**2.223029**	**2.040630**
C	**-6.060900**	**3.593493**	**1.738048**
C	**-6.794065**	**4.386671**	**2.636878**
C	**-7.323181**	**3.844554**	**3.811230**
C	**-7.123971**	**2.491705**	**4.099935**
C	**-6.397276**	**1.663724**	**3.227835**
C	**-5.498860**	**4.237502**	**0.471434**
C	**-4.438798**	**5.307877**	**0.806783**
N	**1.125692**	**0.779006**	**0.455941**
C	**2.528191**	**0.964400**	**0.291236**
C	**3.006849**	**2.220799**	**-0.124060**
C	**4.373940**	**2.430658**	**-0.373294**
C	**5.269068**	**1.366823**	**-0.178981**
C	**4.816723**	**0.103409**	**0.245737**
C	**3.445142**	**-0.091940**	**0.465555**
C	**4.865049**	**3.780088**	**-0.819676**
C	**4.940477**	**4.079325**	**-2.203459**
C	**5.395768**	**5.348359**	**-2.599127**
C	**5.770992**	**6.306794**	**-1.653751**
C	**5.694196**	**6.002743**	**-0.291936**

C	**5.243999**	**4.745900**	**0.146640**
C	**5.793242**	**-1.020079**	**0.463814**
C	**6.340900**	**-1.230597**	**1.754902**
C	**7.254598**	**-2.281593**	**1.941070**
C	**7.629117**	**-3.109032**	**0.879147**
C	**7.087722**	**-2.891886**	**-0.390684**
C	**6.167577**	**-1.854664**	**-0.619069**
C	**5.976300**	**-0.350248**	**2.949602**
C	**7.210516**	**0.389275**	**3.507108**
C	**5.606996**	**-1.662352**	**-2.027255**
C	**4.842523**	**-2.911987**	**-2.511245**
C	**4.538172**	**3.069861**	**-3.277838**
C	**3.322578**	**3.564023**	**-4.090073**
C	**-5.944563**	**-2.934606**	**-0.377234**
C	**-5.079042**	**-4.201640**	**-0.542322**
C	**-6.198614**	**0.193910**	**3.595528**
C	**-7.542557**	**-0.544005**	**3.765267**
C	**5.178367**	**4.466353**	**1.647495**
C	**6.574218**	**4.543542**	**2.300582**
C	**-5.361644**	**1.150529**	**-3.472194**
C	**-4.274771**	**1.149614**	**-4.567863**
Sn	**-0.259498**	**1.132924**	**-1.101589**
C	**-6.615582**	**4.823218**	**-0.417315**
C	**-5.321487**	**0.045525**	**4.856934**
C	**5.720126**	**2.723206**	**-4.206901**
C	**6.714607**	**-1.271031**	**-3.027931**
C	**-7.294643**	**-3.264826**	**0.292812**
C	**4.181911**	**5.407217**	**2.356731**
C	**5.268644**	**-1.159648**	**4.056528**
C	**-6.516062**	**2.106695**	**-3.836978**
H	**2.306884**	**3.047278**	**-0.230382**
H	**3.081589**	**-1.071168**	**0.767105**
H	**-6.953499**	**5.440528**	**2.417101**
H	**2.375107**	**0.186017**	**2.843967**

H	**-3.005418**	**-0.905699**	**-1.321276**
H	**-2.538597**	**-0.625522**	**2.770673**
H	**-6.782868**	**0.730656**	**-0.054379**
H	**-1.225655**	**-1.144014**	**4.807550**
H	**1.239500**	**-0.706346**	**4.851155**
H	**-3.167899**	**1.817934**	**2.017580**
H	**7.385314**	**-3.537712**	**-1.214563**
H	**-4.998696**	**3.457586**	**-0.110510**
H	**-7.167468**	**-3.894120**	**-2.596414**
H	**5.988020**	**6.753176**	**0.439333**
H	**-5.667294**	**-0.291331**	**2.771187**
H	**-7.888100**	**4.472769**	**4.497493**
H	**6.331526**	**1.522369**	**-0.354454**
H	**4.238803**	**2.144216**	**-2.776853**
H	**8.339882**	**-3.917494**	**1.040044**
H	**4.890937**	**-0.835448**	**-1.996307**
H	**-5.405665**	**-2.260703**	**0.295649**
H	**-7.538895**	**2.075254**	**5.015745**
H	**7.679911**	**-2.454962**	**2.927569**
H	**4.812414**	**3.444748**	**1.786228**
H	**-7.352216**	**4.056434**	**-0.683145**
H	**-6.194123**	**5.227611**	**-1.346002**
H	**-7.149005**	**5.637395**	**0.087508**
H	**5.273095**	**0.413952**	**2.604851**
H	**7.232909**	**-0.360551**	**-2.706176**
H	**6.289335**	**-1.088234**	**-4.022556**
H	**7.465224**	**-2.064399**	**-3.125824**
H	**-7.516392**	**-2.797476**	**-4.790473**
H	**6.121571**	**7.285324**	**-1.976666**
H	**5.503552**	**-3.783206**	**-2.589927**
H	**4.406543**	**-2.737421**	**-3.502565**
H	**4.033160**	**-3.170599**	**-1.817518**
H	**-4.899637**	**1.536641**	**-2.558575**
H	**5.457914**	**5.591144**	**-3.658130**

H	**-4.347417**	**0.529882**	**4.721225**
H	**-5.149555**	**-1.014069**	**5.084725**
H	**-5.799694**	**0.501671**	**5.732062**
H	**-4.872328**	**6.135731**	**1.380578**
H	**-4.009876**	**5.727021**	**-0.112026**
H	**-3.622479**	**4.882832**	**1.402187**
H	**-7.892127**	**-2.358885**	**0.448073**
H	**-7.133522**	**-3.738972**	**1.269105**
H	**-7.888561**	**-3.954973**	**-0.318314**
H	**-6.685366**	**-0.494401**	**-5.171308**
H	**4.493492**	**6.455757**	**2.279541**
H	**4.110174**	**5.157962**	**3.422593**
H	**3.180050**	**5.324271**	**1.920036**
H	**-5.573776**	**-4.944772**	**-1.179390**
H	**-4.896781**	**-4.669874**	**0.433399**
H	**-4.112254**	**-3.961008**	**-0.997477**
H	**-8.125038**	**-0.137970**	**4.600759**
H	**-7.372053**	**-1.608918**	**3.966119**
H	**-8.155558**	**-0.462117**	**2.860418**
H	**6.062835**	**3.600594**	**-4.768056**
H	**5.424797**	**1.957423**	**-4.934903**
H	**6.572838**	**2.339294**	**-3.635347**
H	**4.371596**	**-1.658624**	**3.673488**
H	**4.970968**	**-0.500787**	**4.881946**
H	**5.925491**	**-1.934165**	**4.470020**
H	**2.468485**	**3.774452**	**-3.435778**
H	**3.014298**	**2.807293**	**-4.822242**
H	**3.554112**	**4.484297**	**-4.639485**
H	**7.958117**	**-0.311480**	**3.897380**
H	**6.919396**	**1.056532**	**4.327825**
H	**7.693404**	**0.994246**	**2.731066**
H	**7.274118**	**3.849641**	**1.820884**
H	**6.514666**	**4.286356**	**3.365369**
H	**6.999486**	**5.551373**	**2.224492**

H	-7.016697	1.800172	-4.763090
H	-6.138752	3.126345	-3.984544
H	-7.271719	2.134311	-3.043491
H	-3.438065	0.497274	-4.292216
H	-3.883597	2.162816	-4.724489
H	-4.671493	0.793145	-5.525995
H	1.428099	-5.563935	-1.678691
H	2.547675	-6.120744	0.490008
H	0.304543	-2.986708	2.449294
H	-0.821998	-2.445016	0.303627
F	3.218196	-4.025145	3.127043
F	1.357981	-4.791178	3.953689
F	2.724679	-6.134294	2.916232

Table S6. Optimized structure of TS in the closed shell singlet

C	-0.468565	5.132837	0.061247
C	-1.180724	3.979844	0.407989
C	-2.580262	3.962792	0.444765
C	-3.282362	5.127131	0.118215
C	-2.578715	6.286895	-0.238728
C	-1.177288	6.295580	-0.263385
S	-0.265245	2.477655	0.834165
O	1.095325	2.910000	1.229768
C	-3.344845	7.552954	-0.543364
N	-0.233846	1.610650	-0.609869
N	0.624215	2.395245	-1.791467
N	1.129293	1.693700	-2.573337
Sn	0.248107	-0.506653	-1.100990
N	1.662166	-0.963113	0.497282
C	1.167762	-1.758332	1.481934
C	1.943046	-2.331199	2.534810
C	1.337568	-3.085671	3.521468
C	-0.066940	-3.323981	3.499211

C	**-0.853870**	**-2.799456**	**2.492657**
C	**-0.274584**	**-1.994482**	**1.465233**
N	**-0.971740**	**-1.387200**	**0.473299**
C	**-2.380994**	**-1.573838**	**0.319543**
C	**-2.938777**	**-2.828928**	**0.018807**
C	**-4.322442**	**-2.956232**	**-0.182831**
C	**-5.133985**	**-1.811006**	**-0.079483**
C	**-4.588561**	**-0.550262**	**0.216517**
C	**-3.202770**	**-0.440638**	**0.411660**
C	**-4.922200**	**-4.296333**	**-0.507639**
C	**-4.963591**	**-4.742216**	**-1.852897**
C	**-5.519865**	**-6.002009**	**-2.131829**
C	**-6.029288**	**-6.807957**	**-1.110109**
C	**-5.987322**	**-6.358547**	**0.212461**
C	**-5.437853**	**-5.106385**	**0.535543**
C	**-5.451018**	**0.675635**	**0.329682**
C	**-5.813177**	**1.162046**	**1.612388**
C	**-6.585283**	**2.333236**	**1.697736**
C	**-7.001328**	**3.009801**	**0.547346**
C	**-6.644133**	**2.519389**	**-0.711857**
C	**-5.866851**	**1.355833**	**-0.843433**
C	**-5.394741**	**0.457856**	**2.903063**
C	**-6.616468**	**0.056768**	**3.755894**
C	**-5.484774**	**0.879273**	**-2.244328**
C	**-4.616967**	**1.921407**	**-2.980668**
C	**-4.419955**	**-3.901684**	**-3.007635**
C	**-3.203311**	**-4.579667**	**-3.672659**
C	**-5.408073**	**-4.667596**	**1.999054**
C	**-6.828524**	**-4.558841**	**2.591630**
C	**3.064175**	**-0.734612**	**0.338171**
C	**3.524877**	**0.592758**	**0.308064**
C	**4.890084**	**0.860244**	**0.105027**
C	**5.773998**	**-0.217530**	**-0.076911**
C	**5.325433**	**-1.550619**	**-0.064238**

C	**3.961630**	**-1.801187**	**0.144063**
C	**5.400628**	**2.274118**	**0.092742**
C	**5.552453**	**2.977529**	**1.315248**
C	**6.042044**	**4.294035**	**1.281144**
C	**6.380833**	**4.908282**	**0.072963**
C	**6.226993**	**4.207578**	**-1.126033**
C	**5.734981**	**2.891683**	**-1.140084**
C	**6.284356**	**-2.689987**	**-0.271553**
C	**6.441697**	**-3.252311**	**-1.563683**
C	**7.332404**	**-4.326048**	**-1.730895**
C	**8.059892**	**-4.834856**	**-0.651561**
C	**7.902578**	**-4.270417**	**0.617114**
C	**7.019489**	**-3.198282**	**0.829214**
C	**5.670731**	**-2.734042**	**-2.777181**
C	**4.664335**	**-3.785025**	**-3.292258**
C	**5.219134**	**2.355166**	**2.670999**
C	**4.067007**	**3.105938**	**3.372060**
C	**6.876136**	**-2.626527**	**2.239190**
C	**8.208632**	**-2.047677**	**2.758869**
C	**5.575559**	**2.182720**	**-2.485146**
C	**4.636827**	**2.953791**	**-3.435717**
C	**6.614797**	**-2.273218**	**-3.906735**
C	**6.307680**	**-3.674585**	**3.219105**
C	**-5.512765**	**-3.581977**	**-4.048650**
C	**-6.729534**	**0.505549**	**-3.076237**
C	**6.465925**	**2.273671**	**3.576935**
C	**-4.522340**	**-5.601044**	**2.851117**
C	**-4.403087**	**1.314741**	**3.719135**
C	**6.945359**	**1.927099**	**-3.149573**
O	**-1.083525**	**1.692692**	**1.790218**
H	**-2.292713**	**-3.699196**	**-0.075487**
H	**-2.746114**	**0.508945**	**0.672749**
H	**7.461549**	**-4.768430**	**-2.716628**
H	**-1.926668**	**-2.959117**	**2.492205**

H	**2.825755**	**1.408404**	**0.481019**
H	**3.008517**	**-2.132899**	**2.571810**
H	**6.831736**	**-0.016148**	**-0.233791**
H	**1.938231**	**-3.489486**	**4.333266**
H	**-0.525597**	**-3.909830**	**4.292388**
H	**3.590728**	**-2.823684**	**0.136979**
H	**-6.970391**	**3.050983**	**-1.603498**
H	**5.093616**	**-1.858838**	**-2.463833**
H	**6.162301**	**4.844891**	**2.211758**
H	**-6.385988**	**-6.990829**	**1.003355**
H	**6.161119**	**-1.799392**	**2.198908**
H	**8.746855**	**-5.666168**	**-0.798699**
H	**-6.206949**	**-1.906007**	**-0.234205**
H	**-4.075377**	**-2.946730**	**-2.599245**
H	**-7.604026**	**3.912339**	**0.631772**
H	**-4.880700**	**-0.026994**	**-2.141428**
H	**4.879628**	**1.329205**	**2.501307**
H	**8.472772**	**-4.670506**	**1.453200**
H	**-6.868536**	**2.718918**	**2.674848**
H	**-4.963753**	**-3.668656**	**2.044409**
H	**7.310860**	**-1.504828**	**-3.551735**
H	**6.036799**	**-1.851897**	**-4.738435**
H	**7.208700**	**-3.104835**	**-4.303918**
H	**-4.875908**	**-0.466510**	**2.631754**
H	**-7.331407**	**-0.257620**	**-2.569228**
H	**-6.432232**	**0.111212**	**-4.055753**
H	**-7.373837**	**1.375632**	**-3.249415**
H	**6.761048**	**5.928200**	**0.065507**
H	**-6.457420**	**-7.781006**	**-1.343497**
H	**-5.163212**	**2.858036**	**-3.143822**
H	**-4.311071**	**1.540206**	**-3.962817**
H	**-3.711430**	**2.158182**	**-2.410327**
H	**5.115036**	**1.206967**	**-2.304216**
H	**-5.557052**	**-6.357361**	**-3.159679**

H	**5.343116**	**-4.061734**	**2.869404**
H	**6.161385**	**-3.232546**	**4.212590**
H	**6.985434**	**-4.529100**	**3.331632**
H	**5.175341**	**-4.691637**	**-3.637994**
H	**4.085395**	**-3.384755**	**-4.133715**
H	**3.961659**	**-4.080561**	**-2.504362**
H	**7.272940**	**1.709849**	**3.093857**
H	**6.218695**	**1.775779**	**4.522881**
H	**6.854628**	**3.269953**	**3.818952**
H	**6.487566**	**4.692777**	**-2.064455**
H	**-4.918750**	**-6.623110**	**2.870947**
H	**-4.472027**	**-5.243526**	**3.887228**
H	**-3.501289**	**-5.649922**	**2.454490**
H	**4.345846**	**4.143040**	**3.595556**
H	**3.816865**	**2.617534**	**4.322328**
H	**3.165572**	**3.124597**	**2.750817**
H	**8.975518**	**-2.825327**	**2.855755**
H	**8.069696**	**-1.591191**	**3.746604**
H	**8.597260**	**-1.279704**	**2.080400**
H	**-5.893416**	**-4.491540**	**-4.528056**
H	**-5.111470**	**-2.934168**	**-4.837780**
H	**-6.362895**	**-3.068403**	**-3.585183**
H	**-3.492975**	**1.530851**	**3.148793**
H	**-4.107158**	**0.788061**	**4.634869**
H	**-4.853168**	**2.270187**	**4.015333**
H	**-2.407981**	**-4.770610**	**-2.942777**
H	**-2.792982**	**-3.943028**	**-4.466237**
H	**-3.477529**	**-5.540889**	**-4.123463**
H	**-7.171295**	**0.933965**	**4.109048**
H	**-6.294057**	**-0.506890**	**4.640020**
H	**-7.311682**	**-0.570204**	**3.185323**
H	**-7.449588**	**-3.871146**	**2.006347**
H	**-6.787004**	**-4.187232**	**3.622908**
H	**-7.334058**	**-5.531651**	**2.608347**

H	7.458229	2.868539	-3.380302
H	6.820984	1.374490	-4.089165
H	7.603105	1.343740	-2.494563
H	3.649956	3.102172	-2.984806
H	4.499180	2.395818	-4.370108
H	5.042857	3.939000	-3.694012
H	-3.116925	3.063799	0.733047
H	-4.368696	5.123090	0.136041
H	-0.641950	7.199622	-0.539471
H	0.617219	5.118189	0.057124
F	-3.637161	8.246565	0.586695
F	-2.649118	8.390484	-1.345907
F	-4.524652	7.296114	-1.155950

Table S7. Optimized structure of $^{H}2^{N3\text{-}TolCF3}$ in the closed-shell singlet

C	-1.593434	4.417769	0.400489
C	-0.718424	3.708888	-0.428715
C	-0.369157	4.199844	-1.694323
C	-0.901850	5.415410	-2.132140
C	-1.780642	6.131838	-1.303356
C	-2.125656	5.637378	-0.039165
S	0.016357	2.159103	0.179073
O	1.428434	2.512144	0.536000
C	-2.315191	7.463823	-1.764684
N	-0.103869	1.180789	-1.068225
Sn	0.184880	-0.777440	-1.306941
N	1.595226	-0.934916	0.677385
C	1.011810	-0.896716	1.846011
C	1.704570	-0.759605	3.118028
C	1.005905	-0.748658	4.285096
C	-0.441009	-0.881180	4.306414
C	-1.156465	-1.031336	3.160343
C	-0.486069	-1.062088	1.868938

N	**-1.077085**	**-1.288675**	**0.727674**
C	**-2.487955**	**-1.363649**	**0.588910**
C	**-3.034199**	**-2.508352**	**-0.018243**
C	**-4.418809**	**-2.603921**	**-0.222302**
C	**-5.233133**	**-1.521062**	**0.155930**
C	**-4.693873**	**-0.352943**	**0.724397**
C	**-3.309224**	**-0.276694**	**0.943696**
C	**-5.015504**	**-3.837660**	**-0.840111**
C	**-5.048720**	**-3.972262**	**-2.251302**
C	**-5.607140**	**-5.136194**	**-2.806339**
C	**-6.126332**	**-6.146722**	**-1.992789**
C	**-6.091488**	**-6.003532**	**-0.603079**
C	**-5.538949**	**-4.857960**	**-0.006177**
C	**-5.585913**	**0.801580**	**1.088400**
C	**-6.015382**	**0.963027**	**2.429949**
C	**-6.843055**	**2.052032**	**2.750041**
C	**-7.246640**	**2.962587**	**1.769719**
C	**-6.821797**	**2.792374**	**0.449562**
C	**-5.988992**	**1.720420**	**0.086660**
C	**-5.604182**	**-0.002979**	**3.540718**
C	**-6.824828**	**-0.629481**	**4.245688**
C	**-5.553020**	**1.584882**	**-1.371636**
C	**-4.790639**	**2.831607**	**-1.864423**
C	**-4.500219**	**-2.896736**	**-3.188364**
C	**-3.285950**	**-3.412859**	**-3.989169**
C	**-5.520370**	**-4.754975**	**1.518450**
C	**-6.949246**	**-4.710834**	**2.099738**
C	**2.996546**	**-0.782831**	**0.493648**
C	**3.678705**	**0.374498**	**0.911323**
C	**5.054082**	**0.497791**	**0.659033**
C	**5.725138**	**-0.541833**	**-0.009261**
C	**5.048283**	**-1.691995**	**-0.453318**
C	**3.670513**	**-1.796881**	**-0.211703**
C	**5.794180**	**1.731520**	**1.096762**

C	**6.392622**	**1.770937**	**2.381122**
C	**7.069313**	**2.936160**	**2.777842**
C	**7.155990**	**4.041943**	**1.927529**
C	**6.562899**	**3.992336**	**0.663484**
C	**5.876759**	**2.846651**	**0.226182**
C	**5.779304**	**-2.785896**	**-1.180928**
C	**5.880023**	**-2.743649**	**-2.594552**
C	**6.563187**	**-3.778945**	**-3.254913**
C	**7.137179**	**-4.834734**	**-2.541765**
C	**7.034407**	**-4.866297**	**-1.148352**
C	**6.360120**	**-3.851719**	**-0.448390**
C	**5.272272**	**-1.612443**	**-3.422840**
C	**4.171423**	**-2.132855**	**-4.370863**
C	**6.306436**	**0.597086**	**3.356091**
C	**5.436894**	**0.953833**	**4.580931**
C	**6.274910**	**-3.935128**	**1.075071**
C	**7.673098**	**-3.900433**	**1.726629**
C	**5.244638**	**2.849035**	**-1.164757**
C	**4.116129**	**3.896437**	**-1.271379**
C	**6.353205**	**-0.835753**	**-4.203332**
C	**5.481804**	**-5.178265**	**1.530232**
C	**-5.591479**	**-2.349100**	**-4.131473**
C	**-6.757303**	**1.273257**	**-2.285834**
C	**7.699638**	**0.099607**	**3.792530**
C	**-4.697214**	**-5.893353**	**2.156683**
C	**-4.667602**	**0.682796**	**4.558545**
C	**6.306560**	**3.051999**	**-2.266177**
O	**-0.812667**	**1.768489**	**1.375170**
H	**-2.380289**	**-3.328799**	**-0.305058**
H	**-2.843577**	**0.626709**	**1.331532**
H	**6.648196**	**-3.759669**	**-4.339560**
H	**-2.232892**	**-1.155320**	**3.184305**
H	**3.116829**	**1.193859**	**1.352022**
H	**2.785608**	**-0.680966**	**3.111600**

H	**6.791676**	**-0.446296**	**-0.202688**
H	**1.535693**	**-0.655494**	**5.230723**
H	**-0.951329**	**-0.878594**	**5.267072**
H	**3.123429**	**-2.675929**	**-0.545094**
H	**-7.137359**	**3.506379**	**-0.308281**
H	**4.799452**	**-0.903879**	**-2.736259**
H	**7.531190**	**2.982347**	**3.762143**
H	**-6.497527**	**-6.794173**	**0.024766**
H	**5.730658**	**-3.055653**	**1.432572**
H	**7.662883**	**-5.628551**	**-3.069136**
H	**-6.306850**	**-1.583283**	**-0.009270**
H	**-4.152514**	**-2.057961**	**-2.577717**
H	**-7.888455**	**3.801090**	**2.033514**
H	**-4.862661**	**0.739032**	**-1.443284**
H	**5.816694**	**-0.235557**	**2.841120**
H	**7.484778**	**-5.690639**	**-0.598969**
H	**-7.178242**	**2.189943**	**3.776076**
H	**-5.032410**	**-3.813651**	**1.788864**
H	**7.118461**	**-0.435912**	**-3.528295**
H	**5.904148**	**0.005704**	**-4.744885**
H	**6.857055**	**-1.474787**	**-4.938245**
H	**-5.044215**	**-0.824884**	**3.083022**
H	**-7.278543**	**0.364296**	**-1.962754**
H	**-6.426211**	**1.127736**	**-3.321449**
H	**-7.485240**	**2.093375**	**-2.279806**
H	**7.681036**	**4.939193**	**2.249986**
H	**-6.556664**	**-7.041056**	**-2.439534**
H	**-5.426240**	**3.725014**	**-1.856385**
H	**-4.442540**	**2.681903**	**-2.893621**
H	**-3.915626**	**3.035881**	**-1.238526**
H	**4.788016**	**1.868708**	**-1.332680**
H	**-5.639138**	**-5.253393**	**-3.887646**
H	**4.473768**	**-5.184354**	**1.099502**
H	**5.386948**	**-5.195907**	**2.623125**

H	**5.979166**	**-6.106241**	**1.224115**
H	**4.575696**	**-2.836266**	**-5.108567**
H	**3.712615**	**-1.301079**	**-4.919336**
H	**3.381417**	**-2.651373**	**-3.815114**
H	**8.309196**	**-0.179307**	**2.925369**
H	**7.607585**	**-0.779739**	**4.442336**
H	**8.247411**	**0.867661**	**4.350835**
H	**6.630668**	**4.858272**	**0.008318**
H	**-5.140867**	**-6.875111**	**1.953340**
H	**-4.650383**	**-5.769332**	**3.245761**
H	**-3.671710**	**-5.905533**	**1.769620**
H	**5.881481**	**1.772217**	**5.159453**
H	**5.335418**	**0.089161**	**5.249778**
H	**4.435080**	**1.277198**	**4.273947**
H	**8.275129**	**-4.769252**	**1.435383**
H	**7.587747**	**-3.906132**	**2.820380**
H	**8.224183**	**-2.999879**	**1.432391**
H	**-5.972994**	**-3.127094**	**-4.803239**
H	**-5.187631**	**-1.541338**	**-4.754039**
H	**-6.440798**	**-1.950345**	**-3.565287**
H	**-3.775606**	**1.088667**	**4.067553**
H	**-4.346344**	**-0.029438**	**5.330008**
H	**-5.172323**	**1.514196**	**5.064714**
H	**-2.489606**	**-3.762957**	**-3.322091**
H	**-2.875049**	**-2.615887**	**-4.620973**
H	**-3.563118**	**-4.248474**	**-4.642905**
H	**-7.425692**	**0.126242**	**4.764782**
H	**-6.500258**	**-1.363983**	**4.993423**
H	**-7.477920**	**-1.138886**	**3.527839**
H	**-7.522955**	**-3.878339**	**1.676494**
H	**-6.918407**	**-4.585193**	**3.189178**
H	**-7.498118**	**-5.635568**	**1.885667**
H	**6.784572**	**4.035873**	**-2.189185**
H	**5.843357**	**2.986277**	**-3.258441**

H	**7.095726**	**2.292797**	**-2.206566**
H	**3.316010**	**3.691000**	**-0.553048**
H	**3.679630**	**3.877817**	**-2.278400**
H	**4.495406**	**4.910150**	**-1.092794**
H	**0.296482**	**3.622163**	**-2.329567**
H	**-0.646007**	**5.800546**	**-3.115861**
H	**-2.813127**	**6.191740**	**0.593976**
H	**-1.854461**	**4.008553**	**1.372032**
F	**-3.492259**	**7.779295**	**-1.172828**
F	**-1.457918**	**8.481639**	**-1.485789**
F	**-2.521961**	**7.495469**	**-3.104422**

Table S8. Optimized structure of $^{H}2^{N3\text{-}TolCF3}$ in the open-shell singlet

C	**-0.293093**	**4.571986**	**0.617057**
C	**0.326515**	**3.885176**	**-0.433766**
C	**0.475808**	**4.465055**	**-1.699172**
C	**-0.015806**	**5.756690**	**-1.919143**
C	**-0.647008**	**6.448597**	**-0.875824**
C	**-0.781388**	**5.863586**	**0.391469**
S	**0.940650**	**2.205738**	**-0.152749**
O	**2.028029**	**1.982829**	**-1.145865**
C	**-1.132569**	**7.861156**	**-1.101946**
N	**-0.319801**	**1.219484**	**-0.465484**
Sn	**-0.000564**	**-0.818668**	**-1.163325**
N	**1.364069**	**-1.486977**	**0.453995**
C	**0.772585**	**-2.088287**	**1.514091**
C	**1.478300**	**-2.709752**	**2.590535**
C	**0.796504**	**-3.344152**	**3.610341**
C	**-0.626902**	**-3.406891**	**3.601387**
C	**-1.350967**	**-2.831139**	**2.574603**
C	**-0.691411**	**-2.147573**	**1.507894**
N	**-1.320475**	**-1.590796**	**0.442135**
C	**-2.728079**	**-1.442757**	**0.357179**

C	**-3.389291**	**-1.854897**	**-0.815014**
C	**-4.770536**	**-1.656585**	**-0.969728**
C	**-5.487040**	**-1.037395**	**0.067974**
C	**-4.845187**	**-0.610712**	**1.245164**
C	**-3.464299**	**-0.812777**	**1.380467**
C	**-5.466614**	**-2.105381**	**-2.224573**
C	**-5.621949**	**-1.198660**	**-3.303347**
C	**-6.274322**	**-1.638074**	**-4.467712**
C	**-6.762736**	**-2.943247**	**-4.572188**
C	**-6.604056**	**-3.829846**	**-3.503613**
C	**-5.959899**	**-3.431037**	**-2.320262**
C	**-5.622857**	**0.064720**	**2.340767**
C	**-6.276101**	**-0.719211**	**3.324965**
C	**-6.993654**	**-0.068711**	**4.342765**
C	**-7.068870**	**1.325923**	**4.393137**
C	**-6.422138**	**2.089951**	**3.418099**
C	**-5.694054**	**1.479891**	**2.382576**
C	**-6.212824**	**-2.246073**	**3.324348**
C	**-7.615333**	**-2.878975**	**3.213167**
C	**-5.003934**	**2.362150**	**1.343392**
C	**-3.899406**	**3.228374**	**1.984298**
C	**-5.105621**	**0.238229**	**-3.241520**
C	**-4.045900**	**0.510436**	**-4.329486**
C	**-5.813732**	**-4.439460**	**-1.181371**
C	**-7.186196**	**-4.919476**	**-0.665128**
C	**2.769266**	**-1.286204**	**0.359594**
C	**3.469985**	**-0.564100**	**1.343477**
C	**4.842903**	**-0.318511**	**1.197486**
C	**5.501587**	**-0.783403**	**0.044839**
C	**4.813860**	**-1.486043**	**-0.958256**
C	**3.444323**	**-1.740151**	**-0.786825**
C	**5.599113**	**0.441345**	**2.251938**
C	**6.118279**	**-0.249324**	**3.376063**
C	**6.828231**	**0.474397**	**4.348703**

C	**7.030520**	**1.850741**	**4.215797**
C	**6.517530**	**2.521773**	**3.102553**
C	**5.794745**	**1.838403**	**2.109791**
C	**5.521508**	**-1.948015**	**-2.200827**
C	**5.457723**	**-1.153756**	**-3.374233**
C	**6.119286**	**-1.602865**	**-4.529847**
C	**6.832757**	**-2.804634**	**-4.532977**
C	**6.891948**	**-3.578326**	**-3.370571**
C	**6.241501**	**-3.169056**	**-2.194226**
C	**4.696551**	**0.170877**	**-3.422819**
C	**3.497960**	**0.096695**	**-4.391924**
C	**5.931337**	**-1.754379**	**3.566343**
C	**5.047879**	**-2.060946**	**4.794393**
C	**6.330244**	**-4.055169**	**-0.952494**
C	**7.782192**	**-4.171192**	**-0.442871**
C	**5.265147**	**2.618274**	**0.907198**
C	**4.382625**	**3.809802**	**1.329342**
C	**5.623620**	**1.349868**	**-3.783628**
C	**5.717564**	**-5.449205**	**-1.201457**
C	**-6.260764**	**1.257909**	**-3.326776**
C	**-6.016010**	**3.235721**	**0.573452**
C	**7.281414**	**-2.495209**	**3.657780**
C	**-4.928560**	**-5.634328**	**-1.594240**
C	**-5.461667**	**-2.777876**	**4.563415**
C	**6.425270**	**3.082578**	**0.000294**
O	**1.241019**	**2.098283**	**1.298747**
H	**-2.827123**	**-2.354009**	**-1.601961**
H	**-2.949914**	**-0.453967**	**2.268253**
H	**6.078867**	**-1.004399**	**-5.437784**
H	**-2.432563**	**-2.910014**	**2.557585**
H	**2.931856**	**-0.158306**	**2.195664**
H	**2.562430**	**-2.690021**	**2.584915**
H	**6.563974**	**-0.583441**	**-0.078002**
H	**1.351778**	**-3.816241**	**4.417582**

H	**-1.148103**	**-3.929269**	**4.400452**
H	**2.903267**	**-2.303543**	**-1.544596**
H	**-6.484932**	**3.175372**	**3.462864**
H	**4.290699**	**0.375921**	**-2.428632**
H	**7.230329**	**-0.042757**	**5.217789**
H	**-6.987188**	**-4.844592**	**-3.591359**
H	**5.745037**	**-3.583100**	**-0.157597**
H	**7.340816**	**-3.136361**	**-5.436680**
H	**-6.557594**	**-0.878793**	**-0.043235**
H	**-4.617839**	**0.383403**	**-2.273031**
H	**-7.628425**	**1.814723**	**5.188501**
H	**-4.516676**	**1.710938**	**0.611849**
H	**5.411635**	**-2.144472**	**2.685674**
H	**7.449072**	**-4.513164**	**-3.379642**
H	**-7.498478**	**-0.657814**	**5.105899**
H	**-5.312476**	**-3.938829**	**-0.347416**
H	**6.459848**	**1.425164**	**-3.079275**
H	**5.065770**	**2.293469**	**-3.750301**
H	**6.042920**	**1.243900**	**-4.791504**
H	**-5.647077**	**-2.561433**	**2.442311**
H	**-6.781623**	**2.620009**	**0.087347**
H	**-5.504684**	**3.819519**	**-0.201693**
H	**-6.528263**	**3.941961**	**1.237623**
H	**7.585069**	**2.397627**	**4.976246**
H	**-7.264798**	**-3.267804**	**-5.481716**
H	**-4.314959**	**3.927855**	**2.719862**
H	**-3.380828**	**3.814226**	**1.215911**
H	**-3.156450**	**2.605895**	**2.496089**
H	**4.632367**	**1.952388**	**0.313985**
H	**-6.401235**	**-0.952677**	**-5.303323**
H	**4.675089**	**-5.369894**	**-1.530807**
H	**5.740742**	**-6.048526**	**-0.282774**
H	**6.269086**	**-6.000720**	**-1.972115**
H	**3.824449**	**-0.074422**	**-5.425073**

H	**2.930420**	**1.034537**	**-4.365851**
H	**2.817606**	**-0.718922**	**-4.119222**
H	**7.896754**	**-2.305117**	**2.770958**
H	**7.120836**	**-3.577821**	**3.736418**
H	**7.856830**	**-2.180666**	**4.536375**
H	**6.678242**	**3.593417**	**3.005892**
H	**-5.377754**	**-6.200644**	**-2.418749**
H	**-4.793129**	**-6.322910**	**-0.751016**
H	**-3.938104**	**-5.298661**	**-1.922600**
H	**5.516792**	**-1.709303**	**5.721077**
H	**4.884582**	**-3.141942**	**4.893160**
H	**4.071046**	**-1.570057**	**4.712309**
H	**8.429354**	**-4.657589**	**-1.182498**
H	**7.821120**	**-4.766031**	**0.478195**
H	**8.206031**	**-3.183257**	**-0.229065**
H	**-6.787053**	**1.189680**	**-4.286364**
H	**-5.877965**	**2.281007**	**-3.227277**
H	**-6.995967**	**1.090238**	**-2.531261**
H	**-4.451179**	**-2.356445**	**4.624700**
H	**-5.377403**	**-3.871224**	**4.523810**
H	**-5.984477**	**-2.517273**	**5.491305**
H	**-3.209004**	**-0.193605**	**-4.252898**
H	**-3.646567**	**1.527029**	**-4.229054**
H	**-4.468290**	**0.416046**	**-5.336964**
H	**-8.238669**	**-2.634521**	**4.081323**
H	**-7.540118**	**-3.971886**	**3.154898**
H	**-8.138785**	**-2.525049**	**2.317609**
H	**-7.803071**	**-4.074838**	**-0.337397**
H	**-7.059360**	**-5.600174**	**0.185872**
H	**-7.743362**	**-5.457786**	**-1.440943**
H	**7.090611**	**3.777214**	**0.527839**
H	**6.035525**	**3.596459**	**-0.886874**
H	**7.031086**	**2.233199**	**-0.336881**
H	**3.532841**	**3.473332**	**1.932032**

H	3.985791	4.314086	0.439941
H	4.946499	4.551417	1.907960
H	0.981030	3.918059	-2.489894
H	0.088363	6.220407	-2.896245
H	-1.267040	6.409685	1.195543
H	-0.376217	4.106525	1.594947
F	-2.196555	8.162991	-0.322059
F	-0.169576	8.774847	-0.818868
F	-1.502502	8.071162	-2.386692

Table S9. Optimized structure of $^{H}2^{TolCF3\text{-}N\bullet}$ in the triplet state

C	-0.316243	4.556127	0.478780
C	0.314215	3.857900	-0.557796
C	0.471793	4.421047	-1.829798
C	-0.022372	5.707919	-2.070831
C	-0.663822	6.411534	-1.041700
C	-0.806564	5.843053	0.232164
S	0.935723	2.186514	-0.248666
O	2.028874	1.956252	-1.232800
C	-1.151981	7.819497	-1.290572
N	-0.321604	1.191712	-0.564212
Sn	0.008808	-0.894604	-1.144888
N	1.370473	-1.435696	0.524055
C	0.773695	-1.926258	1.638436
C	1.474675	-2.442360	2.771721
C	0.789404	-2.974605	3.846496
C	-0.633504	-3.031698	3.841281
C	-1.353214	-2.553102	2.762517
C	-0.689582	-1.980317	1.635230
N	-1.316254	-1.529717	0.517498
C	-2.724265	-1.395729	0.414917
C	-3.377418	-1.922957	-0.715101
C	-4.760377	-1.756643	-0.890597

C	**-5.487488**	**-1.053460**	**0.084291**
C	**-4.854248**	**-0.511140**	**1.217834**
C	**-3.470943**	**-0.680470**	**1.372546**
C	**-5.447665**	**-2.329090**	**-2.099175**
C	**-5.612395**	**-1.528618**	**-3.257727**
C	**-6.257617**	**-2.082199**	**-4.376473**
C	**-6.730210**	**-3.397240**	**-4.359330**
C	**-6.562256**	**-4.178664**	**-3.212946**
C	**-5.924500**	**-3.663891**	**-2.071609**
C	**-5.645971**	**0.246438**	**2.247883**
C	**-6.266777**	**-0.455907**	**3.311592**
C	**-6.998605**	**0.269510**	**4.266611**
C	**-7.119966**	**1.658994**	**4.178315**
C	**-6.505307**	**2.342222**	**3.125670**
C	**-5.763855**	**1.655493**	**2.149265**
C	**-6.153450**	**-1.972449**	**3.462073**
C	**-7.535336**	**-2.657781**	**3.441038**
C	**-5.105427**	**2.451490**	**1.023636**
C	**-4.017843**	**3.400002**	**1.569921**
C	**-5.114493**	**-0.085721**	**-3.329169**
C	**-4.058545**	**0.099208**	**-4.438883**
C	**-5.768987**	**-4.560340**	**-0.843760**
C	**-7.137661**	**-4.995971**	**-0.280138**
C	**2.775187**	**-1.244030**	**0.414626**
C	**3.482546**	**-0.456959**	**1.342787**
C	**4.856641**	**-0.231471**	**1.178148**
C	**5.510659**	**-0.780238**	**0.060164**
C	**4.816390**	**-1.547198**	**-0.890068**
C	**3.446086**	**-1.781082**	**-0.698364**
C	**5.619904**	**0.595023**	**2.176058**
C	**6.153008**	**-0.023094**	**3.335356**
C	**6.870465**	**0.761562**	**4.253735**
C	**7.066053**	**2.127752**	**4.034055**
C	**6.538330**	**2.727193**	**2.887383**

C	**5.808116**	**1.981271**	**1.946406**
C	**5.518533**	**-2.097811**	**-2.099300**
C	**5.467857**	**-1.378964**	**-3.320982**
C	**6.125672**	**-1.909190**	**-4.443902**
C	**6.822084**	**-3.118620**	**-4.368935**
C	**6.867401**	**-3.818243**	**-3.159931**
C	**6.220744**	**-3.326120**	**-2.013607**
C	**4.723838**	**-0.050610**	**-3.456114**
C	**3.529427**	**-0.170153**	**-4.425914**
C	**5.970237**	**-1.513260**	**3.622077**
C	**5.096141**	**-1.741241**	**4.873779**
C	**6.293412**	**-4.133790**	**-0.718464**
C	**7.742885**	**-4.245005**	**-0.200843**
C	**5.261106**	**2.684076**	**0.704879**
C	**4.367251**	**3.887220**	**1.066073**
C	**5.667872**	**1.092083**	**-3.883619**
C	**5.654654**	**-5.528917**	**-0.880802**
C	**-6.282946**	**0.906649**	**-3.506175**
C	**-6.144301**	**3.224341**	**0.184944**
C	**7.321807**	**-2.245644**	**3.750741**
C	**-4.879230**	**-5.784586**	**-1.145552**
C	**-5.365951**	**-2.352716**	**4.734021**
C	**6.408325**	**3.108961**	**-0.236865**
O	**1.225028**	**2.095946**	**1.205857**
H	**-2.807154**	**-2.487152**	**-1.450569**
H	**-2.963507**	**-0.234309**	**2.223949**
H	**6.095528**	**-1.368910**	**-5.388024**
H	**-2.434916**	**-2.629849**	**2.751453**
H	**2.948216**	**0.013259**	**2.163419**
H	**2.558821**	**-2.429637**	**2.766161**
H	**6.574019**	**-0.595911**	**-0.077952**
H	**1.342259**	**-3.370880**	**4.695121**
H	**-1.158621**	**-3.473524**	**4.685138**
H	**2.900977**	**-2.394372**	**-1.413302**

H	**-6.603657**	**3.424097**	**3.062749**
H	**4.315832**	**0.220150**	**-2.478589**
H	**7.283328**	**0.300448**	**5.148929**
H	**-6.932916**	**-5.201788**	**-3.206007**
H	**5.717179**	**-3.602014**	**0.044676**
H	**7.327357**	**-3.513860**	**-5.248325**
H	**-6.559883**	**-0.920691**	**-0.042063**
H	**-4.628675**	**0.153945**	**-2.378646**
H	**-7.690337**	**2.206470**	**4.926367**
H	**-4.608044**	**1.745504**	**0.352083**
H	**5.444435**	**-1.959211**	**2.772118**
H	**7.410676**	**-4.759811**	**-3.108362**
H	**-7.478622**	**-0.256462**	**5.089498**
H	**-5.267671**	**-3.981264**	**-0.062315**
H	**6.501108**	**1.200578**	**-3.180061**
H	**5.122312**	**2.042999**	**-3.912931**
H	**6.091374**	**0.918022**	**-4.880189**
H	**-5.591327**	**-2.356722**	**2.605407**
H	**-6.899129**	**2.547873**	**-0.232379**
H	**-5.653427**	**3.743216**	**-0.647493**
H	**-6.667521**	**3.978974**	**0.784107**
H	**7.626512**	**2.722280**	**4.753303**
H	**-7.227104**	**-3.810971**	**-5.234870**
H	**-4.445980**	**4.155333**	**2.240157**
H	**-3.517400**	**3.923209**	**0.746435**
H	**-3.257602**	**2.845241**	**2.131857**
H	**4.632009**	**1.978058**	**0.155893**
H	**-6.391524**	**-1.479045**	**-5.272245**
H	**4.613605**	**-5.450693**	**-1.214874**
H	**5.667287**	**-6.070639**	**0.073171**
H	**6.195272**	**-6.137033**	**-1.615814**
H	**3.859274**	**-0.409547**	**-5.444288**
H	**2.973717**	**0.774445**	**-4.462671**
H	**2.837324**	**-0.958709**	**-4.107088**

H	**7.930440**	**-2.112194**	**2.849077**
H	**7.163152**	**-3.321128**	**3.899546**
H	**7.903265**	**-1.875195**	**4.603170**
H	**6.693426**	**3.791449**	**2.723135**
H	**-5.328375**	**-6.428849**	**-1.910759**
H	**-4.737047**	**-6.389514**	**-0.241483**
H	**-3.891729**	**-5.476770**	**-1.508270**
H	**5.572500**	**-1.332515**	**5.772859**
H	**4.932762**	**-2.813681**	**5.041363**
H	**4.119166**	**-1.254977**	**4.768552**
H	**8.380763**	**-4.789668**	**-0.907181**
H	**7.770314**	**-4.780937**	**0.756090**
H	**8.185528**	**-3.253792**	**-0.049422**
H	**-6.808117**	**0.743777**	**-4.454908**
H	**-5.913875**	**1.939596**	**-3.501238**
H	**-7.015930**	**0.802799**	**-2.697836**
H	**-4.368772**	**-1.896561**	**4.733619**
H	**-5.247178**	**-3.441383**	**4.803506**
H	**-5.882514**	**-2.015112**	**5.640355**
H	**-3.212156**	**-0.583358**	**-4.298770**
H	**-3.673087**	**1.126085**	**-4.433281**
H	**-4.479511**	**-0.093349**	**-5.432880**
H	**-8.152820**	**-2.349099**	**4.292762**
H	**-7.423823**	**-3.748068**	**3.489361**
H	**-8.084690**	**-2.411569**	**2.525148**
H	**-7.757139**	**-4.127057**	**-0.029892**
H	**-7.005234**	**-5.594323**	**0.629839**
H	**-7.694877**	**-5.605897**	**-1.000994**
H	**7.069625**	**3.840482**	**0.243809**
H	**6.005490**	**3.566236**	**-1.148833**
H	**7.021393**	**2.248424**	**-0.529769**
H	**3.527790**	**3.575697**	**1.696322**
H	**3.955967**	**4.334510**	**0.153128**
H	**4.926759**	**4.667407**	**1.596192**

H	**0.985505**	**3.865376**	**-2.608894**
H	**0.087852**	**6.158858**	**-3.053222**
H	**-1.300878**	**6.397857**	**1.024893**
H	**-0.406739**	**4.103250**	**1.461872**
F	**-2.222080**	**8.128794**	**-0.522198**
F	**-0.193435**	**8.739598**	**-1.013582**
F	**-1.513673**	**8.010530**	**-2.580564**