Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Redox-switchable bistable nickel corrole

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Contents

1. Materials and methods

General: All reagents and solvents were commercial reagent grade and used without further purification. ESI-HR-MS data were recorded on a Thermo Scientific Q Exactive MS using a positive ion mode. The NMR spectra were measured on a Bruker AVANCE III 400 and HD 500. X-ray diffraction data were collected on a Bruker D8 Venture with GaK\α radiation (λ = 1.34139 Å). MALDI-TOF MS data were measured on a Bruker Daltonics autoflex II spectrometer. The elemental analysis was performed on a Vario Micro Cube elemental analyzer. UV-visible-NIR absorption spectra were measured on a Shimizu UV-3600 spectrophotometer. Cyclic voltammetry measurements were carried out on a CHI650E electrochemical workstation with a standard three-electrode system. Spectroelectrochemistry spectra were measured on Pine spectroelectrochemical intergraded system with honeycomb cell kits and Avaspec ULS2048 UV/vis spectrometer. ESR spectra were obtained using a Bruker EMX-10/12 spectrometer. The VT ESR data were fitted by a modified Bleaney- Bowers equation[1]:

$$IT = \frac{C}{k_B[3 + \exp(-2J / k_B T)]}$$

Where I is the intensity of ESR spectra, C is a constant, k_B is Boltzman's constant, T is the temperature, and $-2J$ is correlated to the excitation energy from the singlet ground state to the triplet excited state.

2. Mass spectra

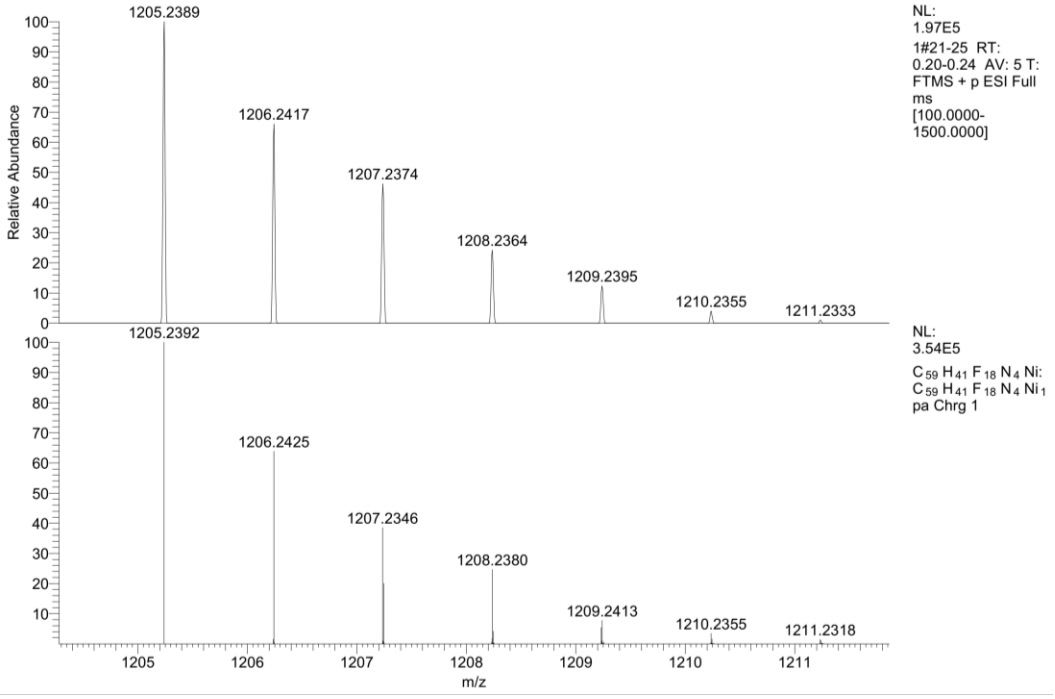

Figure S1. HR-ESI-MS spectrum of **1**.

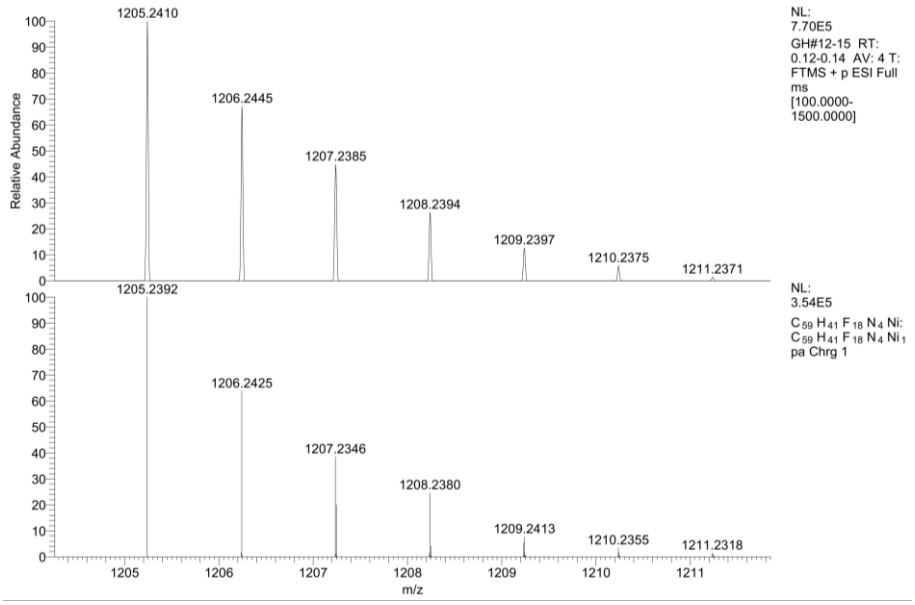

Figure S2. HR-ESI-MS spectrum of $\mathbf{1}^{+}$.

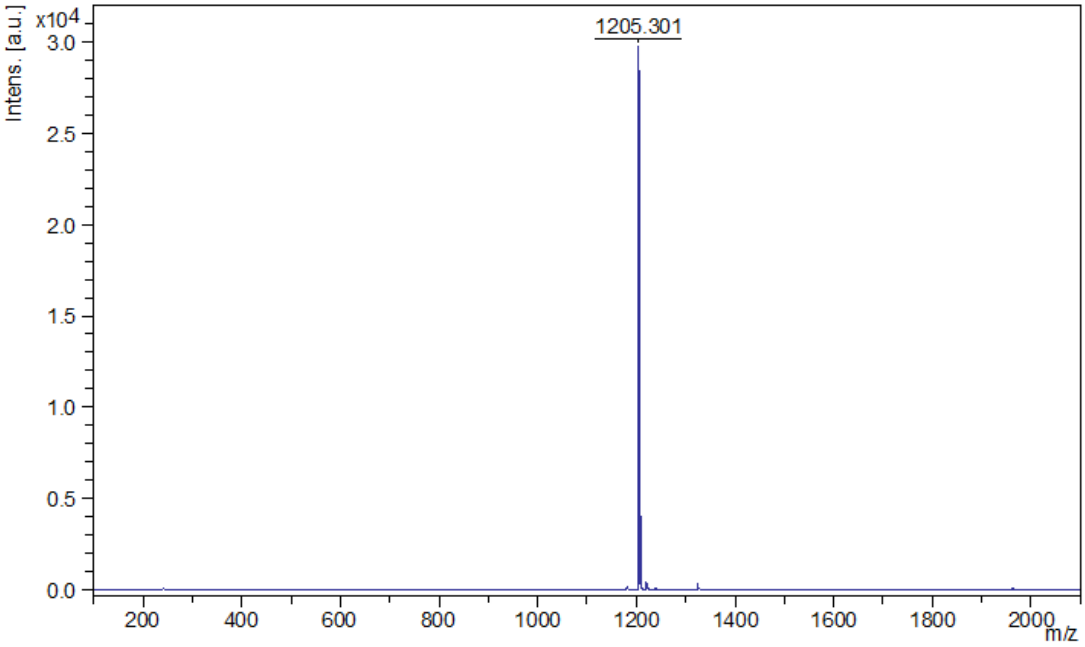

Figure S3. MALDI-TOF mass spectrum of **1**.

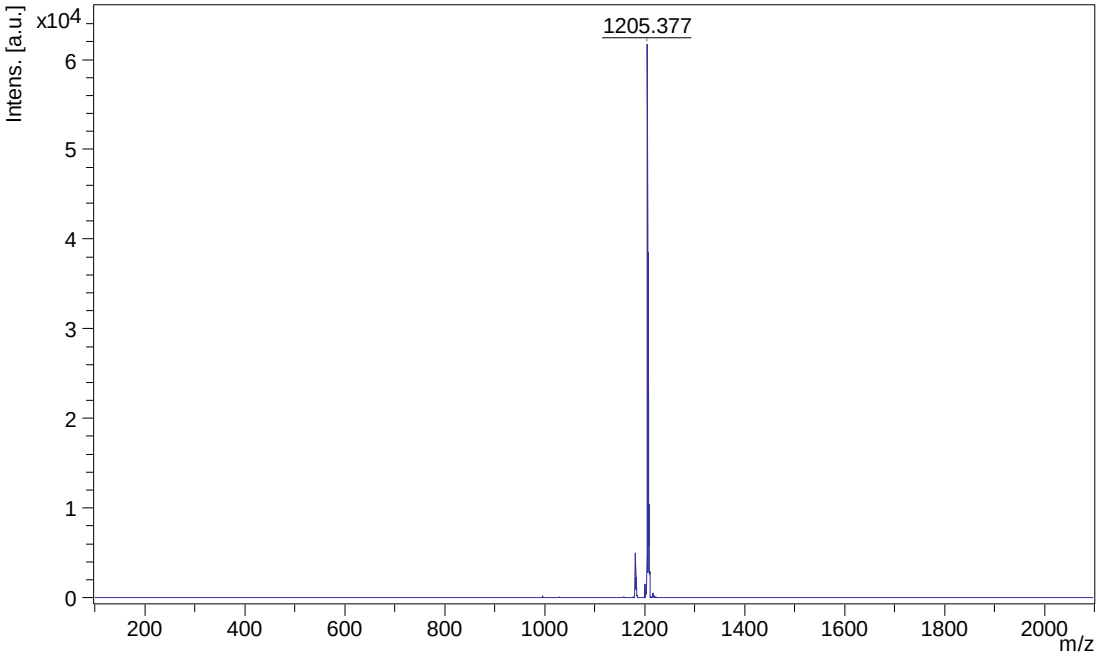

Figure S4. MALDI-TOF mass spectrum of $\mathbf{1}^+$.

3. NMR spectra

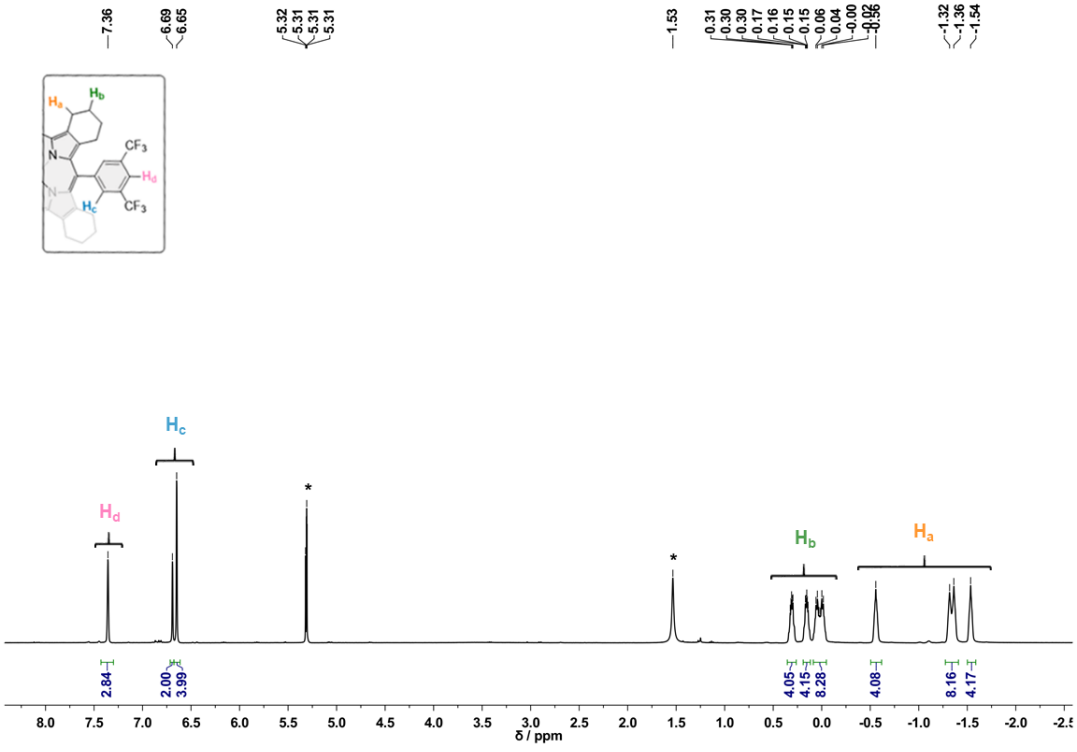

Figure S5. ^{1}H NMR spectrum (400 MHz) of $\mathbf{1}^+$ in CD_2Cl_2. Solvent and water peaks are marked with asterisks.

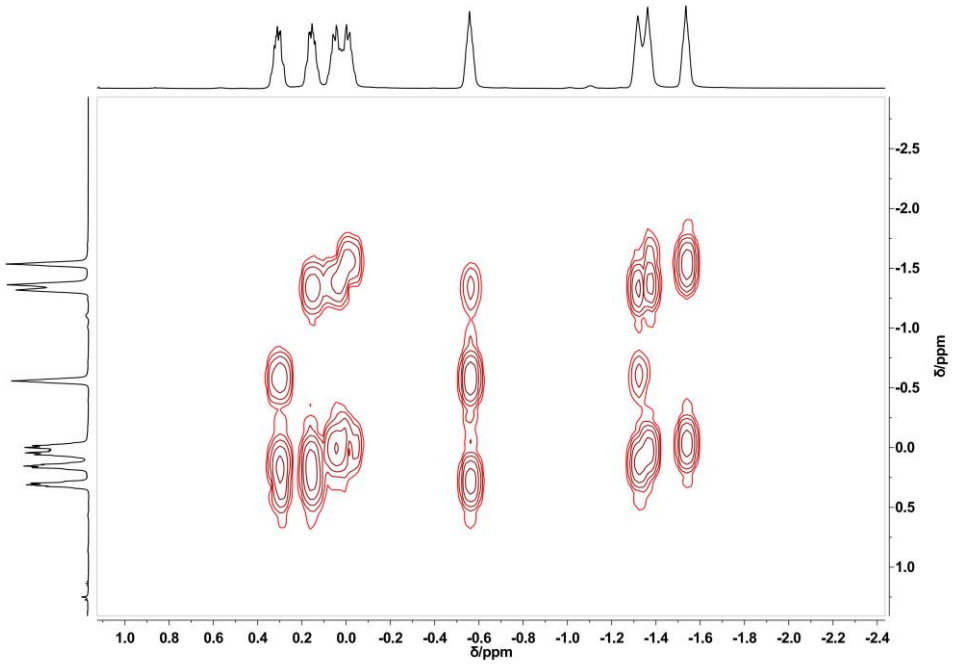

Figure S6. H-H COSY spectrum (400 MHz) of $\mathbf{1}^+$ in CD_2Cl_2.

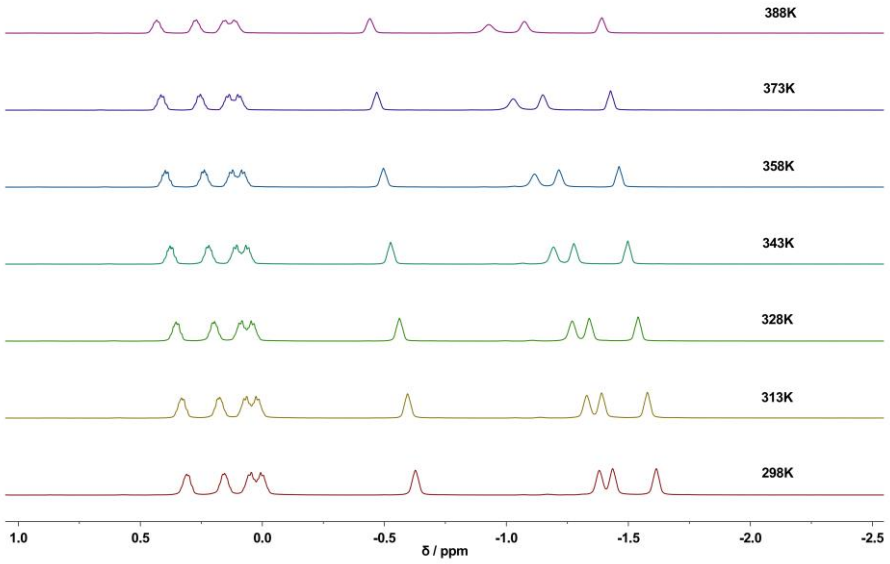

Figure S7. VT-NMR spectrum (500 MHz) of $\mathbf{1}^+$ in $C_2D_2Cl_4$.

^{1}H NMR measurement of $\mathbf{1}^-$. In a glovebox, **1** (10 mg, 0.008 mmol) and Kryptofix 222 (6 mg, 0.016 mmol) were dissolved in 1 mL THF-d_8. KC_8 (2.2 mg, 0.016 mmol) was dispersed in THF-d_8 and added dropwise to the solution of **1**. After stirring for 2 hours, the solution was loaded directly into the NMR tube and sealed for measurement. ^{1}H NMR (400 MHz, THF-d_8): δ 8.47 (s, 4H, aryl-*ortho*), 8.44 (s, 2H, aryl-*ortho*), 8.23 (d, 3H, aryl-*para*), 4.06 (m, 4H, β-butano), 2.94-2.96 (m, 48H, kryp), 2.59 (m, 8H, β-butano), 2.39 (m, 4H, β-butano), 2.13 (m, 4H, β-butano), 2.00 (m, 24H, kryp), 1.88 (m, 4H, β-butano), 1.62 (m, 8H, β-butano).

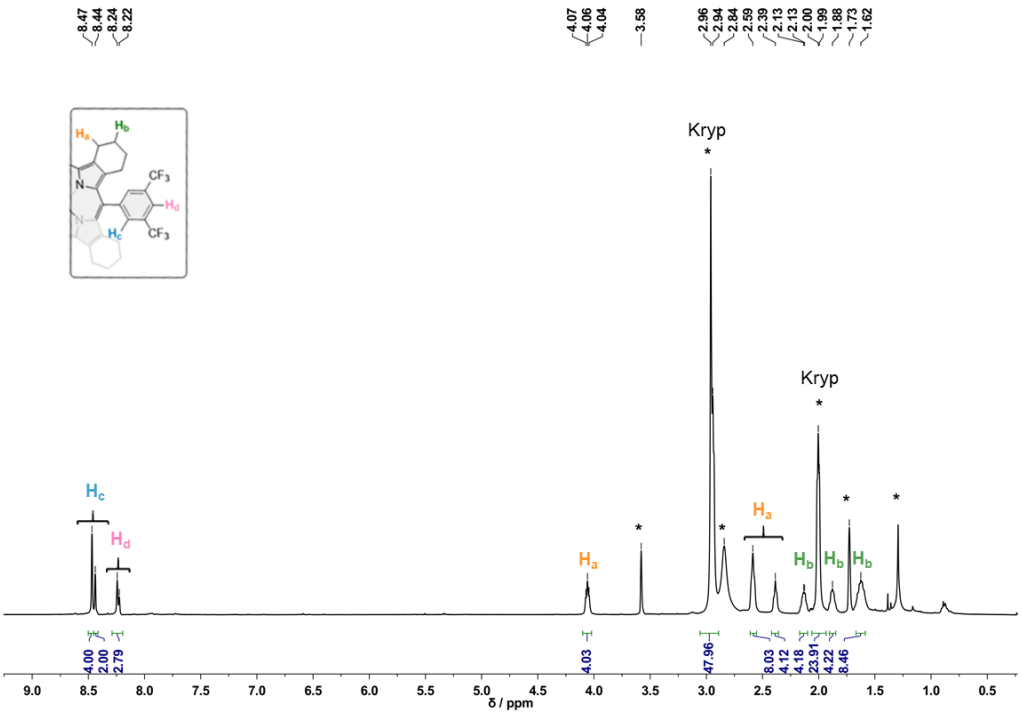

Figure S8. ^{1}H NMR spectrum (400 MHz) of $\mathbf{1}^-$ in THF-d_8. Solvent and Kryptofix-222 resonances are marked with asterisks.

4. UV/vis spectral changes during chemical reduction

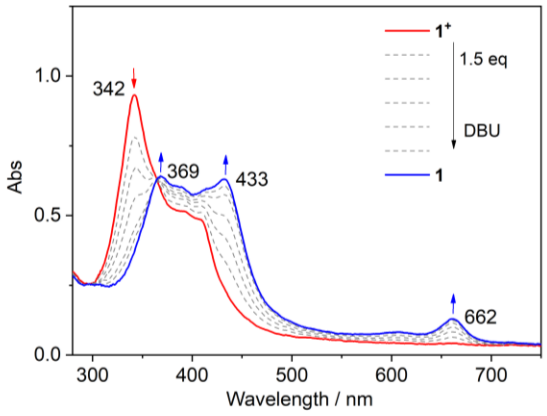

Figure S9. UV-vis spectra change from $\mathbf{1}^+$ to **1** after adding 1.5 eq DBU into the CH_2Cl_2 solution of $\mathbf{1}^+$.

5. Spectroelectrochemistry measurements

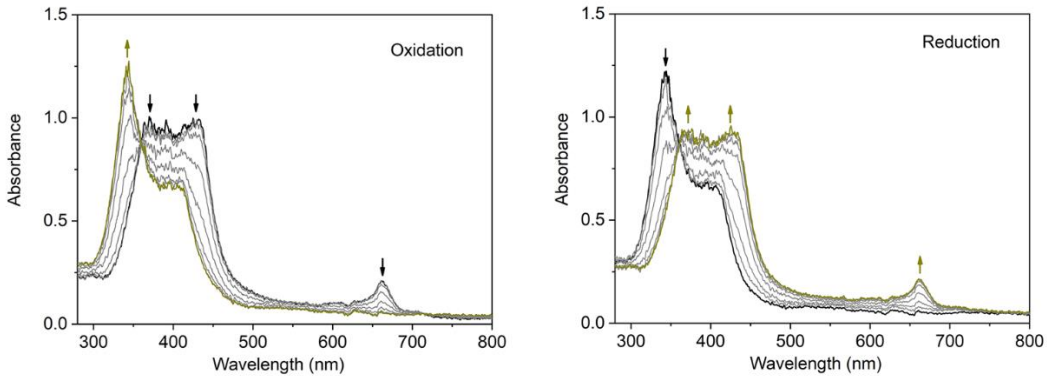

Figure S10. UV−vis spectral changes of from **1 to 1**$^{+}$ (left) and from **1**$^{+}$ to **1** (right) with applying potential positively shifted to 0.3 V (oxidation) and negatively shifted to -0.3 V (reduction) in CH_2Cl_2.

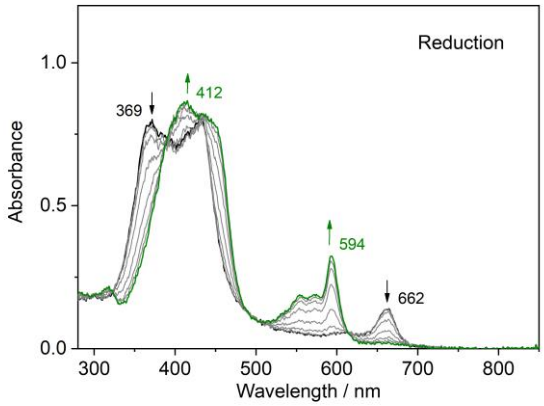

Figure S11. UV−vis spectral changes from **1** to **1**$^{-}$ during the electrochemical reduction with applying potential negatively shifted to -0.8 V in CH_2Cl_2.

6. Stability of 1 and 1^{+}

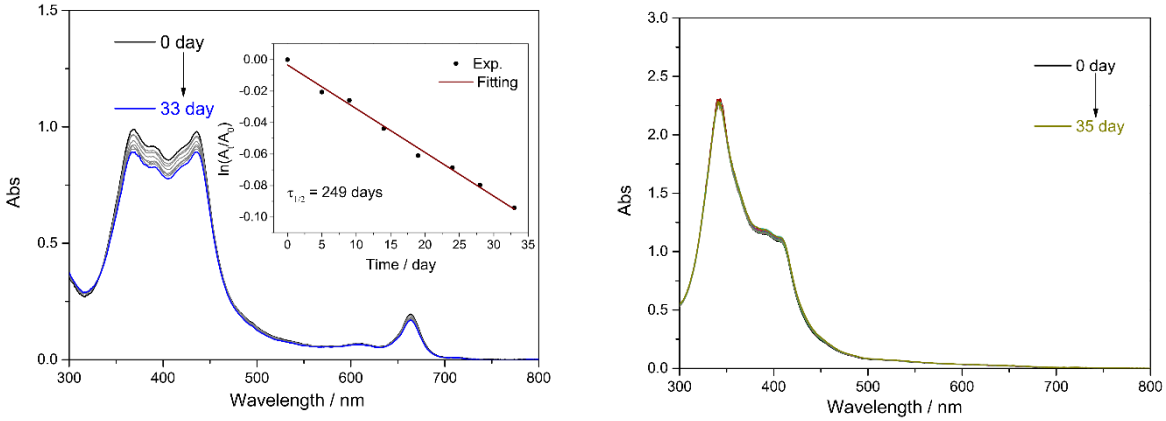

Figure S12. Time course of the absorbance change of **1** (left) in toluene (1.7×10^{-5} mol/L) and **1**$^{+}$ (right) in DCM monitored by UV-vis measurements (3×10^{-5} mol/L).

7. X-ray diffraction analysis

Table S1. Crystallographic data of **1** and $\mathbf{1}^{+}$.

Crystallographic data

Compound	**1**	$\mathbf{1}^{+}\mathbf{SbF_6^-}$
CCDC.No.	2168702	2168703
Formula	$C_{59}H_{41}F_{18}N_4Ni$	$C_{59}H_{41}F_{18}N_4NiF_6Sb$, $2(CH_2Cl_2)$
Formula weight	1206.67	1612.27
Radiation	GaK\α	GaK\α
Temperature [K]	193	173
Crystal system	Monoclinic	Monoclinic
Space group	P 1 21/n 1	C 2/c
a [Å]	23.608(2)	43.583(5)
b [Å]	8.3957(7)	17.614(2)
c [Å]	29.792(3)	16.1794(18)
α [deg]	90	90
β [deg]	101.871(4)	92.066(9)
γ [deg]	90	90
V [$Å^3$]	5778.6(9)	12413(3)
Z	4	8
ρ [gcm^{-3}]	1.387	1.725
μ [mm^{-1}]	2.394	5.751
F (000)	2452	6416
Reflections collected / unique	12893 / 74723	11405 / 64837
R_1	0.0713	0.0490
wR_2	0.2303	0.1533
GOF	1.091	1.074

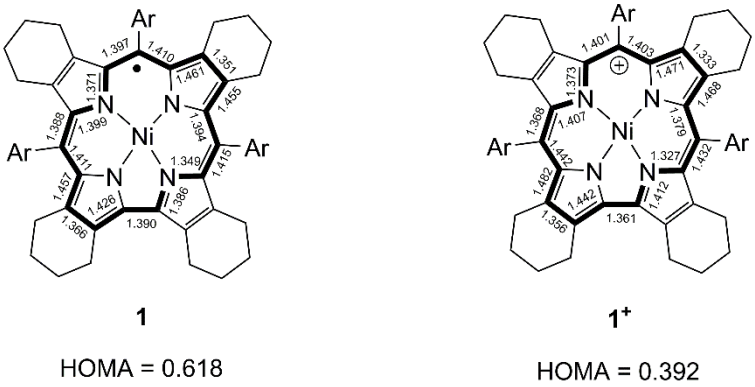

Figure S13. Selected distances and calculated HOMA values for single-crystal structures of **1** and $\mathbf{1}^{+}$.

8. Theoretical analysis

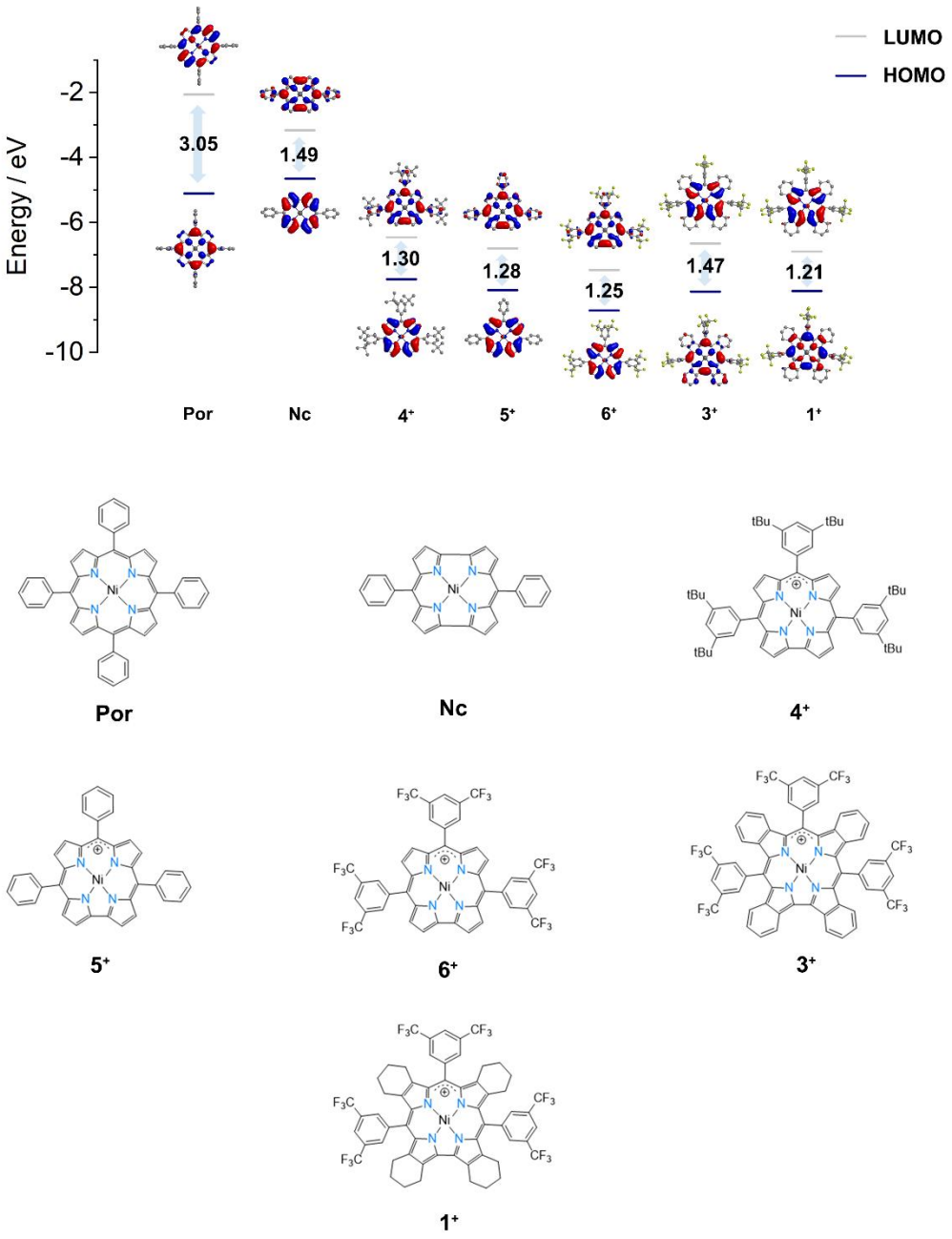

Figure S14. The calculated HOMO-LUMO gaps of meso-phenyl substituted nickel porphyrin and norcorrole, and a series of nickel corroles with various meso- and β, β'-substituents at the (U)B3LYP/6-31G(d,p) (C, N, F, H)+SDD(Ni) level of theory.

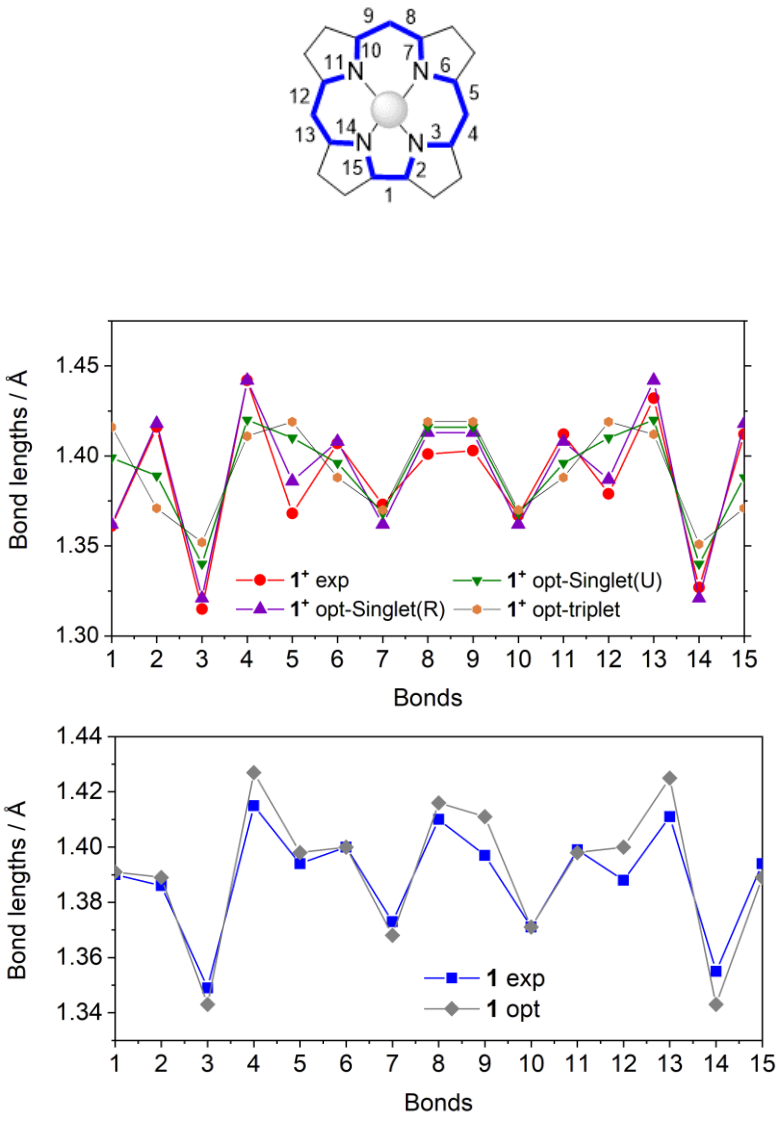

Figure S15. Comparison of selected inner 15 bond lengths of $\mathbf{1}^+$ and **1** between DFT optimized structures and single-crystal X-ray diffraction characterized structures.

The diradical character was evaluated by performing a natural orbital (NO) population analysis. From the occupation numbers n of the highest occupied NO (HONO) and lowest unoccupied NO (LUNO) the diradical character (y_0) was estimated according to Yamaguchi's scheme[2]:

$$y_0 = 1 - \frac{2T}{1+T^2}$$

$$\text{where} \quad T = \frac{n_{HONO} - n_{LUNO}}{2}$$

The singlet-triplet energy gap was estimated using Yamaguchi's approach[3], which includes the energy difference between BS singlet and open-shell triplet and the correction of spin contamination:

$$\Delta E_{S-T} = \frac{2(E_{BS} - E_T)}{\langle S^2 \rangle_T - \langle S^2 \rangle_{BS}}$$

Where the E_{BS} and E_T are the total energy of the broken-symmetry singlet state and triplet state, $\langle S^2 \rangle_{BS}$ and $\langle S^2 \rangle_T$ represent the total spin angular momentums of the calculated broken-symmetry singlet state and triplet states.

Table S2. Calculations of diradical character with different theoretical methods based on open-shell optimized structures of $\mathbf{1}^+$

CAM-B3LYP		BHandHLYP		LC-BLYP		B3LYP	
n_{LUNO}	y	n_{LUNO}	y	n_{LUNO}	y	n_{LUNO}	y
0.74	0.51	0.74	0.52	0.75	0.52	0.67	0.40

Table S3. Calculated total energies (hartree), relative energies, singlet-triplet gap (ΔE_{S-T}) of the closed-shell singlet (CS), open-shell singlet (OS), and triplet states of $\mathbf{1}^+$.

$\mathbf{1}^+$	Singlet (CS)	Singlet (OS)	Triplet
Total energy [Hartree]	-4460.049417	-4460.050766	-4460.048437
Total energy (+ZPVE)[Hartree]	-4459.147003	-4459.149990	-4459.146097
Relative energy [kcal/mol]	0	-0.85	0.61
Relative energy (+ZPVE) [kcal/mol]	0	-1.87	0.57
ΔE_{S-T} /ΔE_{S-T}(+ZPVE) [kcal/mol]	-1.88 / -3.14		

Table S4. Calculated total energies (hartree), relative energies, singlet-triplet gap ($\Delta E_{S\text{-}T}$) of the closed-shell singlet (CS), open-shell singlet (OS), and triplet states of $\mathbf{2}^{+}$.

$\mathbf{2}^{+}$	Singlet (CS)	Singlet (OS)	Triplet
Total energy [Hartree]	-1592.304318	-1592.304631	-1592.301049
Total energy (+ZPVE)[Hartree]	-1591.709142	-1591.711438	-1591.706803
Relative energy [kcal/mol]	0	-0.20	2.05
Relative energy (+ZPVE) [kcal/mol]	0	-1.44	1.46
$\Delta E_{S\text{-}T}$ /$\Delta E_{S\text{-}T}$(+ZPVE) [kcal/mol]		-3.13 / -4.03	

Table S5. Calculated total energies (hartree), relative energies, singlet-triplet gap ($\Delta E_{S\text{-}T}$) of the closed-shell singlet (CS) and triplet states of $\mathbf{3}^{+}$.

$\mathbf{3}^{+}$	Singlet (CS)	Triplet
Total energy [Hartree]	-4450.410748	-4450.398708
Total energy (+ZPVE)[Hartree]	-4449.692746	-4449.681604
Relative energy [kcal/mol]	0	7.56
Relative energy (+ZPVE) [kcal/mol]	0	6.99

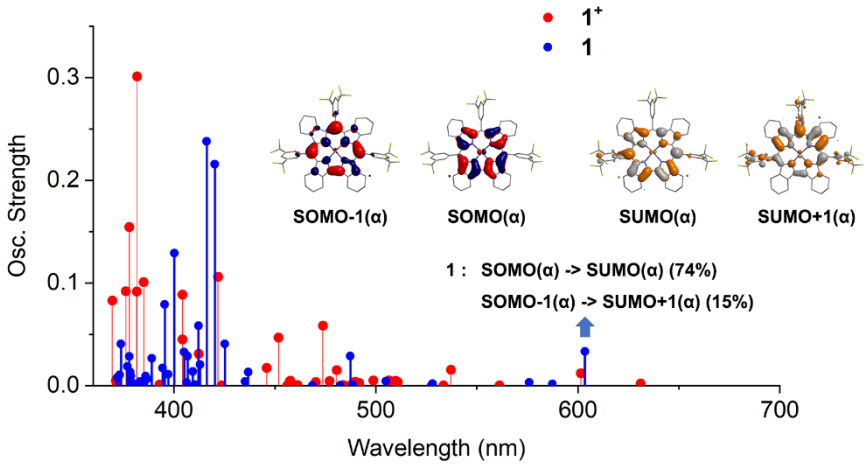

Figure S16. The TD-DFT calculated stick spectra of the excited states of $\mathbf{1}^{+}$ and **1**. The electronic transition compositions of α-spin Q band of **1** is analyzed.

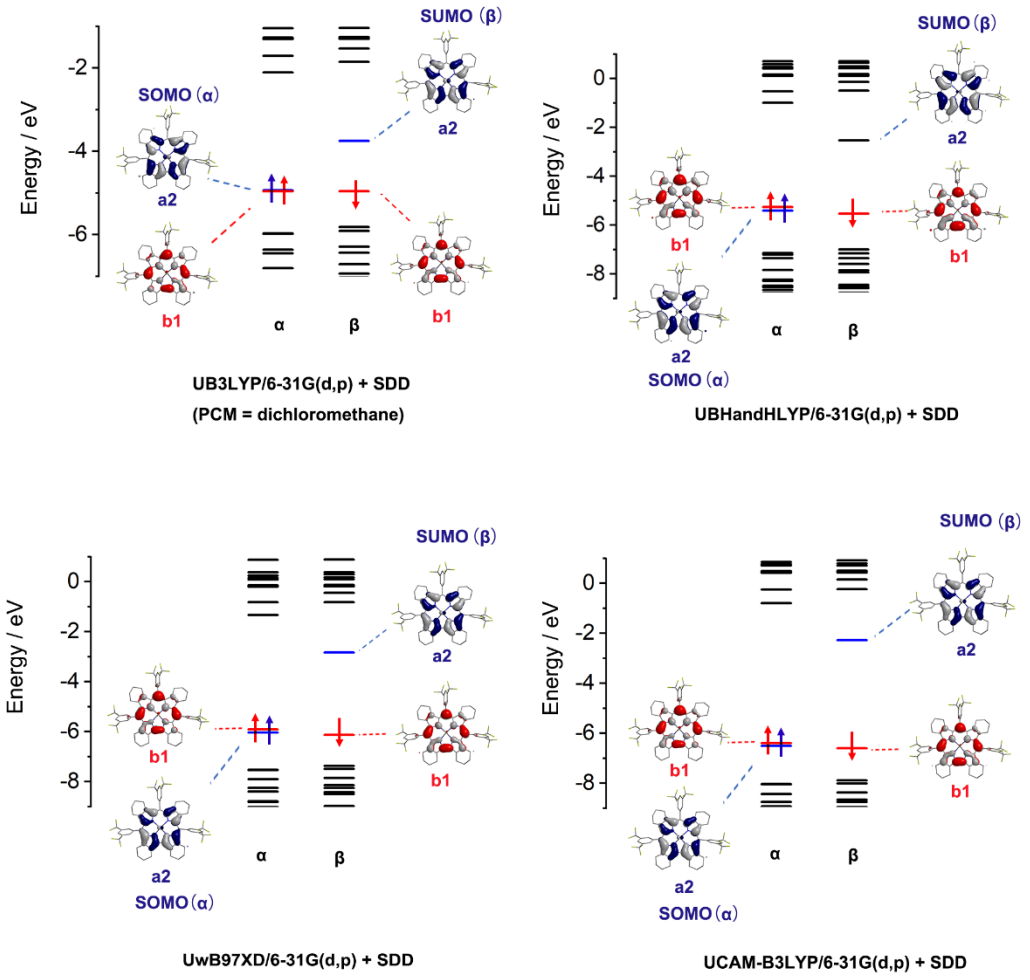

Figure S17. DFT calculated frontier molecular orbital diagrams of **1** using various hybird fuctionals.

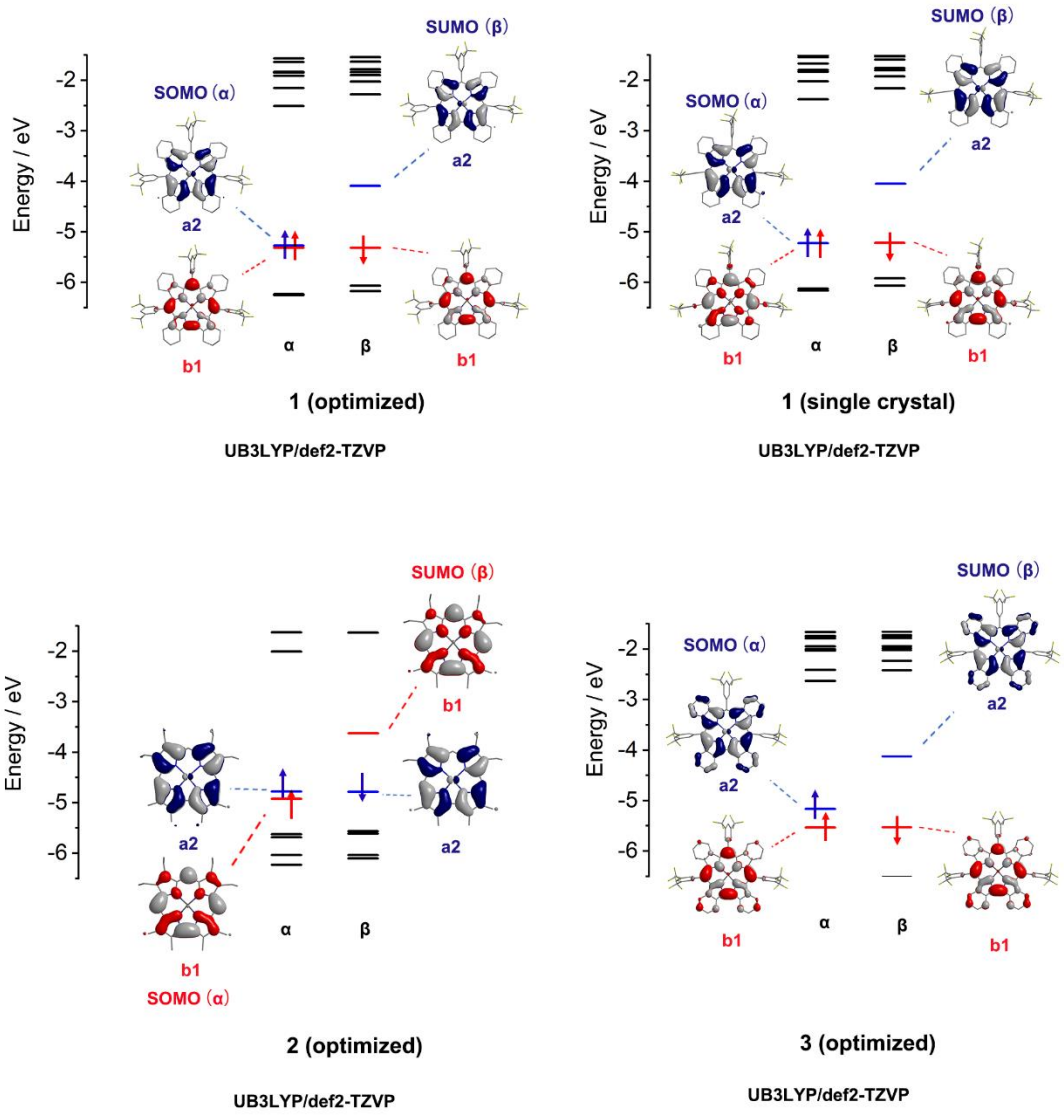

Figure S18. DFT calcualted frontier molecular orbital diagrams of corrole radicals **1**, **2** and **3** using def2-TZVP bias set.

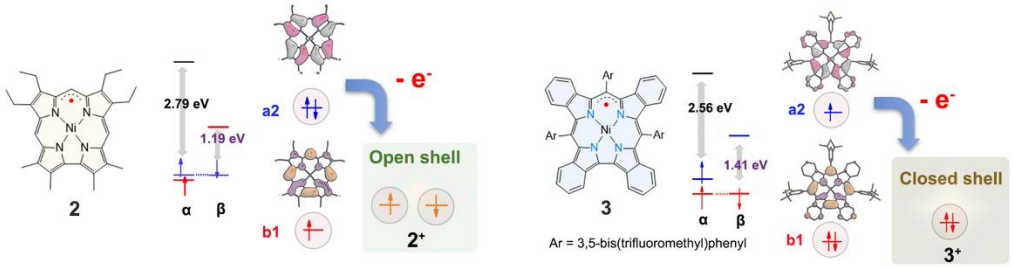

Figure S19. Frontier molecular orbital diagrams and isosurfaces (isovalue = 0.03) of **2** and **3**, and the ground states of their one-electron oxidized products $\mathbf{2}^{+}$ and $\mathbf{3}^{+}$ calculated at a UB3LYP/6-31G(d,p) +SDD level of theory .

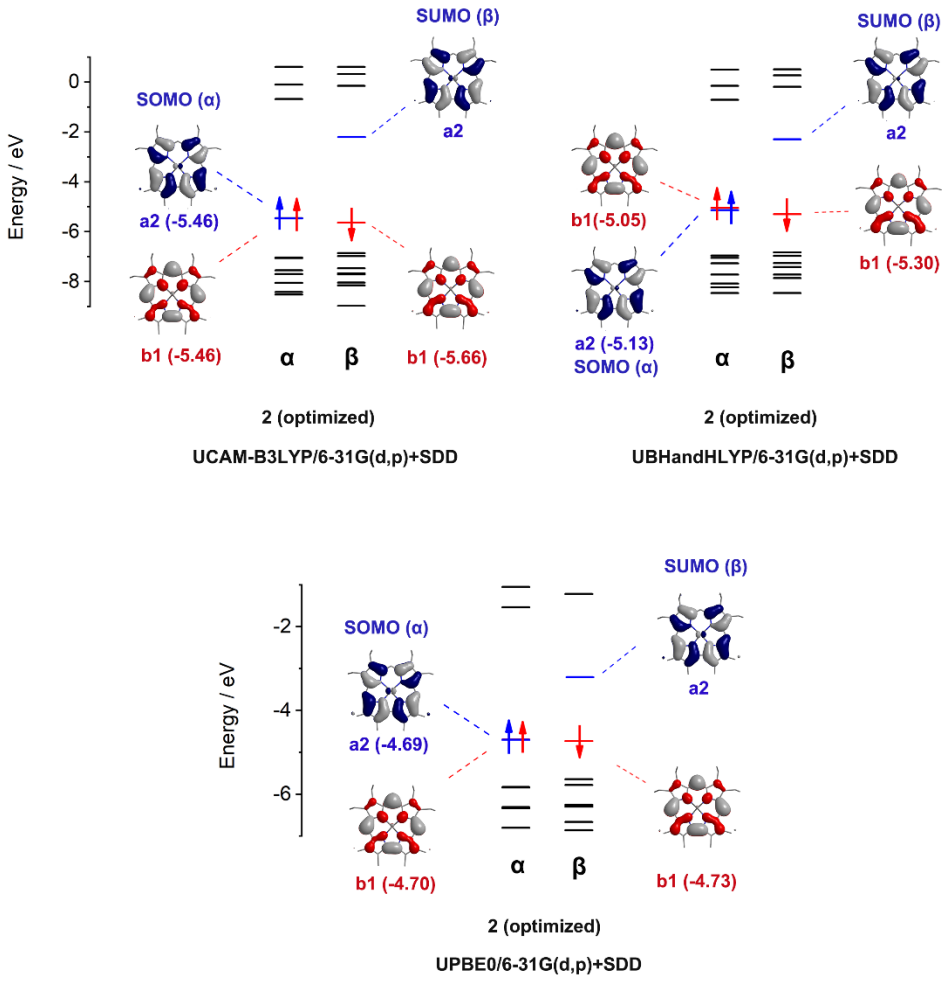

Figure S20. DFT calcualted frontier molecular orbital diagrams of corrole radical **2** with different functionals.

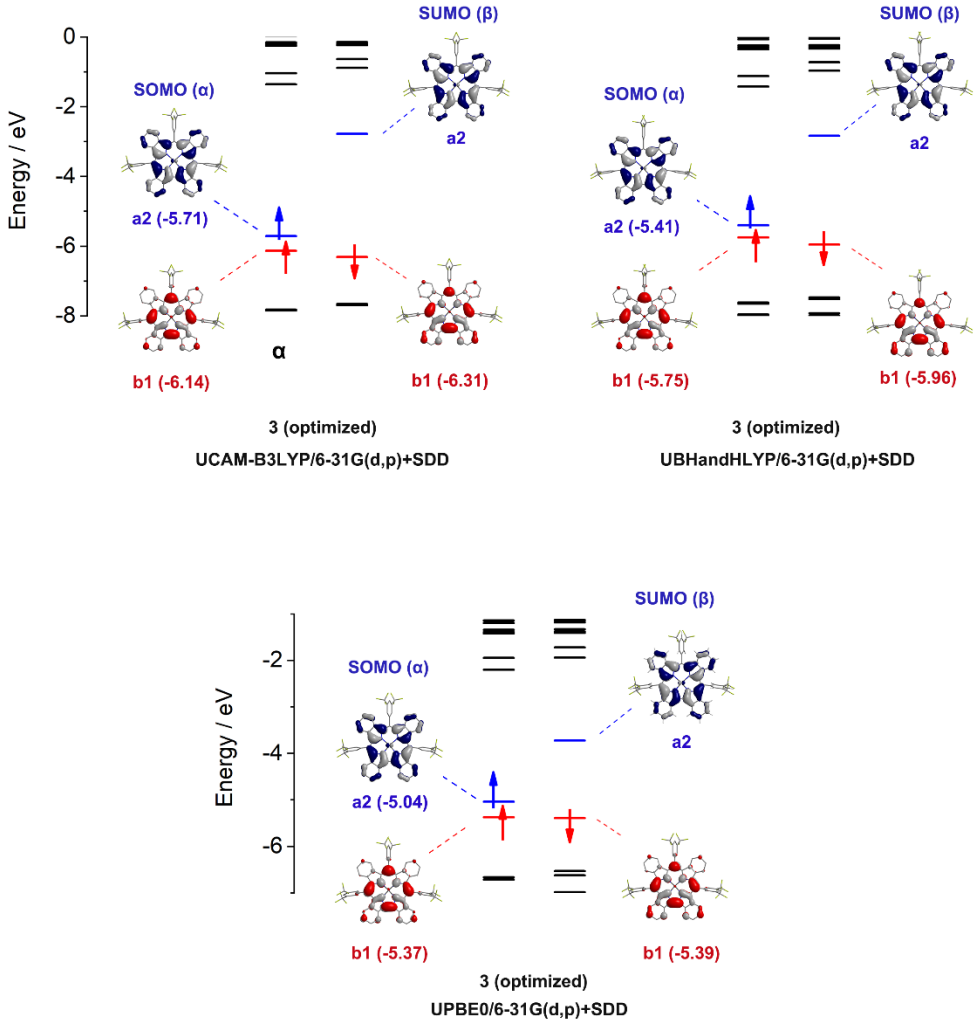

Figure S21. DFT calcualted frontier molecular orbital diagrams of corrole radical **3** with different functionals.

The structures of compounds **2** and **3** were optimized with various functionals. The frequency calculations were carried out to confirm the minimum nature of the stationary point. Compound **2** always shows degenerate or near-degenerate SOMO-HOMO energy levels with all functionals. At a UB3LYP/6-31G(d,p) (C, N, H)+SDD(Ni) level of theory, the b1 SOMO of **2** lies below the a2 HOMO with a small gap of 0.1 eV. The calculation of the cation $\mathbf{2}^{+}$ also shows a low-lying broken-symmetry singlet diradical ground state as that in $\mathbf{1}^{+}$. In contrast, the a2 SOMO of **3** is significantly higher than the b1 HOMO with all the functionals. The cation $\mathbf{3}^{+}$ has a larger closed-shell HOMO-LUMO gap (1.47 eV) than those of $\mathbf{1}^{+}$ (1.21 eV) and $\mathbf{2}^{+}$ (1.31 eV). The wavefunction of closed-shell $\mathbf{3}^{+}$ is stable, and no broken-symmetry singlet diradical state can be found by calculation for $\mathbf{3}^{+}$.

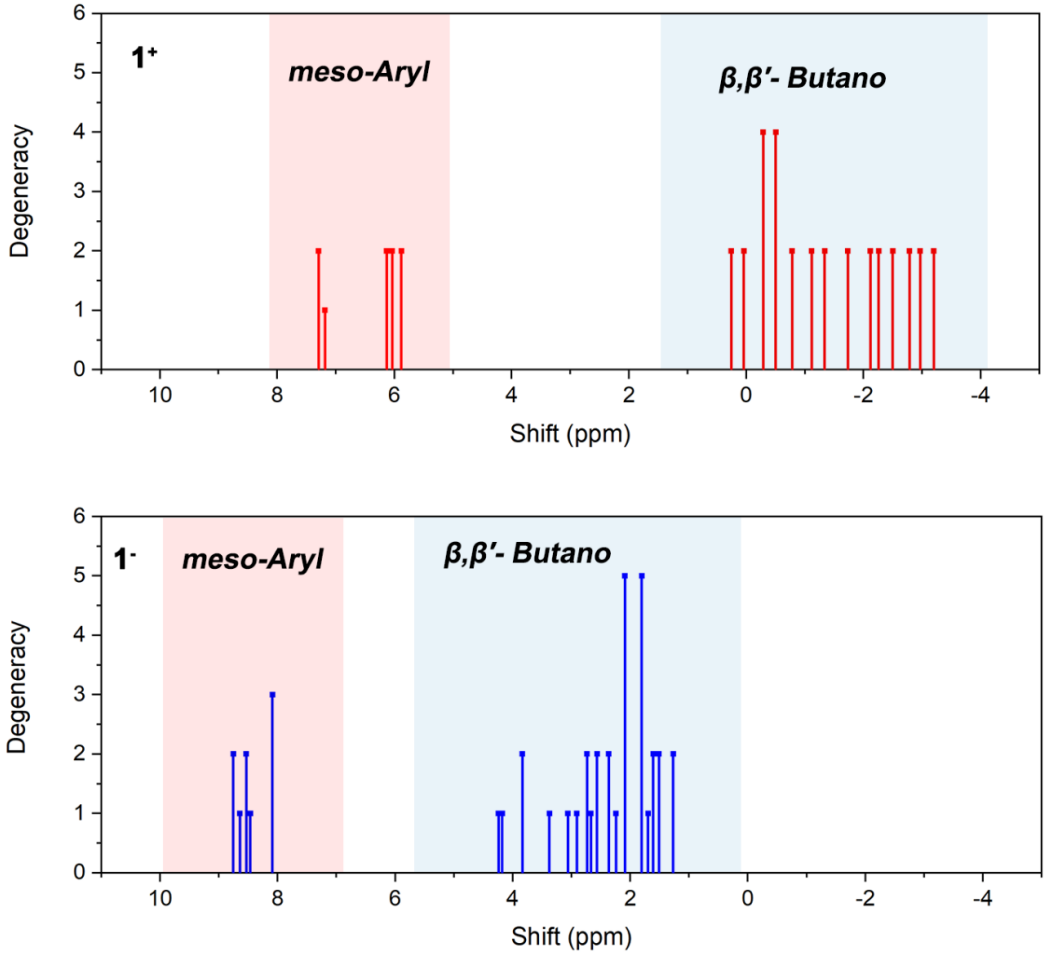

Figure S22. DFT calculated NMR chemical shifts of $\mathbf{1}^{+}$ and $\mathbf{1}^{-}$ with GIAO method at UB3LYP/6-31g(d,p)+SDD level of theory.

NICS values

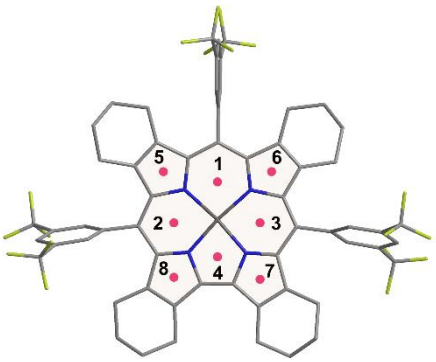

Table S6. Singlet-state NICS values of $\mathbf{1}^{+}$ at various positions calculated at GIAO/RB3LYP (RBHandHLYP) /6-31G(d,p)+SDD level of theory using the closed-shell optimized structure.

Singlet (CS)	RB3LYP		RBHandHLYP	
Positions	NICS(0)	$NICS(1)_{zz}$	NICS(0)	$NICS(1)_{zz}$
1	+ 59.4	+ 160.9	+33.9	+98.5
2	+76.1	+200.6	+41.6	+115.4
3	+76.1	+202.2	+41.6	+114.2
4	+102.1	+268.3	+49.4	+144.7
5	+13.2	+40.1	+10.3	+26.2
6	+13.2	+33.5	+10.3	+22.3
7	+16.3	+49.1	+8.1	+22.1
8	+16.3	+43.6	+8.1	+19.0

Table S7. Singlet-state NICS values of $\mathbf{1}^{+}$ at various positions calculated at GIAO/UB3LYP (UBHandHLYP) /6-31G(d,p)+SDD level of theory using the closed-shell optimized structure.

Singlet (OS)	UB3LYP		UBHandHLYP	
Positions	NICS(0)	$NICS(1)_{zz}$	NICS(0)	$NICS(1)_{zz}$
1	+ 43.1	+ 118.5	+11.9	+41.4
2	+55.6	+149.8	+16.1	+50.4
3	+55.6	+148.5	+16.1	+49.7
4	+74.7	+199.5	+18.1	+64.9
5	+10.2	+29.6	+4.7	+9.0
6	+10.2	+24.8	+4.7	+7.6
7	+12.4	+36.2	+3.8	+7.4
8	+12.4	+32.2	+3.8	+6.3

Table S8. Singlet-state NICS values of $\mathbf{1}^+$ at various positions calculated at GIAO/UB3LYP (UBHandHLYP) /6-31G(d,p)+SDD level of theory using the open-shell optimized structure.

Singlet (OS)	UB3LYP		UBHandHLYP	
Positions	NICS(0)	$NICS(1)_{zz}$	NICS(0)	$NICS(1)_{zz}$
1	+ 46.5	+127.0	+13.5	+45.6
2	+57.1	+153.3	+17.2	+53.2
3	+57.1	+151.9	+17.2	+52.3
4	+71.9	+192.7	+18.1	+65.0
5	+11.0	+32.7	+4.5	+8.8
6	+11.0	+26.6	+4.5	+6.9
7	+9.9	+30.8	+3.2	+6.2
8	+9.9	+26.1	+3.2	+4.7

Table S9. Triplet-state NICS values of $\mathbf{1}^+$ at various positions calculated at GIAO/UB3LYP (UBHandHLYP) /6-31G(d,p)+SDD level of theory using the triplet optimized structure.

Triplet	UB3LYP		UBHandHLYP	
Positions	NICS(0)	$NICS(1)_{zz}$	NICS(0)	$NICS(1)_{zz}$
1	-13.8	-30.2	-19.8	-41.2
2	-17.4	-37.1	-20.3	-42.9
3	-17.4	-36.8	-20.3	-43.0
4	-23.2	-45.7	-26.4	-46.6
5	-1.1	-10.1	-1.9	-14.0
6	-1.1	-7.7	-1.9	-11.3
7	1.7	-2.1	-0.5	-9.2
8	1.7	-0.6	-0.5	-7.3

GIMIC ring currents

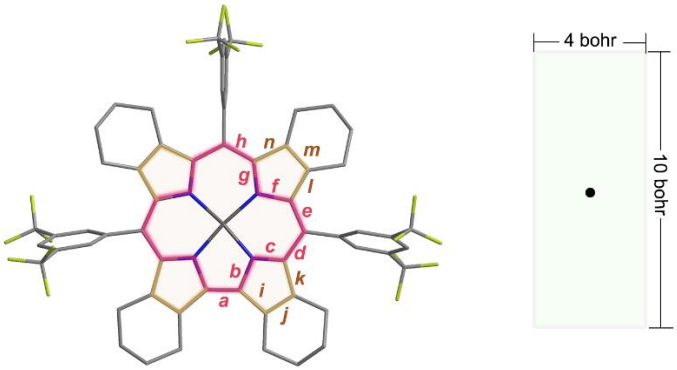

Table S10. The ring-current strengths (nA / T) of selected bonds of $\mathbf{1}^{+\cdot}$ in closed-shell and open-shell states using B3LYP and BHandHLYP functionals.

Bonds	Current strength (nA/T)			
	UBHandHLYP	RBHandHLYP	UB3LYP	RB3LYP
a	-27.4	-63.2	-85.8	-116.2
b	-21.2	-46.0	-61.2	-82.3
c	-16.2	-36.3	-44.5	-60.3
d	-22.6	-53.6	-69.3	-94.4
e	-22.8	-54.0	-69.9	-95.2
f	-15.9	-35.2	-47.4	-64.2
g	-12.8	-29.7	-37.0	-50.6
h	-19.4	-47.8	-58.8	-80.5
i	-6.9	-18.4	-26.5	-36.3
j	-7.3	-19.9	-27.0	-36.8
k	-6.5	-17.6	-25.4	-34.9
l	-7.0	-19.0	-23.0	-31.7
m	-7.3	-19.6	-23.6	-32.3
n	-6.7	-18.6	-22.5	-31.0

ACID ring currents

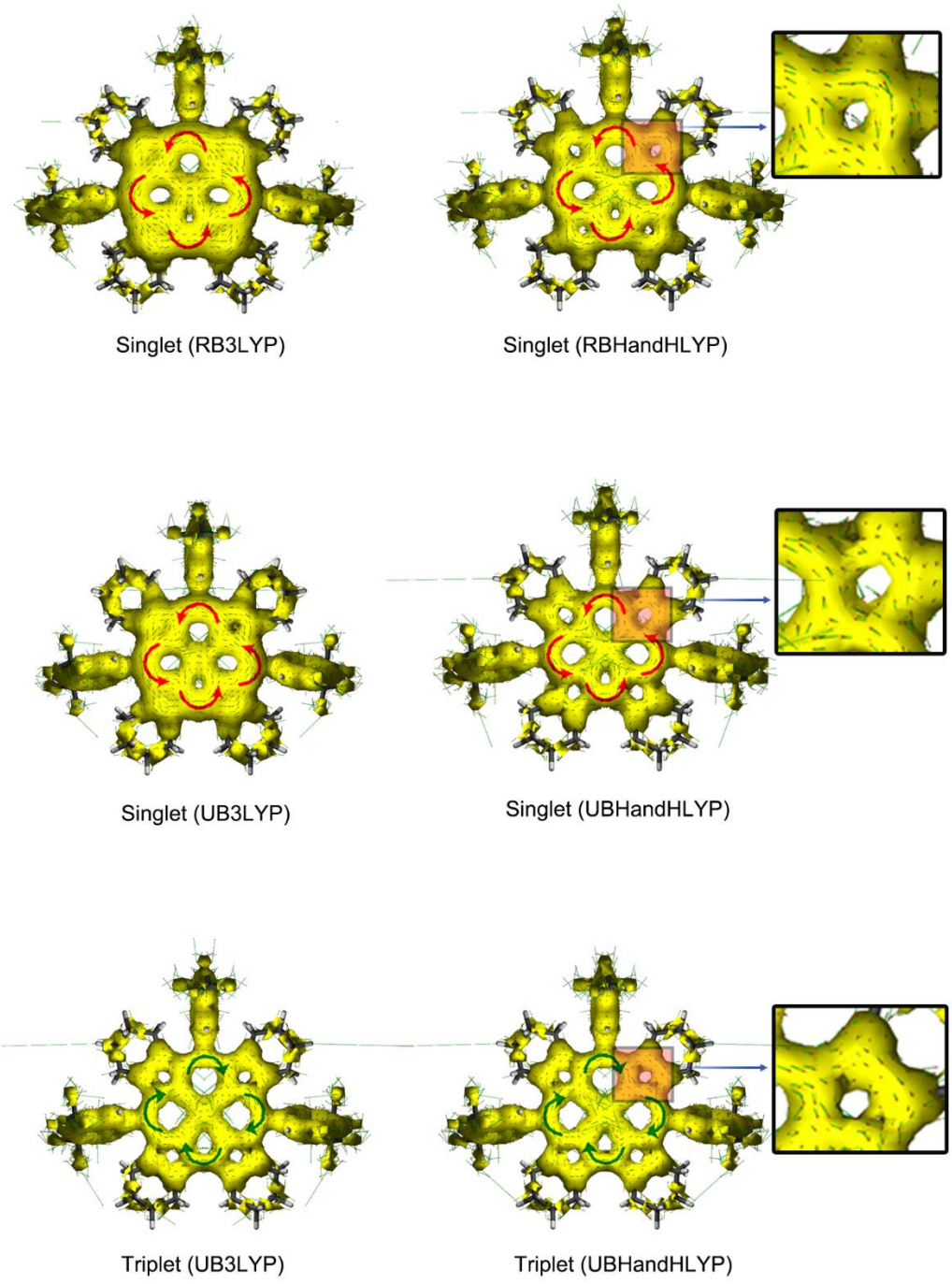

Figure S23. ACID plots (isovalue = 0.03) of $\mathbf{1}^{+}$ calculated in closed-shell singlet, open-shell singlet and triplet states with (U)B3LYP and (U)BHandHLYP functionals, isovalue is 0.03.

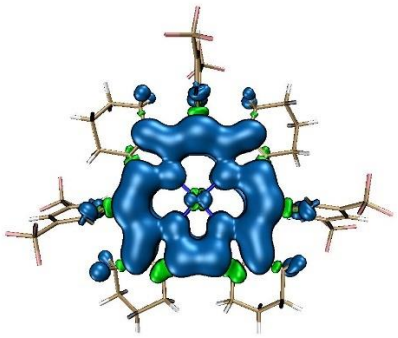

Figure S24. Spin density of $\mathbf{1}^{+}$ in the triplet state (isovalue = 0.001) calculated at UB3LYP/6-31g(d,p)+SDD level of theory.

9. Cartesian coordinates for optimized geometries

Table S11. Coordinates of the optimized structure for **1** at the UB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4460.26687721				Sum of electronic and zero-point Energies = -4459.366263			
symmetry c1				Sum of electronic and thermal Energies = -4459.297873			
Charge = 0, Multiplicity = 2				Sum of electronic and thermal Enthalpies = -4459.296928			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -4459.483205			
Atom	x	y	z	Atom	x	y	z
Ni	0.013677000	-0.854456000	-0.039582000	C	-7.375869000	-3.074065000	2.344786000
N	1.396420000	0.432710000	-0.017054000	C	6.971841000	-1.696918000	-1.051102000
N	1.256612000	-2.232865000	-0.128147000	C	7.612375000	-1.268421000	2.658249000
N	-1.412833000	0.379186000	0.061895000	C	-0.488864000	5.980185000	-1.264955000
N	-1.182742000	-2.278000000	-0.111941000	F	0.179112000	6.360840000	3.369733000
C	2.771481000	0.183275000	-0.040350000	C	7.708058000	-2.048929000	-2.316347000
C	0.754018000	-3.522941000	-0.240279000	C	0.703814000	6.853487000	2.226438000
C	1.208126000	1.787852000	-0.103556000	C	4.289603000	4.029354000	-1.087402000
C	-0.049216000	2.420222000	0.003283000	C	5.266682000	3.245376000	-0.213307000
C	3.469331000	1.468002000	-0.165520000	C	-3.018367000	-6.633055000	-0.511930000
F	6.877290000	-1.791043000	3.663493000	C	-4.087118000	-5.801930000	-1.230617000
C	-0.636583000	-3.546063000	-0.267083000	C	-5.090362000	2.797321000	1.767933000
C	-5.409301000	-2.060854000	1.190291000	C	-4.474295000	3.948774000	0.975419000
F	-9.092259000	-1.059156000	-2.009413000	F	7.419951000	-3.313874000	-2.706593000
C	2.598286000	-2.283699000	-0.074137000	F	9.045870000	-1.968775000	-2.170085000
F	2.050876000	6.784425000	2.353487000	F	7.356513000	-1.237226000	-3.337378000
C	1.857618000	-4.445931000	-0.261968000	F	0.374453000	8.158959000	2.153041000
C	-1.278044000	1.735912000	0.164311000	F	-2.324047000	6.689257000	-2.567879000
C	-0.085420000	3.917113000	-0.041574000	F	-0.549901000	6.022710000	-3.628905000

C	-6.788563000	-2.273144000	1.213570000
C	0.255145000	4.681208000	1.078767000
C	2.519546000	2.443520000	-0.257804000
F	7.838896000	0.028443000	2.969601000
C	5.526543000	-1.200976000	1.272345000
C	-2.522763000	-2.369125000	-0.136642000
C	3.364612000	-1.084645000	-0.014020000
C	-2.885199000	-3.773561000	-0.366773000
F	-8.719353000	-2.976541000	2.398833000
C	-2.768103000	0.065767000	0.221309000
C	-1.708513000	-4.492011000	-0.419888000
C	1.831384000	-5.944876000	-0.382462000
F	-7.296811000	-0.751125000	-3.206661000
F	-6.886097000	-2.681168000	3.540535000
C	-3.325222000	-1.207074000	0.070787000
C	-4.805098000	-1.396277000	0.115436000
C	-4.234280000	-4.411367000	-0.587599000
C	-3.487977000	1.300695000	0.543009000
C	-7.596211000	-1.807140000	0.176298000
C	3.007149000	-3.696643000	-0.133952000
F	-7.072796000	-4.389014000	2.213030000
C	4.377774000	-4.321537000	-0.060145000
C	0.238112000	6.077209000	1.023746000
C	-5.618826000	-0.945069000	-0.931175000
C	-1.632563000	-5.977859000	-0.640780000
F	-7.965373000	0.795355000	-1.836761000
C	-7.001410000	-1.136654000	-0.892382000
C	4.851997000	-1.239426000	0.044468000
C	-2.591668000	2.328515000	0.477310000
C	5.592223000	-1.486477000	-1.116108000
F	8.808509000	-1.893064000	2.656867000
C	7.639650000	-1.648650000	0.171012000
C	-0.136007000	6.736379000	-0.145581000
C	-4.916017000	1.477658000	1.003341000
C	6.908006000	-1.394385000	1.332390000
C	4.951865000	1.741893000	-0.252346000
C	2.859084000	3.887349000	-0.547723000
C	4.286106000	-5.833269000	0.215291000
C	-0.458402000	4.585496000	-1.216124000
F	-0.545852000	7.941440000	-2.593747000
C	-7.845568000	-0.545257000	-1.989919000
C	3.234359000	-6.502054000	-0.676335000
C	-2.958697000	3.759302000	0.795778000
C	-0.971958000	6.663298000	-2.517406000
H	-4.795196000	-2.412927000	2.012915000
H	0.541274000	4.180864000	1.998419000
H	4.965636000	-1.022994000	2.184064000
H	1.134357000	-6.253287000	-1.168582000
H	1.449744000	-6.384636000	0.550803000
H	-4.778332000	-4.512790000	0.361248000
H	-4.862537000	-3.775583000	-1.219877000
H	-8.667113000	-1.964795000	0.199400000
H	4.981548000	-3.844752000	0.717692000
H	4.924293000	-4.156494000	-0.999306000
H	-5.166514000	-0.439140000	-1.777857000
H	-0.935004000	-6.436361000	0.068315000
H	-1.223446000	-6.180209000	-1.641565000
H	5.085519000	-1.521724000	-2.075293000
H	8.708960000	-1.812047000	0.219828000
H	-0.149297000	7.818379000	-0.186608000
H	-5.217048000	0.640309000	1.638186000
H	-5.605630000	1.466248000	0.149024000
H	5.352966000	1.307771000	-1.178079000
H	5.487695000	1.244852000	0.559572000
H	2.154815000	4.309300000	-1.268411000
H	2.758932000	4.498708000	0.358422000
H	5.269387000	-6.290959000	0.061625000
H	4.022466000	-5.996287000	1.268987000
H	-0.722348000	4.008468000	-2.096470000
H	3.238735000	-7.588181000	-0.533929000
H	3.485323000	-6.319847000	-1.729775000
H	-2.437747000	4.071989000	1.711153000
H	-2.614552000	4.440631000	0.015889000
H	4.560682000	5.090115000	-1.124810000
H	4.335204000	3.652089000	-2.117912000
H	5.195247000	3.609029000	0.820521000
H	6.301940000	3.407394000	-0.532554000
H	-2.983785000	-7.652117000	-0.912265000
H	-3.284073000	-6.719547000	0.550070000
H	-5.053723000	-6.316906000	-1.210158000
H	-3.809401000	-5.689443000	-2.287267000
H	-6.155286000	2.975634000	1.953203000
H	-4.603234000	2.722459000	2.749386000
H	-4.661213000	4.910588000	1.465309000
H	-4.955072000	4.000506000	-0.010708000

Table S12. Coordinates of the optimized singlet structure for $\mathbf{1}^{+}$ at the RB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4460.04941679				Sum of electronic and zero-point Energies = -4459.147003			
symmetry c1				Sum of electronic and thermal Energies = -4459.078840			
Charge = 1, Multiplicity =1				Sum of electronic and thermal Enthalpies = -4459.077896			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -4459.260585			
Atom	x	y	z	Atom	x	y	z
C	-2.931418000	3.747887000	0.099641000	F	0.510003000	-6.276645000	-3.463219000
C	-4.294205000	4.371739000	0.235690000	F	-0.073679000	-8.092782000	-2.407150000
C	-1.780668000	4.486112000	0.056260000	F	-1.574456000	-6.610027000	-2.950595000
C	-1.729851000	5.987685000	0.073795000	N	-1.216848000	2.229620000	0.002092000
C	-4.188513000	5.849550000	0.654395000	N	1.217008000	2.229569000	-0.002020000
C	-3.125106000	6.590326000	-0.163266000	N	1.397571000	-0.427681000	0.016313000
C	-2.535214000	2.308676000	0.033667000	N	-1.397521000	-0.427623000	-0.016131000
C	-0.681072000	3.543240000	0.010742000	Ni	0.000051000	0.830555000	0.000067000
C	2.931640000	3.747762000	-0.099648000	C	7.533579000	2.512076000	2.367622000
C	1.780921000	4.486036000	-0.056278000	F	8.870288000	2.383623000	2.333989000
C	1.730162000	5.987610000	-0.073881000	F	7.079065000	1.898882000	3.479837000
C	4.294448000	4.371556000	-0.235760000	F	7.249934000	3.830196000	2.499307000
C	4.188801000	5.849346000	-0.654550000	C	-7.709376000	1.044538000	2.461063000
C	3.125448000	6.590209000	0.163104000	F	-7.864126000	-0.288923000	2.620007000
C	0.681286000	3.543211000	-0.010718000	F	-8.932864000	1.601058000	2.453468000
C	2.535378000	2.308569000	-0.033606000	F	-7.048852000	1.498712000	3.547123000
C	3.346502000	1.118123000	0.009021000	C	-7.533362000	2.512253000	-2.367721000
C	4.830141000	1.308786000	-0.003471000	F	-8.870048000	2.383502000	-2.334259000
C	5.563344000	1.128778000	-1.181710000	F	-7.249998000	3.830443000	-2.499263000
C	6.943577000	1.340400000	-1.194708000	F	-7.078580000	1.899248000	-3.479932000
C	7.607516000	1.763051000	-0.043004000	H	-4.894993000	3.820088000	0.964656000
C	5.500250000	1.722566000	1.153350000	H	-4.839838000	4.294611000	-0.714088000
C	6.875477000	1.958615000	1.128190000	H	-1.027167000	6.351434000	-0.682859000
C	7.709398000	1.044064000	-2.461099000	H	-1.337320000	6.325135000	1.043525000
C	2.777195000	-0.145481000	0.057863000	H	-5.165731000	6.326951000	0.535266000
C	3.508485000	-1.424185000	0.144080000	H	-3.935972000	5.909073000	1.721001000
C	2.590750000	-2.423684000	0.083194000	H	-3.111847000	7.654015000	0.092364000
C	4.988280000	-1.660810000	0.321482000	H	-3.373290000	6.524292000	-1.230194000
C	2.972924000	-3.883279000	0.078493000	H	1.027516000	6.351422000	0.682779000
C	4.481532000	-4.080485000	-0.133841000	H	1.337612000	6.325029000	-1.043615000
C	5.282284000	-3.110371000	0.732957000	H	4.895200000	3.819838000	-0.964707000
C	1.247050000	-1.781839000	0.027935000	H	4.840098000	4.294468000	0.714010000
C	-0.000016000	-2.446372000	0.000104000	H	5.166040000	6.326716000	-0.535479000
C	-0.000058000	-3.946260000	0.000028000	H	3.936227000	5.908816000	-1.721151000
C	0.095347000	-4.658726000	1.200083000	H	3.112223000	7.653885000	-0.092584000

C	-0.095535000	-4.658563000	-1.200127000	H	3.373664000	6.524224000	1.230028000
C	-0.109142000	-6.054864000	-1.197228000	H	5.058297000	0.822338000	-2.092244000
C	-0.000216000	-6.762611000	-0.000155000	H	8.676053000	1.939938000	-0.059183000
C	0.108798000	-6.055035000	1.197003000	H	4.949038000	1.863390000	2.077852000
C	-0.305639000	-6.773070000	-2.509110000	H	5.392570000	-0.973174000	1.068829000
C	0.305031000	-6.773391000	2.508840000	H	5.520291000	-1.432617000	-0.610310000
C	-1.247057000	-1.781786000	-0.027713000	H	2.423262000	-4.420018000	-0.697470000
C	-2.590785000	-2.423578000	-0.082954000	H	2.675361000	-4.348148000	1.026610000
C	-3.508478000	-1.424042000	-0.143868000	H	4.741810000	-5.118663000	0.094087000
C	-2.973030000	-3.883155000	-0.078158000	H	4.730527000	-3.916824000	-1.190480000
C	-5.282367000	-3.110181000	-0.732611000	H	6.356572000	-3.299414000	0.645671000
C	-4.988285000	-1.660605000	-0.321246000	H	5.018617000	-3.256682000	1.788408000
C	-4.481640000	-4.080271000	0.134236000	H	0.163677000	-4.122741000	2.141813000
C	-2.777134000	-0.145366000	-0.057702000	H	-0.163800000	-4.122451000	-2.141787000
C	-3.346388000	1.118262000	-0.008924000	H	-0.000269000	-7.845627000	-0.000225000
C	-4.830021000	1.308990000	0.003511000	H	-2.675521000	-4.348102000	-1.026254000
C	-5.563263000	1.129093000	1.181743000	H	-2.423370000	-4.419872000	0.697821000
C	-6.943488000	1.340776000	1.194689000	H	-5.018732000	-3.256581000	-1.788058000
C	-5.500077000	1.722722000	-1.153358000	H	-6.356663000	-3.299165000	-0.645288000
C	-7.607375000	1.763375000	0.042935000	H	-5.392538000	-0.973003000	-1.068645000
C	-6.875296000	1.958828000	-1.128253000	H	-5.520283000	-1.432311000	0.610529000
F	8.933001000	1.600325000	-2.453490000	H	-4.730597000	-3.916518000	1.190870000
F	7.863864000	-0.289427000	-2.620105000	H	-4.741978000	-5.118453000	-0.093606000
F	7.048960000	1.498422000	-3.547134000	H	-5.058257000	0.822692000	2.092312000
F	1.573506000	-6.609656000	2.951056000	H	-4.948837000	1.863461000	-2.077855000
F	-0.511436000	-6.277649000	3.462601000	H	-8.675907000	1.940305000	0.059071000
F	0.073922000	-8.093219000	2.406501000				

Table S13. Coordinates of the optimized broken-symmetry singlet structure for $\mathbf{1}^{+}$ at the UB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4460.05076593			Sum of electronic and zero-point Energies = -4459.149990			
symmetry c1			Sum of electronic and thermal Energies = -4459.081725			
Charge = 1, Multiplicity =1			Sum of electronic and thermal Enthalpies = -4459.080781			
Number of Imaginary Frequencies = 0			Sum of electronic and thermal Free Energies = -4459.263748			
Atom	x	y	z	Atom	x	y	z
C	-2.944925000	3.749508000	0.097612000	F	0.559187000	-6.264267000	-3.455385000
C	-4.302709000	4.384552000	0.233996000	F	-0.039925000	-8.080176000	-2.407519000
C	-1.782807000	4.483484000	0.058366000	F	-1.532450000	-6.597009000	-2.972409000
C	-1.725666000	5.985787000	0.085066000	N	-1.217674000	2.245194000	-0.006356000
C	-4.185945000	5.858328000	0.663523000	N	1.217683000	2.245187000	0.006294000
C	-3.117957000	6.596008000	-0.150922000	N	1.405464000	-0.422187000	0.020722000
C	-2.556301000	2.319319000	0.027236000	N	-1.405467000	-0.422180000	-0.020806000

C	-0.699486000	3.532674000	0.008900000
C	2.944943000	3.749494000	-0.097647000
C	1.782828000	4.483475000	-0.058405000
C	1.725697000	5.985779000	-0.085077000
C	4.302733000	4.384531000	-0.233996000
C	4.185986000	5.858317000	-0.663493000
C	3.117988000	6.595987000	0.150948000
C	0.699502000	3.532670000	-0.008954000
C	2.556310000	2.319306000	-0.027301000
C	3.346002000	1.139746000	0.016454000
C	4.830372000	1.316043000	-0.002225000
C	5.557369000	1.112626000	-1.180328000
C	6.938796000	1.313950000	-1.199230000
C	7.609325000	1.744292000	-0.053997000
C	5.505070000	1.738926000	1.148096000
C	6.882538000	1.960402000	1.116673000
C	7.699257000	0.996315000	-2.463869000
C	2.772725000	-0.147211000	0.070605000
C	3.505778000	-1.410650000	0.168804000
C	2.584363000	-2.419756000	0.111685000
C	4.985430000	-1.649421000	0.355180000
C	2.973028000	-3.878351000	0.127890000
C	4.483531000	-4.074572000	-0.071000000
C	5.274821000	-3.092784000	0.790830000
C	1.253700000	-1.781845000	0.039928000
C	-0.000006000	-2.437580000	-0.000046000
C	-0.000011000	-3.936225000	-0.000023000
C	0.079156000	-4.646030000	1.202326000
C	-0.079176000	-4.646065000	-1.202352000
C	-0.092111000	-6.042242000	-1.198723000
C	-0.000010000	-6.749529000	0.000017000
C	0.092091000	-6.042207000	1.198737000
C	-0.270168000	-6.760675000	-2.513436000
C	0.270148000	-6.760604000	2.513471000
C	-1.253710000	-1.781839000	-0.040021000
C	-2.584377000	-2.419746000	-0.111728000
C	-3.505789000	-1.410636000	-0.168845000
C	-2.973048000	-3.878339000	-0.127881000
C	-5.274859000	-3.092781000	-0.790765000
C	-4.985448000	-1.649407000	-0.355166000
C	-4.483545000	-4.074548000	0.071066000
C	-2.772729000	-0.147198000	-0.070682000
C	-3.345998000	1.139762000	-0.016521000
C	-4.830367000	1.316062000	0.002196000

Ni	0.000001000	0.839005000	-0.000039000
C	7.548733000	2.520251000	2.349128000
F	8.885100000	2.391561000	2.307067000
F	7.101459000	1.911619000	3.466720000
F	7.265412000	3.838559000	2.476680000
C	-7.699194000	0.996336000	2.463908000
F	-7.848269000	-0.339954000	2.603420000
F	-8.924724000	1.548127000	2.468102000
F	-7.036687000	1.437047000	3.554016000
C	-7.548785000	2.520253000	-2.349100000
F	-8.885152000	2.391574000	-2.307003000
F	-7.265458000	3.838559000	-2.476671000
F	-7.101544000	1.911609000	-3.466698000
H	-4.911720000	3.832242000	0.955843000
H	-4.845137000	4.321174000	-0.718664000
H	-1.021379000	6.353102000	-0.668089000
H	-1.335625000	6.317709000	1.057640000
H	-5.159841000	6.343652000	0.548716000
H	-3.931679000	5.908829000	1.730198000
H	-3.099478000	7.658844000	0.108157000
H	-3.366431000	6.534850000	-1.218179000
H	1.021400000	6.353084000	0.668074000
H	1.335676000	6.317723000	-1.057651000
H	4.911751000	3.832232000	-0.955846000
H	4.845146000	4.321126000	0.718671000
H	5.159883000	6.343632000	-0.548658000
H	3.931740000	5.908842000	-1.730171000
H	3.099521000	7.658828000	-0.108109000
H	3.366443000	6.534806000	1.218208000
H	5.047479000	0.798106000	-2.085330000
H	8.679295000	1.911658000	-0.075074000
H	4.956423000	1.898381000	2.070974000
H	5.391565000	-0.951999000	1.092024000
H	5.521353000	-1.441101000	-0.579028000
H	2.430826000	-4.428625000	-0.643675000
H	2.672642000	-4.331310000	1.081009000
H	4.743927000	-5.109581000	0.170921000
H	4.740798000	-3.922636000	-1.127440000
H	6.350040000	-3.282579000	0.717296000
H	5.000288000	-3.224684000	1.845478000
H	0.135117000	-4.109903000	2.144703000
H	-0.135135000	-4.109964000	-2.144744000
H	-0.000010000	-7.832549000	0.000033000
H	-2.672698000	-4.331324000	-1.080998000

C	-5.557337000	1.112646000	1.180315000	H	-2.430822000	-4.428595000	0.643680000
C	-6.938764000	1.313967000	1.199249000	H	-5.000363000	-3.224712000	-1.845418000
C	-5.505094000	1.738940000	-1.148111000	H	-6.350077000	-3.282570000	-0.717189000
C	-7.609321000	1.744304000	0.054031000	H	-5.391605000	-0.952005000	-1.092016000
C	-6.882561000	1.960412000	-1.116658000	H	-5.521339000	-1.441058000	0.579054000
F	8.924783000	1.548116000	-2.468040000	H	-4.740776000	-3.922582000	1.127511000
F	7.848347000	-0.339975000	-2.603366000	H	-4.743953000	-5.109563000	-0.170817000
F	7.036771000	1.437010000	-3.553997000	H	-5.047425000	0.798128000	2.085307000
F	1.532430000	-6.596925000	2.972439000	H	-4.956469000	1.898392000	-2.071003000
F	-0.559207000	-6.264168000	3.455405000	H	-8.679290000	1.911668000	0.075132000
F	0.039904000	-8.080108000	2.407591000				

Table S14. Coordinates of the optimized triplet structure for $\mathbf{1}^{+}$ at the UB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4460.04843735				Sum of electronic and zero-point Energies = -4459.146097			
symmetry c1				Sum of electronic and thermal Energies = -4459.077970			
Charge = -1, Multiplicity = 3				Sum of electronic and thermal Enthalpies = -4459.077026			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -4459.260990			
Atom	x	y	z	Atom	x	y	z
C	-2.951785000	-3.749365000	-0.096991000	F	0.581380000	6.254611000	3.451773000
C	-4.307048000	-4.390806000	-0.233419000	F	-0.024192000	8.070699000	2.407842000
C	-1.783810000	-4.482072000	-0.060193000	F	-1.513284000	6.587640000	2.982163000
C	-1.723760000	-5.984544000	-0.092908000	N	-1.217652000	-2.254784000	0.011118000
C	-4.184339000	-5.861504000	-0.671483000	N	1.217878000	-2.254703000	-0.011110000
C	-3.114578000	-6.599110000	0.140632000	N	1.410695000	0.417669000	-0.024774000
C	-2.567345000	-2.326525000	-0.023767000	N	-1.410647000	0.417570000	0.024903000
C	-0.707640000	-3.528241000	-0.007875000	Ni	0.000066000	-0.846446000	0.000032000
C	2.952114000	-3.749171000	0.096935000	C	7.557047000	-2.526363000	-2.337640000
C	1.784187000	-4.481955000	0.060149000	F	8.893259000	-2.397906000	-2.290550000
C	1.724242000	-5.984433000	0.092770000	F	7.114404000	-1.920483000	-3.458592000
C	4.307429000	-4.390527000	0.233232000	F	7.273500000	-3.844611000	-2.462429000
C	4.184848000	-5.861264000	0.671204000	C	-7.693518000	-0.965496000	-2.464309000
C	3.115088000	-6.598889000	-0.140893000	F	-7.839409000	0.372578000	-2.590699000
C	0.707952000	-3.528194000	0.007864000	F	-8.920184000	-1.514413000	-2.475793000
C	2.567575000	-2.326352000	0.023830000	F	-7.030056000	-1.396760000	-3.557406000
C	3.346082000	-1.150245000	-0.020654000	C	-7.557009000	-2.526223000	2.337752000
C	4.830598000	-1.318797000	0.001537000	F	-8.893224000	-2.397841000	2.290526000
C	5.554223000	-1.100629000	1.178991000	F	-7.273406000	-3.844424000	2.462907000
C	6.936261000	-1.296240000	1.201236000	F	-7.114481000	-1.920030000	3.458581000

C	7.610280000	-1.732483000	0.060187000	H	-4.921420000	-3.837632000	-0.950154000
C	5.507608000	-1.748923000	-1.144494000	H	-4.847151000	-4.337300000	0.721184000
C	6.886287000	-1.961921000	-1.109599000	H	-1.019111000	-6.354489000	0.658520000
C	7.693853000	-0.964421000	2.464019000	H	-1.334078000	-6.312718000	-1.066929000
C	2.771434000	0.146416000	-0.078220000	H	-5.156583000	-6.351184000	-0.560653000
C	3.505295000	1.404454000	-0.183057000	H	-3.928327000	-5.905161000	-1.738066000
C	2.582370000	2.416942000	-0.127761000	H	-3.093350000	-7.661084000	-0.121966000
C	4.984393000	1.644159000	-0.375148000	H	-3.363911000	-6.542226000	1.207994000
C	2.972829000	3.875446000	-0.154545000	H	1.019577000	-6.354376000	-0.658644000
C	4.484322000	4.071747000	0.036576000	H	1.334637000	-6.312701000	1.066792000
C	5.270880000	3.084326000	-0.822970000	H	4.921802000	-3.837361000	0.949972000
C	1.258879000	1.779421000	-0.047466000	H	4.847471000	-4.336910000	-0.721399000
C	-0.000045000	2.430788000	0.000099000	H	5.157118000	-6.350870000	0.560279000
C	-0.000118000	3.928588000	0.000087000	H	3.928906000	-5.905012000	1.737800000
C	0.071318000	4.636848000	-1.203414000	H	3.093948000	-7.660881000	0.121637000
C	-0.071737000	4.636847000	1.203577000	H	3.364352000	-6.541918000	-1.208267000
C	-0.084453000	6.032935000	1.199531000	H	5.041668000	-0.780514000	2.080476000
C	-0.000418000	6.739991000	0.000070000	H	8.681030000	-1.894344000	0.083956000
C	0.083744000	6.032940000	-1.199384000	H	4.960122000	-1.920598000	-2.065779000
C	-0.253993000	6.751452000	2.515590000	H	5.390517000	0.941505000	-1.106900000
C	0.253097000	6.751475000	-2.515458000	H	5.522918000	1.445384000	0.559617000
C	-1.258918000	1.779330000	0.047641000	H	2.434927000	4.431694000	0.615691000
C	-2.582447000	2.416769000	0.127866000	H	2.670006000	4.322677000	-1.109603000
C	-3.505312000	1.404226000	0.183166000	H	4.744133000	5.105157000	-0.212709000
C	-2.972988000	3.875252000	0.154597000	H	4.746404000	3.925973000	1.092702000
C	-5.271001000	3.084015000	0.823007000	H	6.346462000	3.274692000	-0.756605000
C	-4.984427000	1.643854000	0.375222000	H	4.990604000	3.208881000	-1.877018000
C	-4.484489000	4.071463000	-0.036551000	H	0.121529000	4.100846000	-2.146146000
C	-2.771369000	0.146230000	0.078346000	H	-0.121887000	4.100847000	2.146314000
C	-3.345931000	-1.150471000	0.020755000	H	-0.000532000	7.823021000	0.000064000
C	-4.830435000	-1.319116000	-0.001515000	H	-2.670207000	4.322525000	1.109649000
C	-5.553979000	-1.101276000	-1.179080000	H	-2.435098000	4.431509000	-0.615643000
C	-6.936004000	-1.296970000	-1.201388000	H	-4.990749000	3.208610000	1.877057000
C	-5.507513000	-1.748996000	1.144567000	H	-6.346592000	3.274318000	0.756623000
C	-7.610092000	-1.732958000	-0.060281000	H	-5.390529000	0.941193000	1.106981000
C	-6.886180000	-1.962067000	1.109618000	H	-5.522924000	1.445033000	-0.559548000
F	8.920573000	-1.513216000	2.475518000	H	-4.746545000	3.925648000	-1.092677000
F	7.839625000	0.373695000	2.590113000	H	-4.744364000	5.104863000	0.212707000
F	7.030531000	-1.395515000	3.557269000	H	-5.041369000	-0.781365000	-2.080606000
F	1.512391000	6.587863000	-2.982096000	H	-4.960094000	-1.920406000	2.065942000
F	-0.582244000	6.254493000	-3.451593000	H	-8.680833000	-1.894872000	-0.084091000
F	0.023090000	8.070684000	-2.407707000				

Table S15. Coordinates of the optimized structure for **2** at the UB3LYP/6-31G(d,p) (for C, N, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -1592.50902605				Sum of electronic and zero-point Energies = -1591.916550			
symmetry c1				Sum of electronic and thermal Energies = -1591.880470			
Charge = 0, Multiplicity = 2				Sum of electronic and thermal Enthalpies = -1591.879526			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -1591.984865			
Atom	x	y	z	Atom	x	y	z
C	3.032355000	0.727951000	-0.100334000	H	0.706019000	4.400793000	-0.030345000
C	3.965477000	1.827419000	-0.141484000	H	-3.994331000	-0.003258000	0.134895000
C	3.200443000	2.987902000	-0.115980000	H	0.713166000	-4.399459000	-0.020711000
C	1.812800000	2.581765000	-0.059322000	H	4.690886000	4.498441000	-0.508723000
N	1.772305000	1.211670000	-0.051324000	H	3.029983000	5.043052000	-0.740497000
C	0.639907000	3.317692000	-0.021855000	H	3.673318000	4.842970000	0.890013000
C	-0.656891000	2.746126000	0.025302000	H	5.804703000	1.100836000	-1.016286000
C	-1.900673000	3.478808000	0.067434000	H	5.910557000	2.723155000	-0.332552000
C	-2.915420000	2.540802000	0.098761000	H	5.878941000	1.320286000	0.731727000
C	-2.277646000	1.245737000	0.071697000	H	5.921874000	-2.715943000	-0.074278000
N	-0.912370000	1.399874000	0.028547000	H	5.815934000	-1.322601000	-1.145903000
C	-2.909830000	-0.001932000	0.093138000	H	5.867831000	-1.087623000	0.601001000
C	-2.274381000	-1.250518000	0.070845000	H	3.052341000	-5.052489000	0.470943000
C	-2.910381000	-2.545754000	0.100595000	H	3.670371000	-4.812012000	-1.164011000
C	-1.894097000	-3.482645000	0.070516000	H	4.707133000	-4.496077000	0.227091000
C	-0.651689000	-2.748637000	0.025815000	H	-3.006387000	-5.275889000	-0.255893000
N	-0.910355000	-1.401433000	0.026145000	H	-1.293683000	-5.440918000	-0.558501000
C	0.644887000	-3.316388000	-0.018722000	H	-0.842739000	-5.309858000	1.936361000
C	1.818549000	-2.578589000	-0.062295000	H	-2.576850000	-5.162899000	2.227962000
C	3.205579000	-2.982118000	-0.107371000	H	-1.923266000	-6.655459000	1.527664000
C	3.969228000	-1.819314000	-0.132625000	H	-4.890175000	-2.052546000	0.751404000
C	3.034764000	-0.722778000	-0.102973000	H	-4.598258000	-3.765689000	0.572334000
N	1.774675000	-1.209088000	-0.061459000	H	-6.111152000	-2.936923000	-1.236907000
Ni	0.361011000	0.000043000	-0.012153000	H	-4.591125000	-3.519860000	-1.940265000
C	3.673103000	4.410588000	-0.119199000	H	-4.872682000	-1.785786000	-1.771557000
C	5.461890000	1.736273000	-0.193310000	H	-4.605595000	3.758536000	0.567638000
C	5.465646000	-1.729344000	-0.189455000	H	-4.895094000	2.044887000	0.747174000
C	3.683007000	-4.402986000	-0.145107000	H	-1.303603000	5.436058000	-0.567623000
C	-2.021206000	-4.981137000	0.122315000	H	-3.015569000	5.269957000	-0.261393000
C	-1.829361000	-5.564140000	1.536285000	H	-1.930293000	6.655425000	1.516426000
C	-4.394104000	-2.792736000	0.111241000	H	-2.581413000	5.164215000	2.221858000
C	-5.032081000	-2.756512000	-1.291335000	H	-0.847889000	5.311941000	1.926828000
C	-4.399418000	2.785622000	0.107396000	H	-6.114712000	2.926292000	-1.243172000
C	-2.029384000	4.977276000	0.115774000	H	-4.873570000	1.776922000	-1.775528000
C	-1.835450000	5.564215000	1.527811000	H	-4.594753000	3.511438000	-1.944804000
C	-5.035292000	2.747641000	-1.296132000				

Table S16. Coordinates of the optimized structure for singlet $\mathbf{2}^{+}$ at the RB3LYP/6-31G(d,p) (for C, N, H) and SDD (for Ni) level of theory.

SCF Done: E(RB3LYP) = -1592.30431795				Sum of electronic and zero-point Energies = -1591.709142			
symmetry c1				Sum of electronic and thermal Energies = -1591.673602			
Charge = 1, Multiplicity =1				Sum of electronic and thermal Enthalpies = -1591.672658			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -1591.774912			
Atom	x	y	z	Atom	x	y	z
C	3.066135000	0.684585000	-0.107969000	H	0.706221000	4.388553000	-0.014311000
C	3.991165000	1.816946000	-0.144361000	H	-3.993834000	0.000130000	0.125630000
C	3.218433000	2.948603000	-0.114056000	H	0.705952000	-4.388584000	-0.014014000
C	1.801362000	2.519685000	-0.058670000	H	4.717872000	4.495104000	-0.173127000
N	1.745964000	1.202523000	-0.056319000	H	3.209608000	4.905952000	-0.996938000
C	0.614441000	3.309785000	-0.011851000	H	3.278548000	4.906561000	0.765598000
C	-0.639692000	2.748982000	0.033905000	H	5.818713000	1.198304000	-1.100523000
C	-1.915177000	3.488188000	0.075092000	H	5.935403000	2.723484000	-0.222973000
C	-2.908955000	2.560118000	0.095131000	H	5.889481000	1.199643000	0.663754000
C	-2.256117000	1.232083000	0.070215000	H	5.935074000	-2.723978000	-0.225429000
N	-0.907852000	1.378533000	0.034455000	H	5.818451000	-1.196488000	-1.099006000
C	-2.912294000	0.000095000	0.089965000	H	5.889556000	-1.202427000	0.665234000
C	-2.256233000	-1.231945000	0.069986000	H	3.280261000	-4.905899000	0.767758000
C	-2.909132000	-2.559934000	0.094765000	H	3.206345000	-4.907162000	-0.994547000
C	-1.915397000	-3.488059000	0.074758000	H	4.717095000	-4.495910000	-0.175474000
C	-0.639918000	-2.748928000	0.033736000	H	-3.016467000	-5.283390000	-0.236082000
N	-0.907975000	-1.378467000	0.034183000	H	-1.309278000	-5.427457000	-0.580376000
C	0.614237000	-3.309806000	-0.011634000	H	-0.806674000	-5.306028000	1.917521000
C	1.801204000	-2.519864000	-0.058181000	H	-2.539938000	-5.191612000	2.237396000
C	3.218179000	-2.948913000	-0.113727000	H	-1.871544000	-6.660715000	1.507926000
C	3.990999000	-1.817339000	-0.144103000	H	-4.860783000	-2.074621000	0.807065000
C	3.066035000	-0.684888000	-0.107627000	H	-4.614586000	-3.774628000	0.479573000
N	1.745944000	-1.202628000	-0.055642000	H	-6.120438000	-2.750316000	-1.231509000
Ni	0.352852000	-0.000024000	-0.006977000	H	-4.633354000	-3.329400000	-2.000646000
C	3.633410000	4.383404000	-0.130704000	H	-4.855549000	-1.603050000	-1.700085000
C	5.484109000	1.730216000	-0.203945000	H	-4.614314000	3.774774000	0.480432000
C	5.483939000	-1.730697000	-0.203779000	H	-4.860595000	2.074688000	0.807386000
C	3.632800000	-4.383813000	-0.130115000	H	-1.309248000	5.427472000	-0.580491000
C	-2.026410000	-4.985063000	0.121907000	H	-3.016291000	5.283540000	-0.235398000
C	-1.795694000	-5.569870000	1.530542000	H	-1.870529000	6.661020000	1.507891000
C	-4.394668000	-2.772206000	0.100188000	H	-2.538776000	5.192085000	2.237822000
C	-5.038576000	-2.601624000	-1.291578000	H	-0.805622000	5.306311000	1.917303000
C	-4.394482000	2.772466000	0.100694000	H	-6.120348000	2.751206000	-1.230881000
C	-2.026089000	4.985196000	0.122171000	H	-4.855679000	1.603872000	-1.699856000
C	-1.794757000	5.570173000	1.530636000	H	-4.633236000	3.330262000	-1.999981000
C	-5.038512000	2.602368000	-1.291065000				

Table S17. Coordinates of the optimized structure for broken-symmetry singlet $\mathbf{2}^{+}$ at the UB3LYP/6-31G(d,p) (for C, N, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -1592.30463051				Sum of electronic and zero-point Energies = -1591.711438			
symmetry c1				Sum of electronic and thermal Energies = -1591.675668			
Charge = 1, Multiplicity =1				Sum of electronic and thermal Enthalpies = -1591.674724			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -1591.777797			
Atom	x	y	z	Atom	x	y	z
C	3.058311000	0.693946000	-0.107023000	H	0.707584000	4.388890000	-0.016504000
C	3.987295000	1.817416000	-0.143911000	H	-3.993055000	0.000159000	0.130020000
C	3.216836000	2.955338000	-0.114095000	H	0.707253000	-4.388929000	-0.016613000
C	1.803880000	2.529612000	-0.058793000	H	4.726121000	4.491968000	-0.175282000
N	1.750999000	1.203288000	-0.055761000	H	3.220547000	4.913817000	-0.996957000
C	0.620356000	3.309323000	-0.013258000	H	3.292186000	4.913733000	0.765796000
C	-0.643273000	2.747302000	0.032872000	H	5.815388000	1.195438000	-1.099650000
C	-1.911698000	3.487329000	0.073800000	H	5.933407000	2.720152000	-0.222840000
C	-2.909856000	2.557748000	0.096528000	H	5.885969000	1.197662000	0.664759000
C	-2.258810000	1.235140000	0.071632000	H	5.933110000	-2.720559000	-0.225516000
N	-0.908355000	1.381741000	0.034184000	H	5.815174000	-1.193709000	-1.098634000
C	-2.911066000	0.000118000	0.092642000	H	5.886060000	-1.200206000	0.665752000
C	-2.258901000	-1.234953000	0.071664000	H	3.292791000	-4.913641000	0.766226000
C	-2.910049000	-2.557510000	0.096586000	H	3.219211000	-4.914356000	-0.996446000
C	-1.911970000	-3.487170000	0.073844000	H	4.725721000	-4.492308000	-0.176558000
C	-0.643480000	-2.747240000	0.032855000	H	-3.013980000	-5.281292000	-0.242274000
N	-0.908458000	-1.381661000	0.034193000	H	-1.306290000	-5.428443000	-0.579890000
C	0.620096000	-3.309358000	-0.013346000	H	-0.812220000	-5.310319000	1.919165000
C	1.803683000	-2.529718000	-0.058920000	H	-2.545840000	-5.189471000	2.233819000
C	3.216600000	-2.955562000	-0.114279000	H	-1.880813000	-6.661066000	1.506248000
C	3.987149000	-1.817697000	-0.144105000	H	-4.865131000	-2.075160000	0.804719000
C	3.058275000	-0.694157000	-0.107114000	H	-4.611064000	-3.775864000	0.489708000
N	1.750899000	-1.203407000	-0.055875000	H	-6.120319000	-2.774424000	-1.229792000
Ni	0.354137000	-0.000003000	-0.007123000	H	-4.628474000	-3.346452000	-1.994915000
C	3.640953000	4.387968000	-0.131235000	H	-4.863742000	-1.620249000	-1.703976000
C	5.480623000	1.727533000	-0.203314000	H	-4.610781000	3.776311000	0.489380000
C	5.480484000	-1.727919000	-0.203549000	H	-4.864987000	2.075686000	0.804726000
C	3.640607000	-4.388221000	-0.131384000	H	-1.305734000	5.428561000	-0.579804000
C	-2.024923000	-4.984495000	0.119838000	H	-3.013501000	5.281550000	-0.242526000
C	-1.801065000	-5.570487000	1.528973000	H	-1.880544000	6.661201000	1.506245000
C	-4.395134000	-2.775305000	0.103063000	H	-2.545812000	5.189643000	2.233671000
C	-5.039544000	-2.617952000	-1.289948000	H	-0.812127000	5.310359000	1.919311000
C	-4.394921000	2.775658000	0.102941000	H	-6.120082000	2.774637000	-1.229948000
C	-2.024540000	4.984665000	0.119777000	H	-4.863568000	1.620295000	-1.703895000
C	-1.800887000	5.570616000	1.528961000	H	-4.628185000	3.346429000	-1.995148000
C	-5.039316000	2.618084000	-1.290056000				

Table S18. Coordinates of the optimized structure for triplet $\mathbf{2}^{+}$ at the UB3LYP/6-31G(d,p) (for C, N, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -1592.30104876				Sum of electronic and zero-point Energies = -1591.706803			
symmetry c1				Sum of electronic and thermal Energies = -1591.671747			
Charge = 1, Multiplicity = 3				Sum of electronic and thermal Enthalpies = -1591.670802			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -1591.773918			
Atom	x	y	z	Atom	x	y	z
C	3.040123000	0.714174000	-0.103978000	H	0.708879000	4.390506000	-0.022789000
C	3.978038000	1.821399000	-0.139928000	H	-3.990421000	0.000134000	0.136371000
C	3.212487000	2.972101000	-0.112609000	H	0.708588000	-4.390550000	-0.022865000
C	1.810284000	2.554557000	-0.060002000	H	4.744153000	4.486485000	-0.171052000
N	1.762908000	1.204976000	-0.056378000	H	3.250609000	4.931300000	-0.999057000
C	0.633364000	3.309047000	-0.017929000	H	3.316301000	4.933035000	0.764768000
C	-0.650761000	2.743411000	0.028756000	H	5.808228000	1.191221000	-1.091500000
C	-1.905452000	3.485860000	0.070332000	H	5.929014000	2.714540000	-0.215142000
C	-2.912418000	2.553596000	0.098465000	H	5.874996000	1.194084000	0.673100000
C	-2.264479000	1.243305000	0.072609000	H	5.928730000	-2.714911000	-0.218098000
N	-0.908820000	1.389917000	0.031274000	H	5.807938000	-1.189389000	-1.090631000
C	-2.907382000	0.000097000	0.095502000	H	5.875181000	-1.196662000	0.673935000
C	-2.264560000	-1.243153000	0.072655000	H	3.317040000	-4.932932000	0.765085000
C	-2.912583000	-2.553401000	0.098574000	H	3.249239000	-4.931829000	-0.998661000
C	-1.905678000	-3.485731000	0.070433000	H	4.743797000	-4.486799000	-0.172579000
C	-0.650940000	-2.743365000	0.028787000	H	-3.008467000	-5.277893000	-0.256132000
N	-0.908912000	-1.389854000	0.031290000	H	-1.299055000	-5.431611000	-0.576344000
C	0.633144000	-3.309085000	-0.017973000	H	-0.826892000	-5.316086000	1.925132000
C	1.810113000	-2.554673000	-0.060085000	H	-2.561644000	-5.181489000	2.226340000
C	3.212282000	-2.972309000	-0.112853000	H	-1.902480000	-6.659377000	1.506052000
C	3.977909000	-1.821658000	-0.140173000	H	-4.876002000	-2.070316000	0.790389000
C	3.040074000	-0.714372000	-0.104023000	H	-4.604886000	-3.774732000	0.519495000
N	1.762829000	-1.205089000	-0.056369000	H	-6.118277000	-2.839164000	-1.229171000
Ni	0.358633000	-0.000010000	-0.009494000	H	-4.615660000	-3.404205000	-1.978076000
C	3.657264000	4.399857000	-0.130538000	H	-4.878466000	-1.676049000	-1.725590000
C	5.471870000	1.723765000	-0.196079000	H	-4.604660000	3.775065000	0.519236000
C	5.471743000	-1.724116000	-0.196472000	H	-4.875890000	2.070686000	0.790251000
C	3.656961000	-4.400096000	-0.130826000	H	-1.298671000	5.431671000	-0.576499000
C	-2.022264000	-4.983511000	0.115861000	H	-3.008106000	5.278083000	-0.256353000
C	-1.814764000	-5.569377000	1.527448000	H	-1.902099000	6.659568000	1.505817000
C	-4.396738000	-2.782475000	0.107625000	H	-2.561402000	5.181760000	2.226141000
C	-5.039867000	-2.667200000	-1.289904000	H	-0.826627000	5.316219000	1.925007000
C	-4.396559000	2.782763000	0.107449000	H	-6.118050000	2.839455000	-1.229410000
C	-2.021939000	4.983650000	0.115695000	H	-4.878293000	1.676225000	-1.725697000
C	-1.814462000	5.569563000	1.527265000	H	-4.615373000	3.404346000	-1.978308000
C	-5.039648000	2.667420000	-1.290093000				

Table S19. Coordinates of the optimized structure for **3** at the UB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4450.62157920				Sum of electronic and zero-point Energies = -4449.905149			
symmetry c1				Sum of electronic and thermal Energies = -4449.841102			
Charge = 0, Multiplicity = 2				Sum of electronic and thermal Enthalpies = -4449.840158			
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies = -4450.016244			
Atom	x	y	z	Atom	x	y	z
C	-0.690824000	-3.618768000	0.042596000	C	2.913637000	3.649055000	0.764021000
C	-1.770218000	-4.565859000	0.181021000	C	4.255855000	3.928954000	1.006631000
C	-2.971229000	-3.798560000	0.199257000	C	5.217159000	2.915293000	0.947367000
C	-2.571707000	-2.390236000	0.066935000	C	4.848409000	1.603776000	0.660784000
N	-1.226931000	-2.340031000	0.011608000	C	-0.913741000	6.710605000	2.336935000
C	-3.353872000	-1.215366000	-0.042171000	F	-2.239166000	6.957660000	2.240044000
C	-2.780228000	0.052991000	-0.165809000	F	-0.720600000	6.016912000	3.477938000
C	-3.498729000	1.307239000	-0.418170000	F	-0.297821000	7.904710000	2.472223000
C	-2.530215000	2.335197000	-0.453724000	C	0.913697000	6.710678000	-2.336670000
C	-1.233410000	1.696556000	-0.180669000	F	2.239178000	6.957483000	-2.239935000
N	-1.416056000	0.340015000	-0.074283000	F	0.297969000	7.904901000	-2.471784000
C	0.000021000	2.350464000	0.000065000	F	0.720285000	6.017110000	-3.477706000
C	1.233451000	1.696576000	0.180797000	C	7.622666000	-2.246254000	2.488879000
C	2.530252000	2.335186000	0.453888000	F	7.925847000	-1.122488000	3.176935000
C	3.498759000	1.307221000	0.418310000	F	6.868114000	-3.015750000	3.301118000
C	2.780254000	0.052998000	0.165864000	F	8.782270000	-2.899522000	2.263912000
N	1.416092000	0.340029000	0.074335000	C	7.730174000	-1.166682000	-2.420482000
C	3.353900000	-1.215351000	0.042101000	F	8.914166000	-1.814548000	-2.417590000
C	2.571722000	-2.390227000	-0.066842000	F	7.993892000	0.146555000	-2.601422000
C	2.971231000	-3.798553000	-0.199212000	F	7.036527000	-1.582457000	-3.501385000
C	1.770236000	-4.565868000	-0.180623000	C	-7.622462000	-2.245683000	-2.489469000
C	0.690859000	-3.618775000	-0.042022000	F	-6.868053000	-3.015501000	-3.301543000
N	1.226963000	-2.340042000	-0.011194000	F	-7.925002000	-1.121791000	-3.177597000
Ni	0.000001000	-0.929211000	0.000113000	F	-8.782387000	-2.898460000	-2.264758000
C	0.000011000	3.847763000	0.000091000	C	-7.730374000	-1.167320000	2.420117000
C	-4.840751000	-1.378399000	-0.043058000	F	-7.036222000	-1.581754000	3.501197000
C	4.840783000	-1.378369000	0.042838000	F	-8.913619000	-1.816574000	2.417565000
C	0.409752000	4.560942000	-1.133613000	F	-7.995663000	0.145692000	2.600414000
C	0.408769000	5.957288000	-1.132337000	H	0.724942000	4.022319000	-2.020507000
C	-0.000024000	6.663273000	0.000137000	H	-0.000042000	7.746986000	0.000155000
C	-0.408794000	5.957236000	1.132597000	H	-0.724925000	4.022236000	2.020700000
C	-0.409740000	4.560899000	1.133829000	H	-5.060660000	-0.947971000	2.055366000
C	-5.574947000	-1.212776000	1.137689000	H	-8.704133000	-1.908782000	-0.014471000
C	-6.959505000	-1.399384000	1.145174000	H	-4.963183000	-1.885133000	-2.133329000
C	-7.632264000	-1.752524000	-0.024652000	H	4.963322000	-1.885653000	2.132979000
C	-6.904641000	-1.921095000	-1.203957000	H	8.704169000	-1.908714000	0.013930000

C	-5.520293000	-1.739522000	-1.214127000	H	5.060586000	-0.947373000	-2.055467000
C	5.520392000	-1.739800000	1.213794000	H	5.133086000	-3.892434000	-0.395652000
C	6.904724000	-1.921362000	1.203513000	H	5.182753000	-6.335658000	-0.626124000
C	7.632301000	-1.752477000	0.024205000	H	3.088512000	-7.658870000	-0.613785000
C	6.959494000	-1.399027000	-1.145478000	H	0.900474000	-6.542340000	-0.371419000
C	5.574919000	-1.212422000	-1.137882000	H	-0.900455000	-6.542280000	0.372333000
C	4.204287000	-4.444681000	-0.361690000	H	-3.088529000	-7.658828000	0.614318000
C	4.229728000	-5.831178000	-0.498993000	H	-5.182803000	-6.335660000	0.625934000
C	3.044356000	-6.580984000	-0.489784000	H	-5.133135000	-3.892473000	0.395140000
C	1.810442000	-5.956320000	-0.337053000	H	-5.611105000	0.841217000	-0.644204000
C	-1.810429000	-5.956287000	0.337654000	H	-6.261053000	3.145683000	-1.137451000
C	-3.044367000	-6.580959000	0.490171000	H	-4.552517000	4.945011000	-1.248388000
C	-4.229757000	-5.831177000	0.498976000	H	-2.196238000	4.450995000	-0.838354000
C	-4.204311000	-4.444695000	0.361509000	H	2.196260000	4.450961000	0.838622000
C	-4.848403000	1.603835000	-0.660445000	H	4.552502000	4.944895000	1.249037000
C	-5.217173000	2.915392000	-0.946837000	H	6.261016000	3.145549000	1.138149000
C	-4.255862000	3.929040000	-1.006123000	H	5.611106000	0.841151000	0.644509000
C	-2.913617000	3.649096000	-0.763698000				

Table S20. Coordinates of the optimized structure for single $\mathbf{3}^{+}$ at the RB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level of theory.

SCF Done: E(UB3LYP) = -4450.41074818				Sum of electronic and zero-point Energies=			-4449.692746
symmetry c1				Sum of electronic and thermal Energies=			-4449.628725
Charge = 1, Multiplicity = 1				Sum of electronic and thermal Enthalpies=			-4449.627781
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies=			-4449.803643
Atom	x	y	z	Atom	x	y	z
C	0.680209000	-3.627509000	-0.049680000	C	-2.915778000	3.655239000	-0.716493000
C	1.770274000	-4.571909000	-0.180826000	C	-4.265988000	3.938473000	-0.940500000
C	2.962275000	-3.798916000	-0.197897000	C	-5.224971000	2.929411000	-0.875852000
C	2.550406000	-2.383755000	-0.073742000	C	-4.853584000	1.610237000	-0.602684000
N	1.224061000	-2.326256000	-0.027258000	C	0.846361000	6.713909000	-2.368236000
C	3.352044000	-1.201641000	0.032171000	F	2.176385000	6.936955000	-2.312324000
C	2.781092000	0.054773000	0.150498000	F	0.602242000	6.017355000	-3.497068000
C	3.504357000	1.317409000	0.383550000	F	0.239777000	7.910776000	-2.476932000
C	2.537086000	2.341179000	0.424020000	C	-0.846302000	6.714186000	2.367890000
C	1.231327000	1.695889000	0.168711000	F	-2.176324000	6.937226000	2.311947000
N	1.406949000	0.344487000	0.071083000	F	-0.239717000	7.911066000	2.476455000
C	0.000008000	2.358332000	0.000075000	F	-0.602186000	6.017757000	3.496801000
C	-1.231321000	1.695894000	-0.168503000	C	-7.607622000	-2.198075000	-2.512549000
C	-2.537073000	2.341176000	-0.423853000	F	-7.885914000	-1.058217000	-3.179268000
C	-3.504363000	1.317429000	-0.383251000	F	-6.846771000	-2.961352000	-3.324426000
C	-2.781104000	0.054793000	-0.150172000	F	-8.770600000	-2.842125000	-2.303996000

N	-1.406971000	0.344507000	-0.070675000
C	-3.352062000	-1.201628000	-0.031937000
C	-2.550427000	-2.383755000	0.073813000
C	-2.962299000	-3.798932000	0.197790000
C	-1.770301000	-4.571929000	0.180594000
C	-0.680235000	-3.627512000	0.049573000
N	-1.224080000	-2.326252000	0.027332000
Ni	0.000000000	-0.921099000	0.000140000
C	0.000026000	3.856753000	-0.000005000
C	4.838494000	-1.375280000	0.038310000
C	-4.838512000	-1.375261000	-0.038152000
C	-0.375555000	4.566516000	1.147287000
C	-0.375311000	5.962759000	1.144855000
C	0.000036000	6.667700000	-0.000171000
C	0.375375000	5.962620000	-1.145113000
C	0.375606000	4.566376000	-1.147382000
C	5.570089000	-1.241930000	-1.147949000
C	6.953324000	-1.436398000	-1.148972000
C	7.622422000	-1.765033000	0.030483000
C	6.894721000	-1.900059000	1.214267000
C	5.511444000	-1.710765000	1.220356000
C	-5.511409000	-1.710738000	-1.220231000
C	-6.894683000	-1.900037000	-1.214205000
C	-7.622439000	-1.765018000	-0.030453000
C	-6.953399000	-1.436378000	1.149031000
C	-5.570162000	-1.241905000	1.148072000
C	-4.199766000	-4.427891000	0.351191000
C	-4.235052000	-5.819950000	0.482428000
C	-3.059464000	-6.575733000	0.474207000
C	-1.815294000	-5.957939000	0.328655000
C	1.815259000	-5.957899000	-0.329069000
C	3.059431000	-6.575685000	-0.474648000
C	4.235024000	-5.819909000	-0.482726000
C	4.199742000	-4.427863000	-0.351334000
C	4.853567000	1.610197000	0.603071000
C	5.224966000	2.929384000	0.876166000
C	4.266006000	3.938477000	0.940648000
C	2.915804000	3.655258000	0.716566000

C	-7.725550000	-1.236705000	2.432428000
F	-8.902387000	-1.888701000	2.412034000
F	-7.986081000	0.071333000	2.637260000
F	-7.022107000	-1.675847000	3.496846000
C	7.607711000	-2.198103000	2.512581000
F	6.846920000	-2.961442000	3.324451000
F	7.885955000	-1.058244000	3.179332000
F	8.770718000	-2.842079000	2.303982000
C	7.725433000	-1.236722000	-2.432395000
F	7.021892000	-1.675715000	-3.496810000
F	8.902198000	-1.888861000	-2.412097000
F	7.986109000	0.071293000	-2.637152000
H	-0.662457000	4.031095000	2.045938000
H	0.000041000	7.751614000	-0.000240000
H	0.662492000	4.030845000	-2.045973000
H	5.061043000	-0.996507000	-2.074129000
H	8.693748000	-1.926910000	0.024823000
H	4.956842000	-1.829814000	2.145213000
H	-4.956761000	-1.829787000	-2.145061000
H	-8.693765000	-1.926898000	-0.024844000
H	-5.061162000	-0.996473000	2.074276000
H	-5.123882000	-3.869209000	0.382076000
H	-5.192083000	-6.317142000	0.602328000
H	-3.111205000	-7.653401000	0.591157000
H	-0.911745000	-6.552974000	0.360897000
H	0.911704000	-6.552917000	-0.361450000
H	3.111168000	-7.653341000	-0.591716000
H	5.192060000	-6.317091000	-0.602629000
H	5.123864000	-3.869186000	-0.382130000
H	5.616711000	0.848884000	0.578341000
H	6.270742000	3.162022000	1.049242000
H	4.563674000	4.956594000	1.169715000
H	2.199221000	4.457083000	0.790933000
H	-2.199179000	4.457040000	-0.790974000
H	-4.563649000	4.956581000	-1.169618000
H	-6.270758000	3.162067000	-1.048838000
H	-5.616752000	0.848952000	-0.577803000

Table S21. Coordinates of the optimized structure for triplet $\mathbf{3}^{+}$ at the UB3LYP/6-31G(d,p) (for C, N, F, H) and SDD (for Ni) level.

SCF Done: E(UB3LYP) = -4450.39870845				Sum of electronic and zero-point Energies=	-4449.681604		
symmetry c1				Sum of electronic and thermal Energies=	-4449.617489		
Charge = 1, Multiplicity = 3				Sum of electronic and thermal Enthalpies=	-4449.616545		
Number of Imaginary Frequencies = 0				Sum of electronic and thermal Free Energies=	-4449.793481		
Atom	x	y	z	Atom	x	y	z
C	0.709108000	-3.610242000	-0.045745000	C	-2.886423000	3.624534000	-0.891962000
C	1.774341000	-4.566981000	-0.214771000	C	-4.222760000	3.890760000	-1.184523000
C	2.980206000	-3.807400000	-0.226463000	C	-5.183198000	2.875080000	-1.138584000
C	2.588744000	-2.399891000	-0.060424000	C	-4.823925000	1.569611000	-0.813154000
N	1.225978000	-2.353716000	0.006170000	C	1.025096000	6.691205000	-2.296471000
C	3.352744000	-1.237686000	0.067511000	F	2.346485000	6.915071000	-2.138265000
C	2.764961000	0.047996000	0.219111000	F	0.868805000	5.994452000	-3.440562000
C	3.481061000	1.286703000	0.519549000	F	0.427480000	7.887384000	-2.450950000
C	2.512778000	2.318590000	0.545559000	C	-1.025653000	6.691302000	2.296006000
C	1.229572000	1.687471000	0.222595000	F	-2.347014000	6.915225000	2.137670000
N	1.416750000	0.329319000	0.097119000	F	-0.427998000	7.887461000	2.450510000
C	-0.000090000	2.338542000	-0.000070000	F	-0.869498000	5.994570000	3.440129000
C	-1.229707000	1.687383000	-0.222720000	C	-7.641256000	-2.327488000	-2.446696000
C	-2.512949000	2.318395000	-0.545746000	F	-7.930991000	-1.229980000	-3.176256000
C	-3.481156000	1.286431000	-0.519741000	F	-6.889513000	-3.137167000	-3.221107000
C	-2.764977000	0.047796000	-0.219199000	F	-8.800018000	-2.959355000	-2.184314000
N	-1.416801000	0.329230000	-0.097125000	C	-7.706963000	-1.015094000	2.417587000
C	-3.352659000	-1.237953000	-0.067619000	F	-8.896901000	-1.642164000	2.447302000
C	-2.588549000	-2.400118000	0.059917000	F	-7.938841000	0.308836000	2.535221000
C	-2.979849000	-3.807667000	0.225990000	F	-7.005253000	-1.396530000	3.505064000
C	-1.773932000	-4.567157000	0.213901000	C	7.640904000	-2.326540000	2.447734000
C	-0.708812000	-3.610304000	0.044732000	F	6.888910000	-3.135715000	3.222420000
N	-1.225792000	-2.353830000	-0.007018000	F	7.930832000	-1.228785000	3.176858000
Ni	0.000042000	-0.938824000	-0.000198000	F	8.799548000	-2.958777000	2.185723000
C	-0.000137000	3.836053000	-0.000110000	C	7.707486000	-1.015487000	-2.416918000
C	4.841578000	-1.382829000	0.052721000	F	7.006340000	-1.398193000	-3.504320000
C	-4.841477000	-1.383153000	-0.052481000	F	8.897861000	-1.641753000	-2.445856000
C	-0.465131000	4.543435000	1.115052000	F	7.938458000	0.308518000	-2.535445000
C	-0.462415000	5.939479000	1.112644000	H	-0.822918000	4.008419000	1.988090000
C	-0.000269000	6.644037000	-0.000225000	H	-0.000319000	7.727936000	-0.000273000
C	0.461936000	5.939434000	-1.113038000	H	0.822599000	4.008328000	-1.988334000
C	0.464780000	4.543387000	-1.115334000	H	5.042414000	-0.846928000	-2.028152000
C	5.561480000	-1.148714000	-1.124509000	H	8.704129000	-1.857475000	-0.018973000
C	6.947889000	-1.317590000	-1.145892000	H	4.978873000	-1.988676000	2.120370000
C	7.630004000	-1.716840000	0.003650000	H	-4.979185000	-1.989544000	-2.119935000
C	6.912464000	-1.950905000	1.178378000	H	-8.704016000	-1.857740000	0.020108000

C	5.526036000	-1.791248000	1.204744000	H	-5.041894000	-0.846693000	2.028296000
C	-5.526166000	-1.791869000	-1.204253000	H	-5.137165000	-3.910013000	0.443534000
C	-6.912598000	-1.951501000	-1.177568000	H	-5.158537000	-6.350698000	0.737827000
C	-7.629894000	-1.717117000	-0.002765000	H	-3.058626000	-7.656353000	0.740498000
C	-6.947539000	-1.317577000	1.146547000	H	-0.878422000	-6.529239000	0.449722000
C	-5.561144000	-1.148721000	1.124841000	H	0.879031000	-6.529097000	-0.451062000
C	-4.204013000	-4.454988000	0.415274000	H	3.059411000	-7.656056000	-0.741164000
C	-4.211848000	-5.841618000	0.588061000	H	5.159235000	-6.350254000	-0.737718000
C	-3.023051000	-6.582713000	0.587378000	H	5.137596000	-3.909588000	-0.443367000
C	-1.793639000	-5.952416000	0.406780000	H	5.583859000	0.804852000	0.807791000
C	1.794200000	-5.952222000	-0.407765000	H	6.219106000	3.100494000	1.369726000
C	3.023715000	-6.582426000	-0.588002000	H	4.515711000	4.899930000	1.456424000
C	4.212459000	-5.841250000	-0.588245000	H	2.168374000	4.427205000	0.957096000
C	4.204472000	-4.454625000	-0.415397000	H	-2.168692000	4.427019000	-0.957377000
C	4.823838000	1.570016000	0.812783000	H	-4.516028000	4.899528000	-1.456879000
C	5.183029000	2.875531000	1.138122000	H	-6.219271000	3.099947000	-1.370299000
C	4.222508000	3.891129000	1.184121000	H	-5.583875000	0.804378000	-0.808220000
C	2.886169000	3.624779000	0.891675000				

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