Supplementary Information

A Series of 4- and 5-Coordinate Ni(II) Complexes: Synthesis, Characterization, and Spectroscopic Studies

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Table S1. Crystal data and structure refinement details for **1**, **2**, and **3**.

	1	**2**	**3**
Empirical formula	$C_{32}H_{40}N_5NiCl$, 0.234(C_7H_8), 0.266(C_5H_{12})	2($C_{32}H_{40}N_5NiBr$), C_7H_8	$C_{32}H_{40}N_5NiI$, C_7H_8
Formula weight	629.58	1358.75	772.43
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
a/Å	11.1388(6)	11.2050(15)	12.8495(5)
b/Å	11.6220(7)	11.7440(15)	26.7024(9)
c/Å	13.6030(8)	13.5601(18)	11.1200(4)
a/°	108.012(2)	108.6744(19)	90
b/°	93.703(2)	93.629(2)	107.6829(14)
g/°	100.966(2)	100.789(2)	90
V/Å^3	1629.67(16)	1646.0(4)	3635.1(2)
Z	2	1	4
D_{calcd}, g cm^{-3}	1.283	1.371	1.411
F(000)	669.7	710.0	1592.0
Temp, K	100	100	100
R(F), %	5.76	4.67	3.33
R_w(F), %	13.68	10.88	6.53

Table S2. Crystal data and structure refinement details for **1**·THF, **2**·THF[a], and **3**·THF.

	1·THF[b]	**2**·THF[c]	**3**·THF[d]
Empirical formula	$C_{36}H_{48}N_5NiClO$	$C_{36}H_{48}N_5NiBrO$, $C_{32}H_{40}Br_2N_5Ni$, $C_{16}H_{32}LiO_4$, $2(C_4H_8O)$	$C_{36}H_{48}N_5NiIO$
Formula weight	660.94	1858.19	752.40
Space group	$P2_1$	$P\bar{1}$	$P\bar{1}$
a/Å	9.9148(14)	16.2231(13)	8.3512(3)
b/Å	13.8947(17)	18.6247(13)	13.7092(6)
c/Å	24.971(3)	18.7192(13)	15.8646(7)
a/°	90	61.585(2)	106.5272(11)
b/°	90.426(5)	77.286(3)	90.1491(11)
g/°	90	71.732(3)	99.9851(9)
V/Å^3	3440.0(8)	4706.8(6)	1712.30(12)
Z	4	2	2
D_{calcd}, g cm^{-3}	1.276	1.311	1.459
F(000)	1408.0	1956.0	776.0
Temp, K	100	150	100
R(F), %	7.33	6.97	6.92
R_w(F), %	19.50	21.97	17.75

[a] Only [**2**·THF]·[$Cz^{tBu}(Pyr^{iPr})_2NiBr_2$][$Li(THF)_4$] was grown and suitable for crystallographic analysis.

[b] ***1**·THF*

The structure exhibits pseudo-orthorhombic symmetry with a beta angle of 90.426(5) and is twinned by that symmetry. The twin matrix 1 0 0, 0 -1 0, 0 0 -1 was applied to account for twinning effects.

The structure also exhibits a pseudo inversion center and a pseudo glide plane, complicating refinement causing large correlation effects between parameters of the two molecules related by the pseudo symmetry elements. Two independent molecules are related by a pseudo-glide plane and a pseudo-inversion center. One of the molecules does however exhibit whole molecule disorder (the Ni coordinated chloro and THF molecules are swapped, inducing substantial shifts for most other atoms) with a close to 1:1 disorder ratio. The other molecule is not disordered. Attempts were made to refine the structure in *P*21/c, with only one molecule site and with ca. 75:25 disorder. The fit of model to data was however substantially worse, with R1 > 20% even after inclusion of disorder.

In the final model disorder was included for one tert-butyl molecule of the otherwise not disordered molecule. The two disordered tert-butyl moieties were restrained to have similar geometries. The two completely disordered molecule moieties were restrained to have a similar

geometry as the mostly not disordered molecule. Uij components of all disordered atoms were restrained to be similar for atoms closer to each other than 1.7 Angstrom. The tert-butyl atoms of C19 to C22 of all moieties were affected by large correlation effects and were restrained to be close to isotropic.

Subject to these conditions the occupancy ratio refined to 0.56(3) to 0.44(3) for the disordered tert-butyl group, and to 0.531(4) to 0.469(4) for the whole molecule disorder

The structure was refined as a 4-component inversion twin, twin matrix TWIN 1 0 0 0 -1 0 0 0 -1 -4. BASF values refined to 0.28(2), 0.23(2) and 0.11(2).

[c] ***2**·THF*

Three types of THF molecules are present in this structure. One molecule is coordinated to a Ni atom. Four molecules coordinate to a lithium cation, and two THF molecules occupy interstitial sites. All seven THF molecules were refined as disordered. The atoms of the $Li(THF)_4$ cluster were refined with a common disorder over two sites that includes the lithium cation. The minor site of one of the THF molecules (that of O4) was refined as additionally disordered. One of the interstitial THF molecules (that of O5) was refined with the same disorder ratio as the $Li(THF)_4$ unit. The disorder of other (of O6) and of the Ni coordinated THF were refined independently. All disordered THF moieties were restrained to have similar geometries. U_{ij} components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. O4D and O4E were constrained to have identical ADPs. Subject to these conditions the occupancy ratios refined to 0.57(3) to 0.43(3) for the Ni coordinated molecule, to 0.47(3) to 0.53(3) for the $Li(THF)_4$ unit, to 0.300(3) to 0.230(3) for the additionally split minor O4 moiety, and to 0.477(11) to 0.523(11) for the interstitial THF molecule of O6.

One tert-butyl group is rotationally disordered. The two moieties were restrained to have similar geometries. U_{ij} components of ADPs for disordered atoms closer toeach other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy ratios refined to 0.529(9) to 0.471(9).

[d] ***3**·THF*

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180 degree rotation around the real a-axis.

The two components were integrated using Saint and corrected for absorption using twinabs, resulting in the following statistics:

11285 data (3787 unique) involve domain 1 only, mean I/sigma 77.3

11243 data (3765 unique) involve domain 2 only, mean I/sigma 48.6

16393 data (5155 unique) involve 2 domains, mean I/sigma 91.5

3 data (3 unique) involve 3 domains, mean I/sigma 64.8

The exact twin matrix identified by the integration program was found to be

-1.00019 -0.00066 -0.00033

0.56992 0.99976 0.49357

0.00111 0.00174 -0.99957

The structure was solved using direct methods with only the non-overlapping reflections of component 1. The structure was refined using the hklf 5 routine with all reflections of component 1 (including the overlapping ones), resulting in a BASF value of 0.257(2).

The R_{int} value given is for all reflections and is based on agreement between observed single and composite intensities and those calculated from refined unique intensities and twin fractions (TWINABS (Sheldrick, 2012)).

The crystal is further affected by slight non-Bragg behavior with streaks between spots not caused by the twinning described above. Relatively large residual electron densities observed might be due to the non-Bragg behavior. The largest residual electron density peak is located close to nitrogen atom N3. To avoid unreasonable thermal ellipsoid behavior N3 was constrained to have the same ADP as the nickel atom it is bonded to.

The two isopropyl groups are disordered with a shared disorder ratio. The disorder was modeled to include the pyrazole moieties. The four units were restrained to have similar geometries, Uij components of ADPs were restrained to be similar for disordered atoms closer than 1.7 Angstrom, and the ADPs substantially overlapping atoms were constrained to be identical to those of their disordered counterparts (N1 and N1B, N2 and N2B, C21 and C21B, C22 and C22B, and C30 and C30B). Subject to these conditions the occupancy ratio refined to 0.499(12) to 0.501(12). The Ni-coordinated THF molecule is disordered with two moieties. The two units were restrained to have similar geometries, and U_{ij} components of ADPs were restrained to be similar for atoms closer than 1.7 Angstrom. Subject to these conditions the occupancy ratio refined to 0.518(14) to 0.482(14).

Table S3. $\lambda_{max}(\varepsilon)$ of four-coordinate complexes at 40 °C and five-coordinate complexes at 40 and −80 °C.

1	305(15730), 319(15470), 373(6350), 395(6370), 630(2010)
1[*]	276, 305, 378, 636
2	320(17010), 396(7840), 651(2590)
2[*]	277. 305, 378, 650
3	321(15410), 399(7200), 680(2410)
3[*]	278, 307, 378, 683
2·THF	319(14730), 403(6780), 418(sh)(6400), 629(900)
2·THF (–80 °C)	305(11370), 325(20590), 348(10420), 403(9440), 424(11680)
1·THF[*]	301, 340, 386, 635
2·THF	303(18000), 327(17360), 351(11530), 371(sh)(7240), 404(7930), 427(10470), 653(310)
2·THF (–80 °C)	304(20040), 327(19290), 351(12810), 371(8040), 404(8820), 427(11640)
2·THF[*]	302, 340, 388, 635
3·THF	303(17570), 320(11950), 352(9690), 369(sh)(8700), 399(6030), 426(sh)(4970), 685(730)
3·THF (–80 °C)	303(15590), 326(14190), 353(10760), 371(7770), 405(7370), 427(8940)
3·THF[*]	306, 343, 389, 635

[*] Computed λ_{max} values in nm.

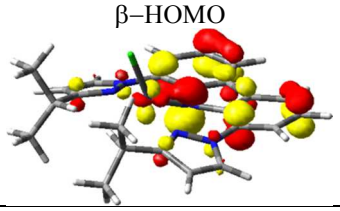
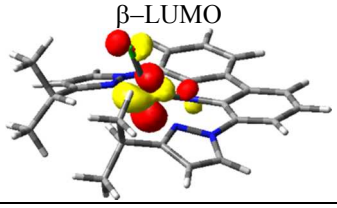
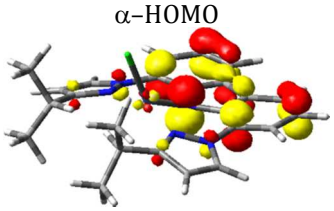
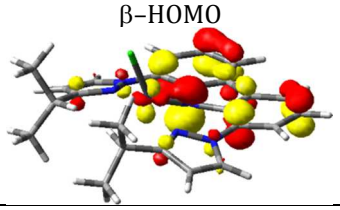
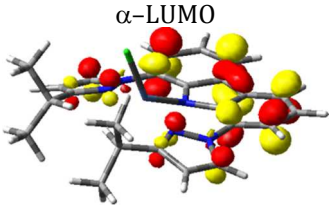
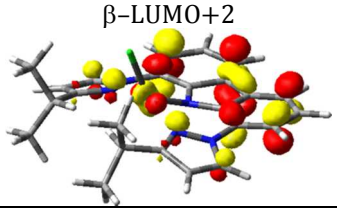
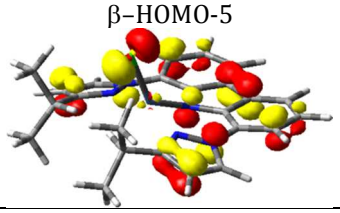
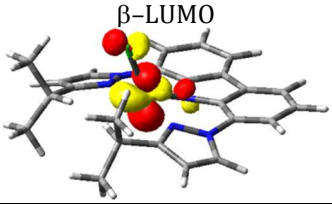
Table S4. Comparison of selected bond distances (Å) and angles (°) for **1**, **2**, and **3**.

	1	**1(calc)**	**2**	**2(calc)**	**3**	**3(calc)**
Ni1–N3	1.879(2)	1.920	1.874(2)	1.922	1.871(1)	1.923
Ni1–N5	2.071(2)	2.092	2.055(2)	2.092	2.044(1)	2.089
Ni1–N1	2.056(2)	2.092	2.041(2)	2.091	2.029(1)	2.089
Ni1–X1	2.2423(7)	2.273	2.3807(5)	2.405	2.5658(4)	2.603
N3–Ni1–X1	129.44(7)	133.2	127.42(7)	129.8	124.25(4)	126.4

Table S5. Comparison of selected bond distances (Å) and angles (°) for **1**·THF, **2**·THF, and **3**·THF.

	1·THF	**1**·THF **(calc)**	**2**·THF	**2**·THF **(calc)**	**3**·THF	**3**·THF **(calc)**
Ni1–N3	1.90(1)	1.951	1.906(4)	1.948	1.911(6)	1.941
Ni1–N5	2.04(1)	2.140	2.044(3)	2.133	1.95(2)	2.118
Ni1–N1	2.05(1)	2.150	2.045(8)	2.148	2.13(2)	2.137
Ni1–X1	2.319(5)	2.326	2.4355(7)	2.471	2.719(1)	2.690
Ni1–O1	2.23(3)	2.235	2.26(2)	2.258	2.21(3)	2.290
N3–Ni1–X1	109.9(4)	114.4	111.4(1)	111.9	103.4(2)	108.4
N3–Ni1–O1	94.3(5)	97.4	95.0(4)	96.7	91.8(7)	96.0

Table S6. Donor and acceptor orbitals of **1** for the excited states responsible for the absorption spectra in Figure 6 (left) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	**Donor**	**Acceptor**
636.11 (f = 0.0490)	β–HOMO 	β–LUMO 
377.79 (f = 0.1690)	α–HOMO  β–HOMO 	α–LUMO  β–LUMO+2 
344.37 (f = 0.0404)	β–HOMO-5 	β–LUMO 
329.56 (f = 0.1420)	α–HOMO	α–LUMO+1

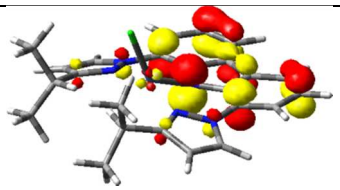
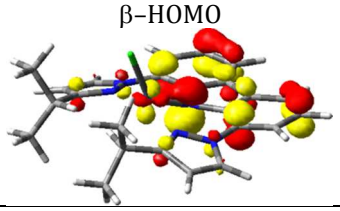
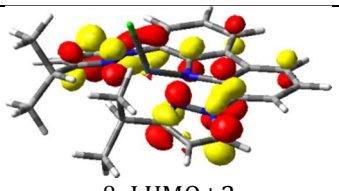
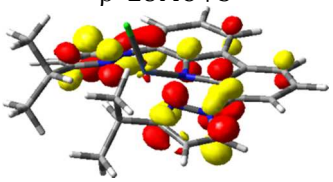
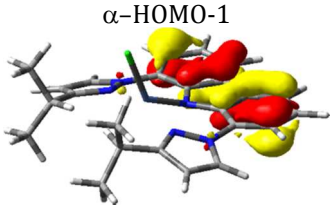
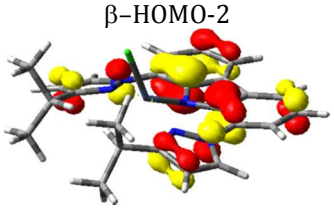
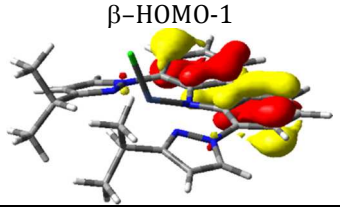
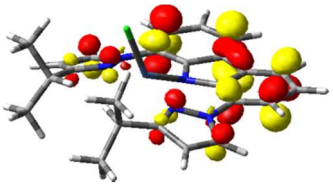
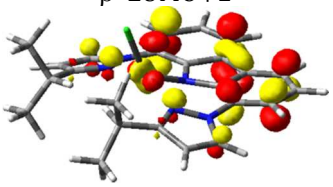
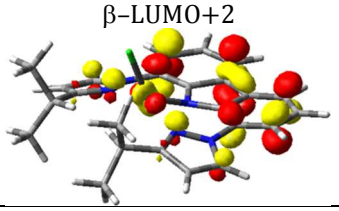
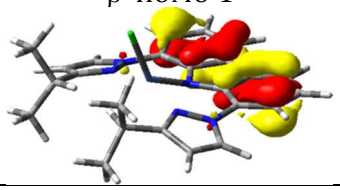
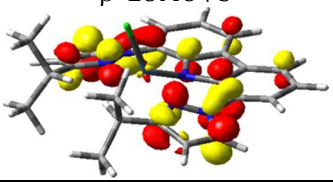
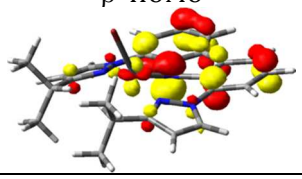
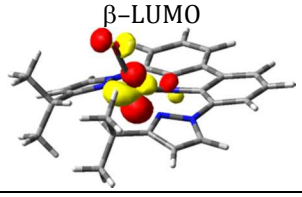
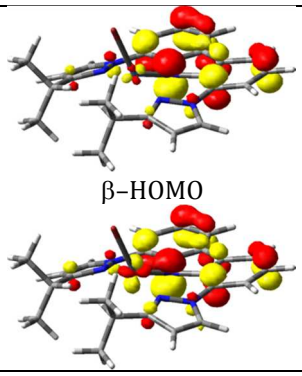
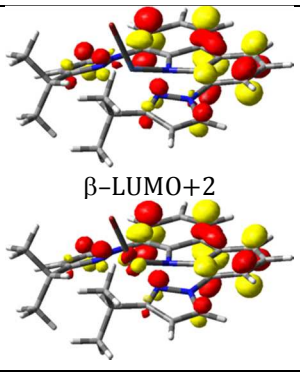
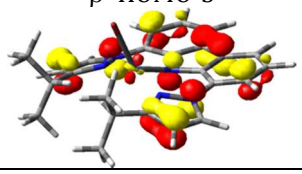
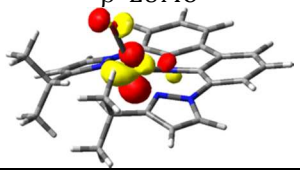
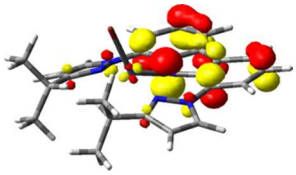
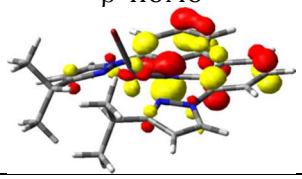
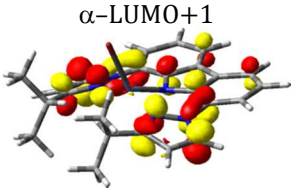
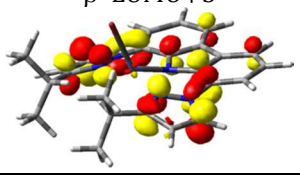
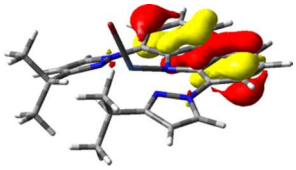
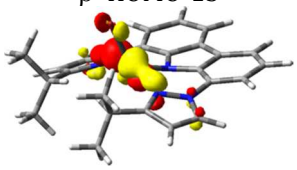
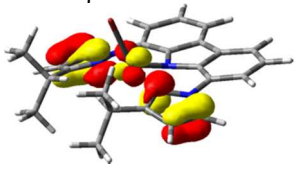
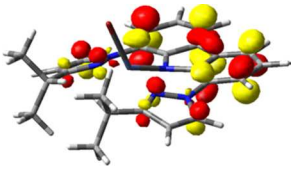
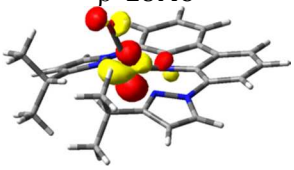
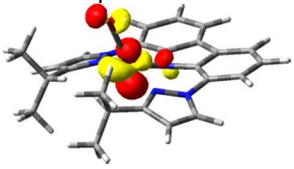
	 β–HOMO 	 β–LUMO+3 
304.60 (f = 0.2294)	α–HOMO-1  β–HOMO-2  β–HOMO-1 	α–LUMO  β–LUMO+2  β–LUMO+2 
275.58 (f = 0.1446)	β–HOMO-1 	β–LUMO+3 

Table S7. Donor and acceptor orbitals of **2** for the excited states responsible for the absorption spectra in Figure 6 (left) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	**Donor**	**Acceptor**
650.93 (f = 0.0472)	β–HOMO 	β–LUMO 
379.07 (f = 0.1796)	α–HOMO	α–LUMO

	β–HOMO 	β–LUMO+2 
348.28 (f = 0.0370)	β–HOMO-5 	β–LUMO 
330.66 (f = 0.1346)	α–HOMO  β–HOMO 	α–LUMO+1  β–LUMO+3 
304.78 (f = 0.1817)	α–HOMO-1  β–HOMO-13  β–HOMO-6  β–HOMO-1	α–LUMO  β–LUMO  β–LUMO  β–LUMO+2

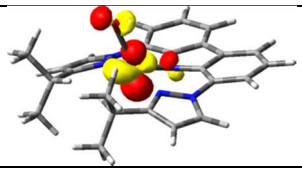
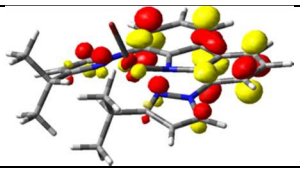
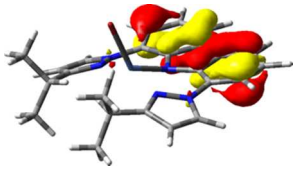
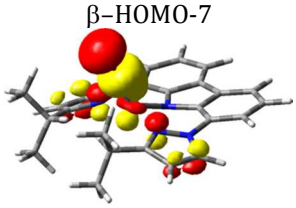
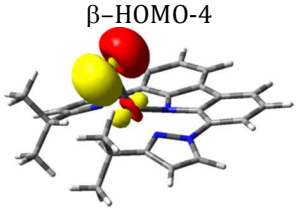
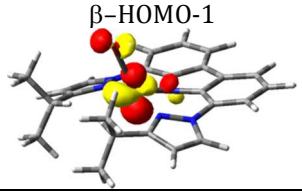
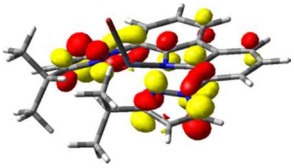
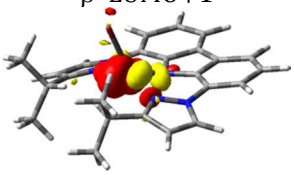
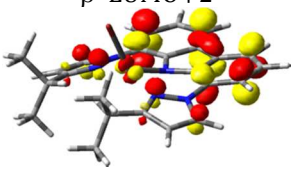
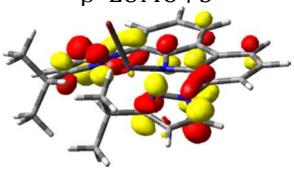
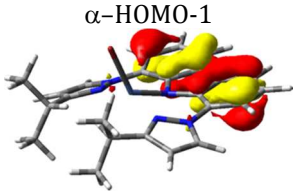
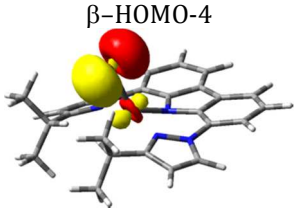
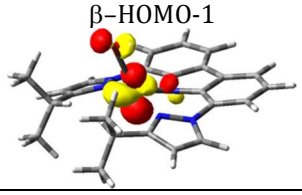
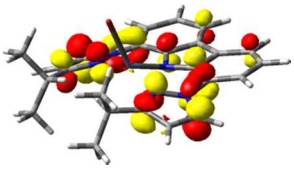
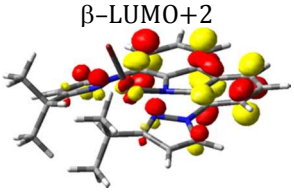
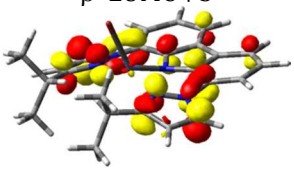
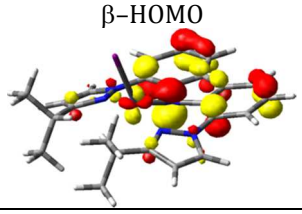
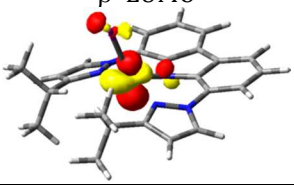
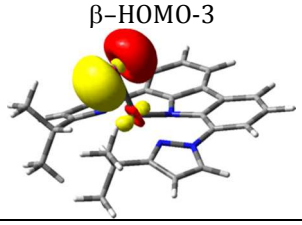
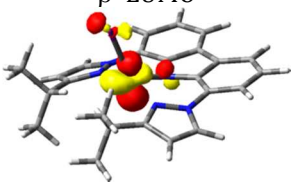
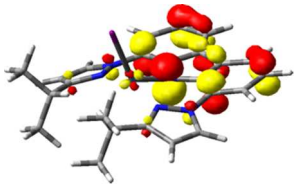
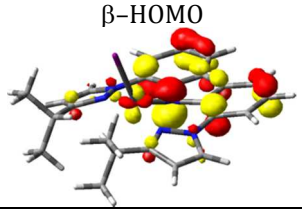
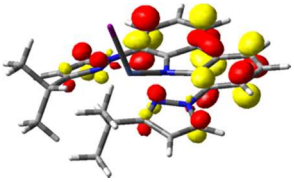
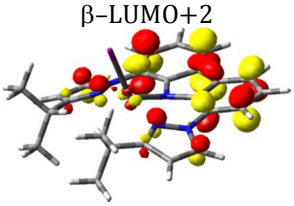
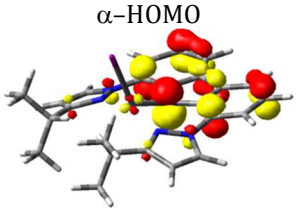
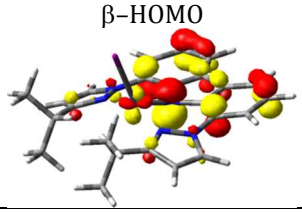
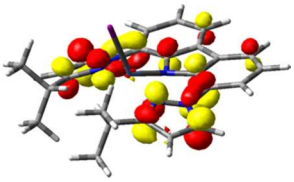
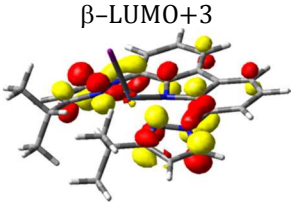
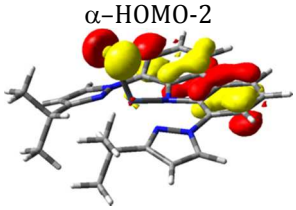
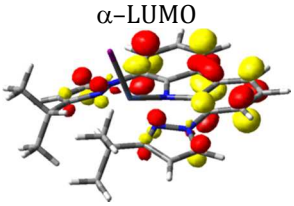
		
277.46 (f = 0.0994)	α–HOMO-1  β–HOMO-7  β–HOMO-4  β–HOMO-1 	α–LUMO+1  β–LUMO+1  β–LUMO+2  β–LUMO+3 
275.37 (f = 0.1016)	α–HOMO-1  β–HOMO-4  β–HOMO-1 	α–LUMO+1  β–LUMO+2  β–LUMO+3 

Table S8. Donor and acceptor orbitals of **3** for the excited states responsible for the absorption spectra in Figure 6 (left) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	Donor	Acceptor
684.46 (f = 0.0480)	β–HOMO 	β–LUMO 
522.67 (f = 0.0145)	β–HOMO-3 	β–LUMO 
380.12 (f = 0.1652)	α–HOMO  β–HOMO 	α–LUMO  β–LUMO+2 
331.82 (f = 0.1253)	α–HOMO  β–HOMO 	α–LUMO+1  β–LUMO+3 
305.48 (f = 0.2736)	α–HOMO-2  β–HOMO-2	α–LUMO  β–LUMO+2

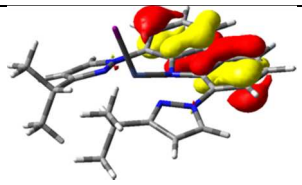
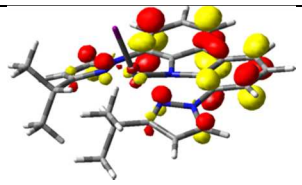
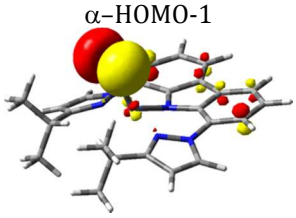
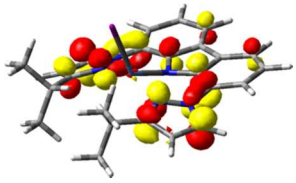
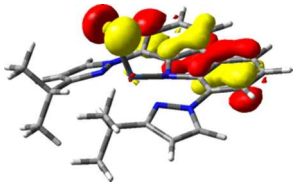
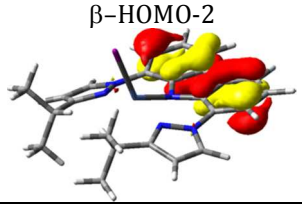
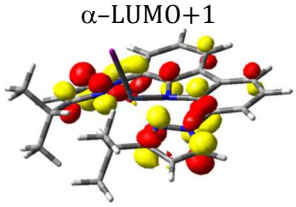
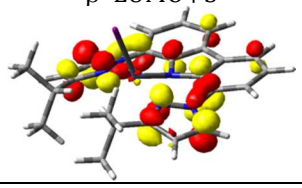
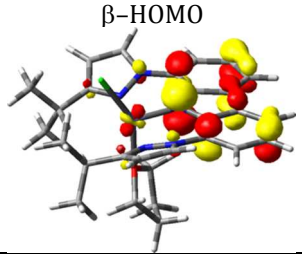
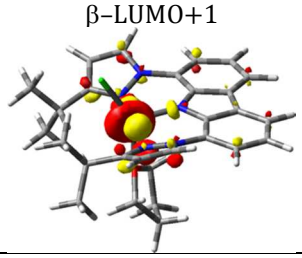
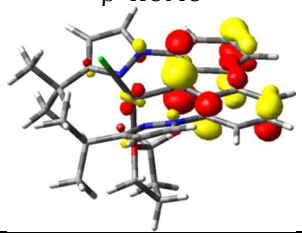
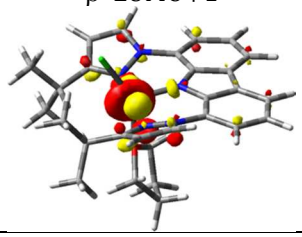
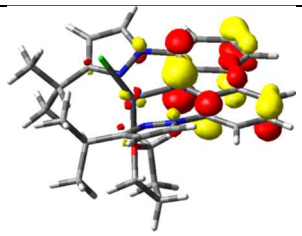
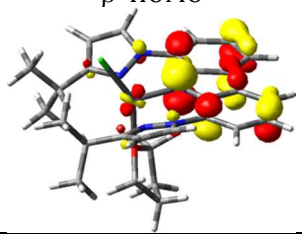
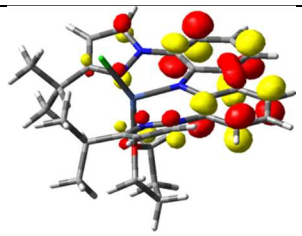
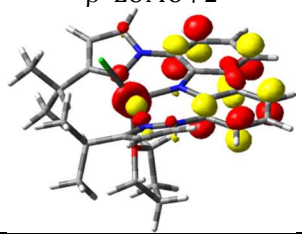
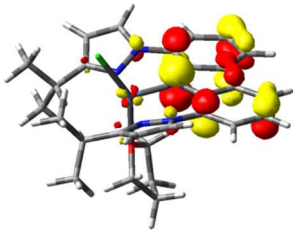
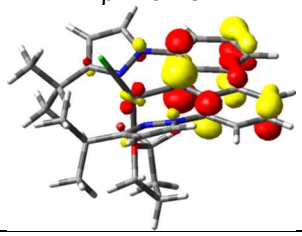
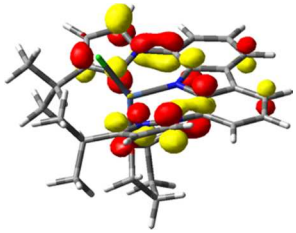
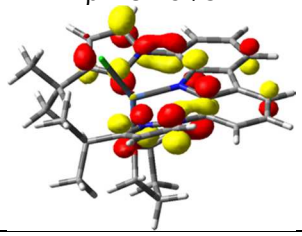
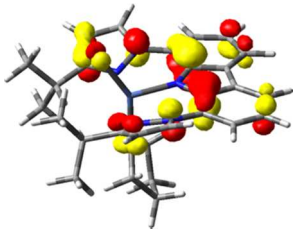
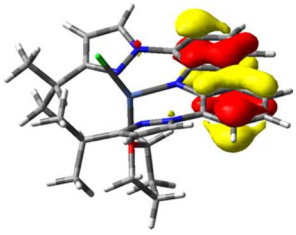
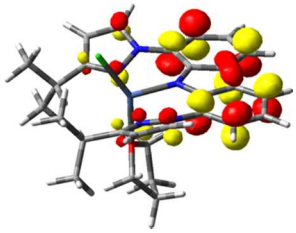
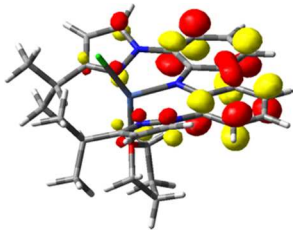
		
277.69 (f = 0.0840)	α–HOMO-1 	α–LUMO+1 
275.37 (f = 0.0593)	α–HOMO-2  β–HOMO-2 	α–LUMO+1  β–LUMO+3 

Table S9. Donor and acceptor orbitals of **1**·THF for the excited states responsible for the absorption spectra in Figure 6 (right) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	**Donor**	**Acceptor**
631.18 (f = 0.0035)	β–HOMO 	β–LUMO+1 
413.39 (f = 0.0501)	β–HOMO 	β–LUMO+1 
383.35 (f = 0.1206)	α–HOMO	α–LUMO

	 β–HOMO 	 β–LUMO+2 
336.42 (f = 0.1159)	α–HOMO  β–HOMO 	α–LUMO+1  β–LUMO+3 
303.62 (f = 0.0965)	α–HOMO-2  α–HOMO-1  β–HOMO-1	α–LUMO  α–LUMO  β–LUMO+2

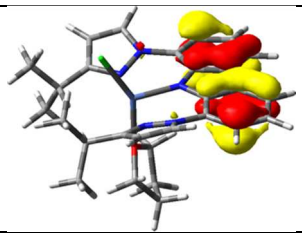
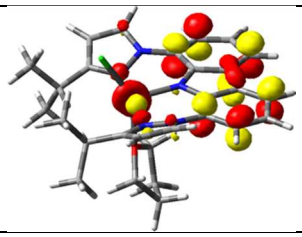
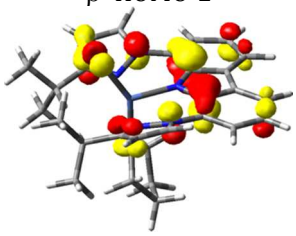
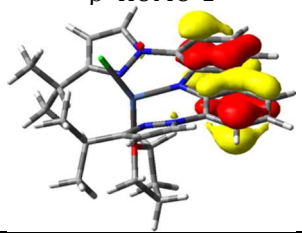
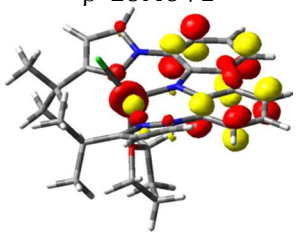
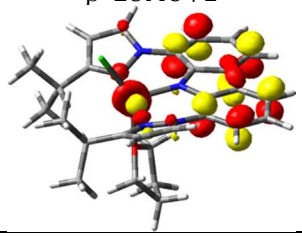
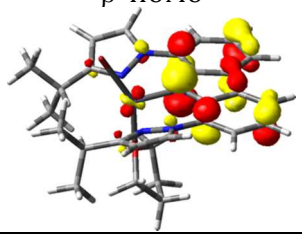
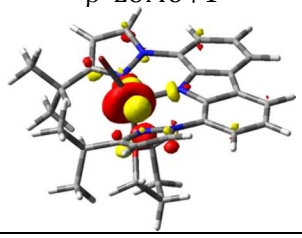
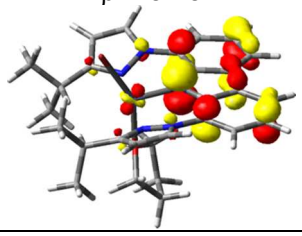
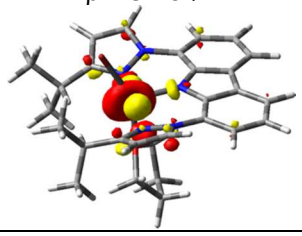
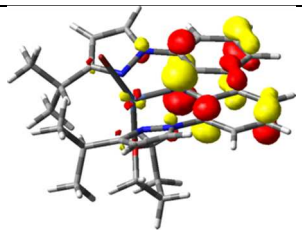
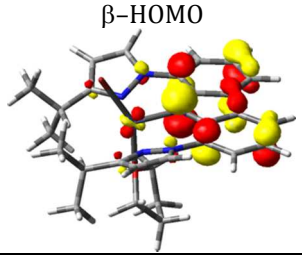
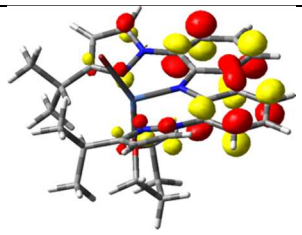
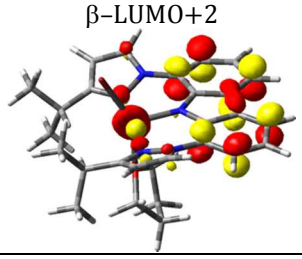
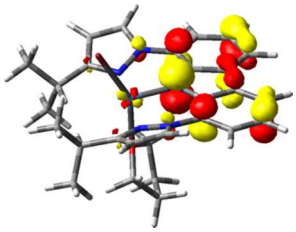
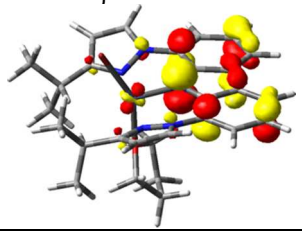
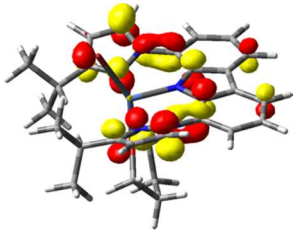
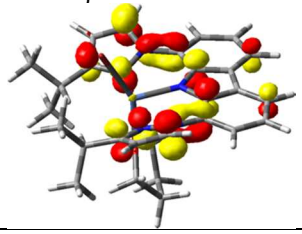
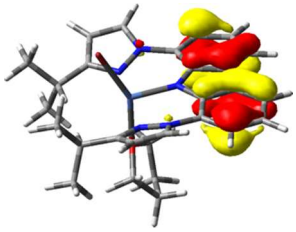
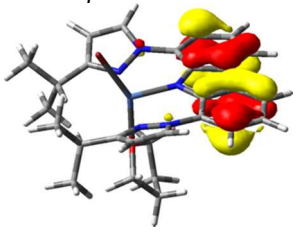
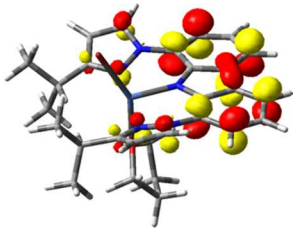
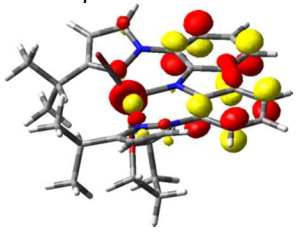
		
298.85 (f = 0.0843)	β–HOMO-2  β–HOMO-1 	β–LUMO+2  β–LUMO+2 

Table S10. Donor and acceptor orbitals of **2**·THF for the excited states responsible for the absorption spectra in Figure 6 (right) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	**Donor**	**Acceptor**
635.81 (f = 0.0035)	β–HOMO 	β–LUMO+1 
422.67 (f = 0.0332)	β–HOMO 	β–LUMO+1 
387.65 (f = 0.1392)	α–HOMO	α–LUMO

	 β–HOMO 	 β–LUMO+2 
338.50 (f = 0.1213)	α–HOMO  β–HOMO 	α–LUMO+1  β–LUMO+3 
302.97 (f = 0.1005)	α–HOMO-1  β–HOMO-1  β–HOMO	α–LUMO  β–LUMO+2  β–LUMO+5

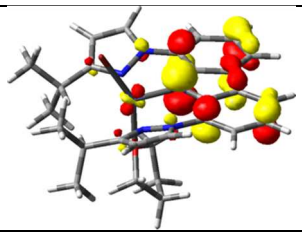
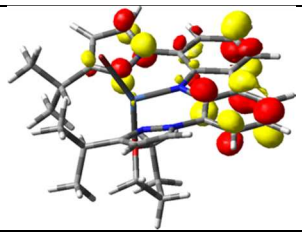
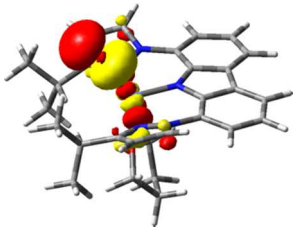
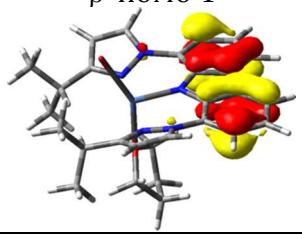
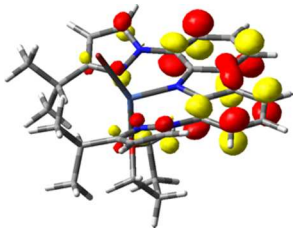
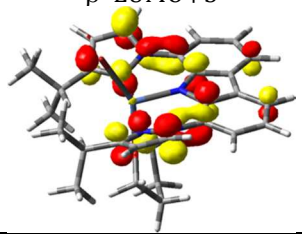
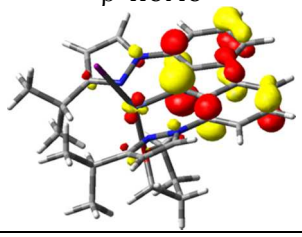
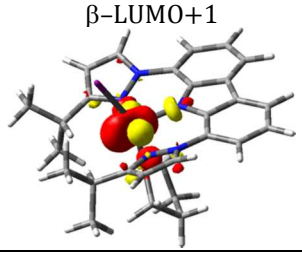
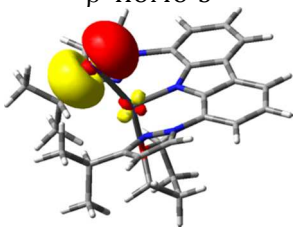
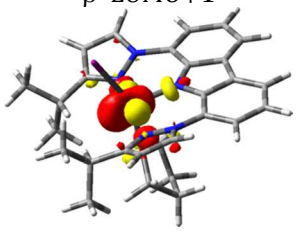
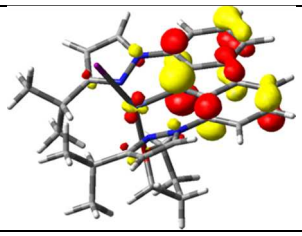
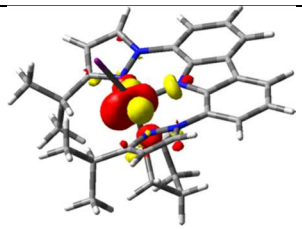
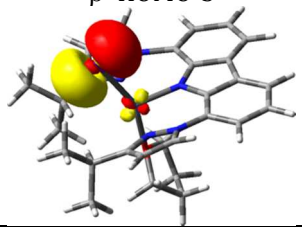
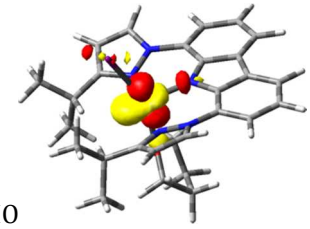
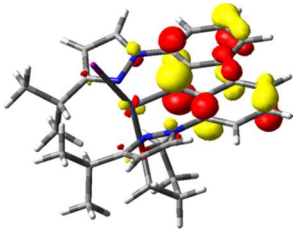
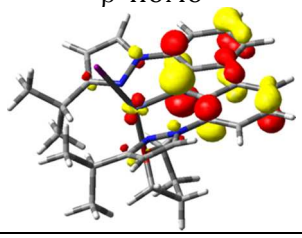
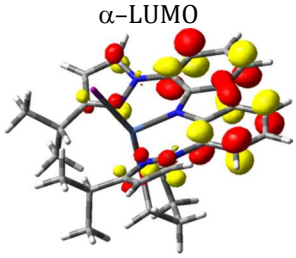
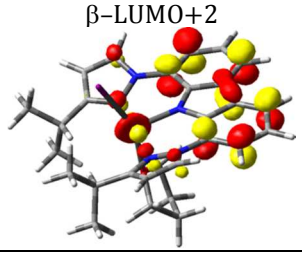
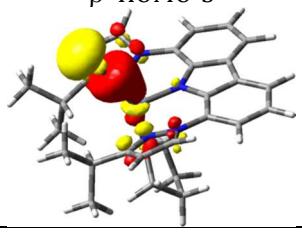
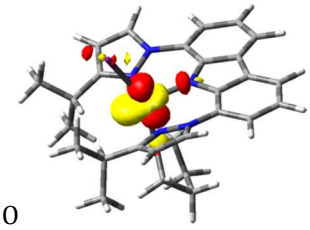
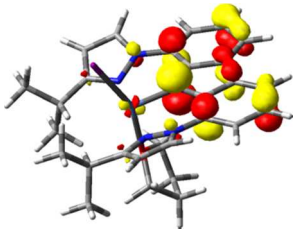
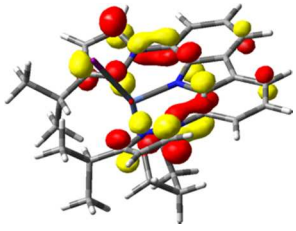
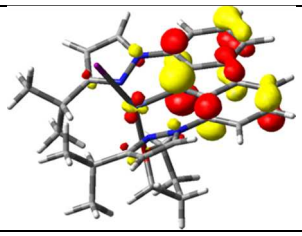
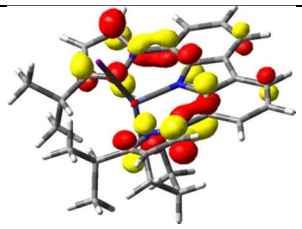
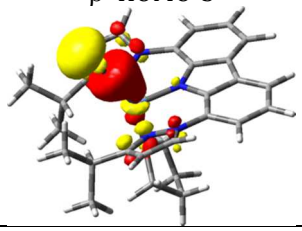
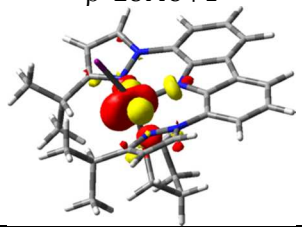
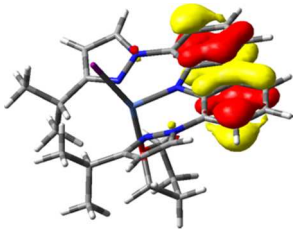
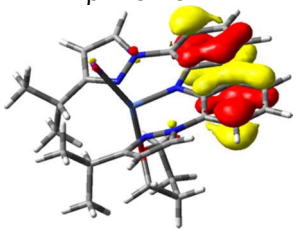
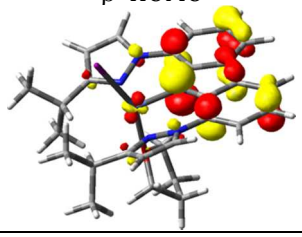
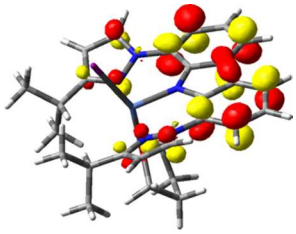
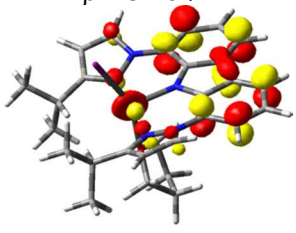
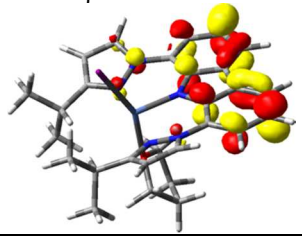
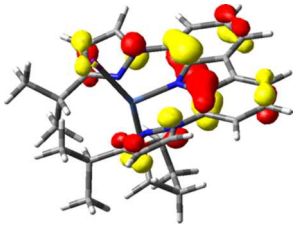
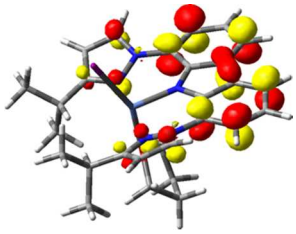
		
276.17 (f = 0.1010)	α–HOMO-4  β–HOMO-1 	α–LUMO  β–LUMO+3 

Table S11. Donor and acceptor orbitals of **3**·THF for the excited states responsible for the absorption spectra in Figure 6 (right) of the manuscript.

Excited State Wavelength / nm (Oscillator Strength)	Donor	Acceptor
637.50 (f = 0.0040)	β–HOMO 	β–LUMO+1 
431.07 (f = 0.0142)	β–HOMO-3  β–HOMO	β–LUMO+1  β–LUMO+1

		
407.75 (f = 0.0173)	β–HOMO-3 	 β–LUMO
390.36 (f = 0.1449)	α–HOMO  β–HOMO 	α–LUMO  β–LUMO+2 
366.72 (f = 0.0346)	β–HOMO-5 	 β–LUMO
342.64 (f = 0.1242)	α–HOMO  β–HOMO	α–LUMO+1  β–LUMO+3

		
316.91 (f = 0.0478)	β–HOMO-5 	β–LUMO+1 
305.08 (f = 0.1181)	α–HOMO-1  β–HOMO-1  β–HOMO 	α–LUMO  β–LUMO+2  β–LUMO+5 
279.43 (f = 0.0944)	α–HOMO–5  α–HOMO-1	α–LUMO  α–LUMO+1

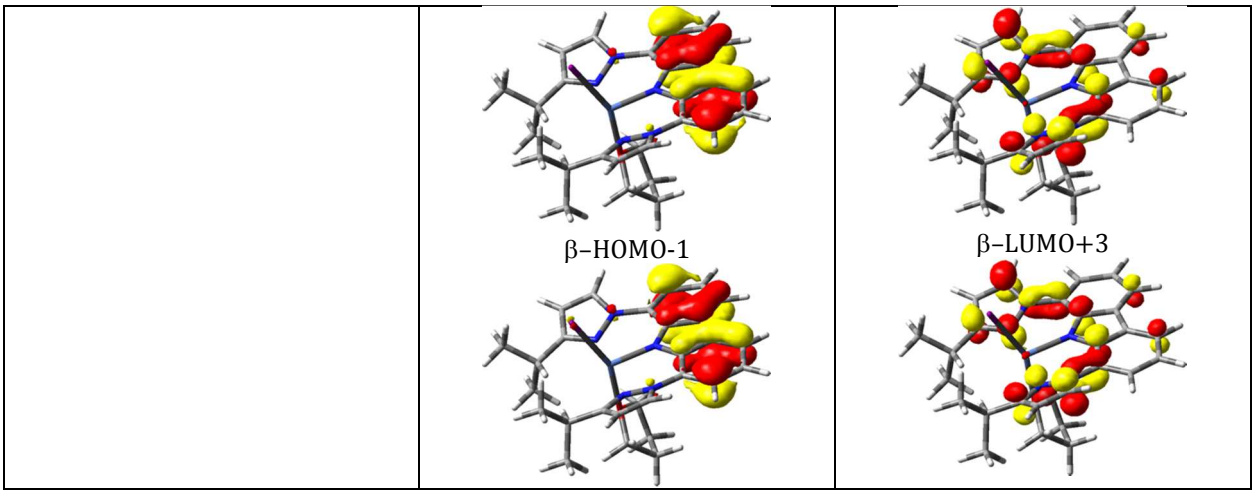


Table S12. Cartesian coordinates (Å) of all optimized species.

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C    0.026654  -4.076305  -0.771883
C   -1.347764  -4.063133  -0.778089
H    0.722859  -4.852069  -1.041263
H   -1.999607  -4.876359  -1.053943
N   -0.617302   2.035775  -0.134307
C   -1.715124   2.764950  -0.373579
C   -1.348325   4.062919  -0.778604
C    0.026086   4.076416  -0.772025
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H    0.722182   4.852313  -1.041306
N    1.357028   0.000185  -0.232859
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C    3.545432   0.723823  -0.033273
C    1.811138   2.452577  -0.176213
C    4.538348   1.696932   0.077412
C    2.816054   3.408625  -0.028907
C    4.160790   3.034840   0.086739
H    5.583826   1.421159   0.171250
H    2.562566   4.460763   0.018966
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C    1.811482  -2.452165  -0.176193
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H    4.911321  -3.809448   0.197181
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H   -3.005975  -1.135942  -0.020623
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H   -4.786422   2.390481   1.163545
H   -3.211082   2.594351   1.937846
H   -3.890490   3.899273   0.943856
C   -3.948719   2.410651  -1.471567
H   -4.933377   1.951481  -1.349126
H   -4.107714   3.472003  -1.684014
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H   -4.933459  -1.952605  -1.347861
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N    0.457100   2.852382  -0.372311

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2 S=1
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C    0.017612  -4.063536  -0.774524
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H    0.710668  -4.836945  -1.058691
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C    1.810706   2.450728  -0.176942
C    4.540428   1.699102   0.054122
C    2.814406   3.408850  -0.036884
C    4.160628   3.036594   0.067463
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C    2.179669  -1.097878  -0.161512
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C    4.540717  -1.698318   0.054460
C    4.161141  -3.035872   0.068052
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H    5.587420  -1.424559   0.140221
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H   -2.994843  -1.141769   0.111573
C   -3.830896   2.893980   0.996720
H   -4.824603   2.460103   1.138571
H   -3.276158   2.778082   1.929029
H   -3.958143   3.962855   0.799528
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H   -4.896837  -1.815598  -1.335522
H   -3.407969  -1.755826  -2.289515
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N    0.453761   2.845667  -0.363612

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3 S=1
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C    0.009671  -4.054916  -0.772645
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H    0.700110  -4.827626  -1.065084
H   -2.023936  -4.843492  -1.039177
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C    0.009252   4.054978  -0.772276
H   -2.024441   4.843322  -1.038842
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C    2.181218   1.097535  -0.169510
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C    2.812508   3.408754  -0.041920
C    4.159845   3.037826   0.053645
H    5.589443   1.429073   0.115527
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N    0.450650   2.840374  -0.356989

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1THF S=1
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C    0.696158  -4.036336  -1.071586
C    2.053152  -3.831814  -0.989266
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H    2.829334  -4.518572  -1.286486
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C    1.088888  -0.860813   2.795963
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C    0.115825  -0.929853   3.968178
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H   -0.211736   2.017327   2.463536
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H   -1.294085   0.642695   4.608143
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H    4.462874   3.195643  -0.682407
H    3.239672   2.788133  -1.897453
H    3.353867   4.440937  -1.259072
C    2.743929   3.779964   1.411396
H    3.773099   3.606243   1.738933
H    2.620716   4.856823   1.262649
H    2.076394   3.477122   2.222500
C    4.411454  -1.754009  -1.416055
H    3.906451  -1.254681  -2.242003
H    5.324804  -1.198579  -1.183372
H    4.709071  -2.757106  -1.737449
C    4.223680  -2.467657   1.009702
H    4.515974  -3.495779   0.776754
H    5.134518  -1.912775   1.252382
H    3.598286  -2.497258   1.905382
N    0.074927  -2.919949  -0.614607
N   -1.074850   2.733779  -0.645939
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2THF S=1
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Ni   0.529753   0.118489  -0.348901
N    1.008612  -1.974189  -0.266237
C    2.211511  -2.532975  -0.473039
C    0.700825  -4.046450  -1.045907
C    2.057836  -3.843716  -0.960527
H    0.136057  -4.891669  -1.400800
H    2.833643  -4.536873  -1.243276
N    0.117808   2.208398  -0.231133
C    1.023853   3.188947  -0.335225
C    0.411400   4.360743  -0.818764
C   -0.910550   4.031807  -1.007202
H    0.877145   5.308955  -1.033629
H   -1.731823   4.613188  -1.390287
N   -1.372599  -0.270713  -0.502213
C   -2.391202   0.640642  -0.471840
C   -3.662139  -0.003626  -0.357036
C   -2.321021   2.046173  -0.509675
C   -4.839499   0.743689  -0.294263
C   -3.508886   2.769370  -0.413606
C   -4.752689   2.128715  -0.321793
H   -5.805663   0.254896  -0.215254
H   -3.480789   3.852025  -0.386755
H   -5.650321   2.734057  -0.257613
C   -1.947884  -1.506050  -0.417930
C   -1.326644  -2.768341  -0.415223
C   -3.370250  -1.414272  -0.314998
C   -2.126604  -3.897924  -0.248914
C   -4.152624  -2.563440  -0.189327
C   -3.521585  -3.799302  -0.146340
H   -1.667997  -4.877376  -0.182125
H   -5.233631  -2.495709  -0.115129
H   -4.103850  -4.706384  -0.026083
Br   1.596902   0.393322  -2.560828
C    2.465545   2.986337   0.052030
H    2.631537   1.906999   0.127463
C    3.503793  -1.815092  -0.180455
H    3.256851  -0.771152   0.039207
O    0.599997   0.204054   1.905948
C    1.078992  -0.848738   2.782548
C   -0.406436   0.998857   2.599787
C    0.088400  -0.906803   3.940550
H    1.135372  -1.765679   2.201259
H    2.083510  -0.576284   3.124652
C   -0.345504   0.559258   4.060047
H   -0.171403   2.049872   2.442700
H   -1.377335   0.783112   2.149975
H    0.539318  -1.302440   4.852999
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H   -0.765133  -1.539438   3.680745
H    0.404798   1.136764   4.609043
H   -1.304556   0.686772   4.565715
C    3.422593   3.530201  -1.018888
H    4.459869   3.325695  -0.738859
H    3.230833   3.061224  -1.984560
H    3.322157   4.614250  -1.131706
C    2.754588   3.608502   1.431024
H    3.794784   3.431663   1.719944
H    2.591669   4.690300   1.420529
H    2.113128   3.180340   2.205335
C    4.446830  -1.828129  -1.394485
H    3.968474  -1.377363  -2.263471
H    5.356746  -1.263550  -1.171432
H    4.748159  -2.848745  -1.650321
C    4.199347  -2.419516   1.054794
H    4.485316  -3.460036   0.875363
H    5.110939  -1.862154   1.288754
H    3.556981  -2.401091   1.938123
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N   -1.078063   2.736670  -0.636308
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3THF S=1
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Ni   0.521958   0.117041  -0.382859
N    1.010383  -1.960417  -0.268811
C    2.216379  -2.520664  -0.456700
C    0.712527  -4.049885  -1.003186
C    2.068613  -3.841683  -0.915420
H    0.153358  -4.905167  -1.342041
H    2.847451  -4.538773  -1.179377
N    0.124804   2.193888  -0.260012
C    1.032714   3.174276  -0.354422
C    0.413085   4.362313  -0.783980
C   -0.914410   4.043604  -0.950460
H    0.876508   5.315410  -0.980785
H   -1.740666   4.641043  -1.295577
N   -1.376732  -0.271885  -0.489400
C   -2.394340   0.639304  -0.461693
C   -3.664993  -0.006743  -0.351083
C   -2.322908   2.044995  -0.496798
C   -4.842458   0.739801  -0.288189
C   -3.512055   2.766674  -0.401524
C   -4.755339   2.124991  -0.312572
H   -5.808768   0.250952  -0.211829
H   -3.487581   3.849214  -0.373944
H   -5.653117   2.730145  -0.249059
C   -1.949013  -1.507830  -0.410299
C   -1.323793  -2.768111  -0.408214
C   -3.371746  -1.417578  -0.311113
C   -2.122834  -3.899161  -0.246107
C   -4.152101  -2.568272  -0.189260
C   -3.518177  -3.802816  -0.147101
H   -1.664691  -4.878686  -0.179329
H   -5.233425  -2.503288  -0.117676
H   -4.098837  -4.711339  -0.030198
I    1.478073   0.365034  -2.885286
C    2.483275   2.947998  -0.015139
H    2.662579   1.868939  -0.071053
C    3.504981  -1.791368  -0.175011
H    3.254306  -0.740256   0.006182
O    0.614100   0.230544   1.902139
C    1.072109  -0.826200   2.784553
C   -0.400411   1.027170   2.581611
C    0.065034  -0.880191   3.928701
H    1.130608  -1.743444   2.203756
H    2.073383  -0.561462   3.141996
C   -0.362587   0.587986   4.042737
H   -0.161119   2.078084   2.429111
H   -1.365554   0.813837   2.118783
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H	0.500949	-1.278906	4.847092
H	-0.788193	-1.507992	3.656473
H	0.382971	1.161503	4.602351
H	-1.328065	0.720769	4.534656
C	3.415603	3.622371	-1.031513
H	4.458952	3.393131	-0.798102
H	3.208983	3.271688	-2.043680
H	3.308790	4.711446	-1.012600
C	2.792107	3.406804	1.422225
H	3.842451	3.221026	1.665330
H	2.606113	4.477848	1.545561
H	2.178926	2.870639	2.150099
C	4.464194	-1.847047	-1.375172
H	3.999152	-1.433223	-2.269679
H	5.369385	-1.271528	-1.161427
H	4.771830	-2.875707	-1.587033
C	4.188403	-2.350495	1.088162
H	4.478332	-3.395721	0.946762
H	5.096370	-1.783160	1.311822
H	3.537241	-2.303415	1.963445
N	0.084651	-2.918517	-0.595582
N	-1.079208	2.737731	-0.617571

1Me S=1

Ni	0.000003	-1.069731	0.259012
N	2.030520	-1.182511	-0.200453
C	2.752997	-2.274911	-0.482876
C	4.069227	-0.527155	-0.830946
C	4.047605	-1.902159	-0.883407
H	4.848047	0.174314	-1.076588
H	4.852220	-2.554822	-1.183083
N	-2.030508	-1.182523	-0.200493
C	-2.752981	-2.274919	-0.482946
C	-4.047602	-1.902164	-0.883432
C	-4.069237	-0.527163	-0.830912
H	-4.852215	-2.554822	-1.183120
H	-4.848066	0.174308	-1.076517
N	-0.000002	0.788562	-0.223216
C	-1.099061	1.606019	-0.123202
C	-0.723726	2.969190	0.044819
C	-2.452843	1.241018	-0.162622
C	-1.697393	3.957722	0.185068
C	-3.409512	2.240631	0.013288
C	-3.035596	3.580325	0.176358
H	-1.422252	4.999591	0.314185
H	-4.461986	1.986018	0.046206
H	-3.811200	4.326631	0.308501
C	1.099055	1.606025	-0.123216
C	2.452837	1.241031	-0.162653
C	0.723715	2.969194	0.044809
C	3.409505	2.240649	0.013241
C	1.697380	3.957732	0.185040
C	3.035584	3.580341	0.176311
H	4.461980	1.986040	0.046144
H	1.422235	4.999599	0.314160
H	3.811186	4.326652	0.308440
Cl	0.000001	-2.246576	2.206998
N	2.849814	-0.105565	-0.409229
N	-2.849818	-0.105577	-0.409206
C	-2.180205	-3.652307	-0.381189
H	-1.477451	-3.853813	-1.196658
H	-1.647341	-3.783048	0.561812
H	-2.975631	-4.396530	-0.442479
C	2.180223	-3.652297	-0.381067
H	1.646977	-3.782864	0.561742
H	1.477816	-3.853984	-1.196792
H	2.975698	-4.396507	-0.441880

1H S=1

Ni	-0.000001	-1.367568	0.184860
N	2.076041	-1.382761	-0.082724
C	2.811005	-2.467491	-0.331162
C	4.110678	-0.732554	-0.731378
C	4.101858	-2.110343	-0.743680
H	4.884375	-0.031658	-0.994290
H	4.911860	-2.764793	-1.022445
N	-2.076039	-1.382765	-0.082725
C	-2.811000	-2.467497	-0.331160
C	-4.101856	-2.110353	-0.743675
C	-4.110678	-0.732564	-0.731374
H	-4.911857	-2.764805	-1.022437
H	-4.884378	-0.031670	-0.994285
N	-0.000001	0.539437	-0.099310
C	-1.102711	1.367684	-0.025609
C	-0.722594	2.730057	0.127044
C	-2.463775	1.028756	-0.090513
C	-1.681847	3.735297	0.241095
C	-3.409748	2.043886	0.053700
C	-3.024508	3.379475	0.212315
H	-1.390188	4.773850	0.359368
H	-4.465461	1.801814	0.062800
H	-3.792301	4.137587	0.320034
C	1.102708	1.367686	-0.025608
C	2.463772	1.028761	-0.090511
C	0.722588	2.730058	0.127045
C	3.409744	2.043893	0.053703
C	1.681839	3.735300	0.241096
C	3.024501	3.379481	0.212317
H	4.465457	1.801822	0.062803
H	1.390178	4.773853	0.359368
H	3.792293	4.137594	0.320037
Cl	0.000010	-3.437117	1.151822
N	2.883460	-0.310607	-0.322706
N	-2.883461	-0.310613	-0.322706
H	-2.364191	-3.438377	-0.189346
H	2.364199	-3.438373	-0.189348

1tri S=1

Ni	0.000000	-1.434535	0.161283
N	2.008026	-1.493487	-0.317598
C	4.068772	-0.892993	-0.811656
C	3.920718	-2.255880	-0.926923
H	4.905337	-0.241891	-0.990523
H	4.641898	-3.003854	-1.213525
N	-2.008026	-1.493485	-0.317598
C	-3.920720	-2.255879	-0.926916
C	-4.068773	-0.892991	-0.811650
H	-4.641900	-3.003853	-1.213514
H	-4.905340	-0.241891	-0.990516
N	0.000000	0.460269	-0.246984
C	-1.097293	1.273074	-0.130478
C	-0.723560	2.635767	0.059466
C	-2.454866	0.916393	-0.169959
C	-1.697251	3.619684	0.217634
C	-3.413319	1.912047	0.013676
C	-3.038013	3.246636	0.200444
H	-1.421761	4.658822	0.366190
H	-4.466447	1.658256	0.032603
H	-3.811328	3.993128	0.341697
C	1.097295	1.273072	-0.130475
C	2.454867	0.916390	-0.169956
C	0.723563	2.635766	0.059468
C	3.413321	1.912042	0.013683
C	1.697255	3.619681	0.217639
C	3.038016	3.246632	0.200452
H	4.466448	1.658249	0.032612

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H    1.421766   4.658820   0.366194
H    3.811332   3.993122   0.341708
Cl  -0.000003  -2.323850   2.222953
N    2.853366  -0.431761  -0.423487
N   -2.853366  -0.431758  -0.423487
N    2.647689  -2.584398  -0.621550
N   -2.647690  -2.584396  -0.621546


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4 S=1
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Ni  -0.595325   0.000040   0.556227
N   -0.712781  -2.062549   0.072578
C   -1.813765  -2.795315  -0.125552
C   -0.087655  -4.082679  -0.643367
C   -1.461677  -4.081998  -0.579697
H    0.600483  -4.846480  -0.963251
H   -2.120125  -4.895048  -0.841319
N   -0.712588   2.062659   0.072654
C   -1.813504   2.795543  -0.125424
C   -1.461306   4.082160  -0.579670
C   -0.087288   4.082684  -0.643441
H   -2.119682   4.895270  -0.841288
H    0.600917   4.846395  -0.963398
N    1.245110  -0.000043  -0.071120
C    2.068641   1.096451  -0.047174
C    3.443397   0.722476   0.013712
C    1.709680   2.454296  -0.078920
C    4.442855   1.694089   0.068635
C    2.722803   3.408275   0.010141
C    4.071035   3.033129   0.076804
H    5.490898   1.415382   0.116818
H    2.473732   4.462116   0.047148
H    4.827100   3.807913   0.142920
C    2.068539  -1.096615  -0.047162
C    1.709455  -2.454428  -0.078895
C    3.443330  -0.722765   0.013719
C    2.722495  -3.408496   0.010177
C    4.442701  -1.694466   0.068656
C    4.070760  -3.033472   0.076839
H    2.473333  -4.462315   0.047191
H    5.490769  -1.415852   0.116837
H    4.826755  -3.808324   0.142965
C   -3.187382   2.235394   0.129813
H   -3.049236   1.208942   0.487185
C   -3.187598  -2.235048   0.129667
H   -3.049428  -1.208268   0.486083
C   -3.904206   3.014993   1.245112
H   -4.882910   2.573414   1.453143
H   -3.323470   3.001528   2.169674
H   -4.065007   4.059438   0.961136
C   -4.027464   2.194872  -1.158069
H   -5.003026   1.738891  -0.966949
H   -4.204674   3.201355  -1.548775
H   -3.531935   1.617314  -1.942518
C   -3.903935  -3.013729   1.245926
H   -3.322869  -2.999342   2.170265
H   -4.882625  -2.572091   1.453901
H   -4.064684  -4.058451   0.962942
C   -4.028153  -2.195722  -1.157935
H   -4.205450  -3.202558  -1.547692
H   -5.003677  -1.739645  -0.966851
H   -3.532959  -1.618817  -1.943076
N    0.351568  -2.862564  -0.236233
N    0.351828   2.862545  -0.236266
H   -1.125653   0.000013   2.037904

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5 S=1
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Ni  -0.506662  -0.000021   0.330935
N   -0.627920  -2.040894  -0.135471
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C    0.013782  -4.092684  -0.732367
C   -1.360828  -4.078498  -0.739882
H    0.708062  -4.875516  -0.985367
H   -2.012793  -4.896994  -0.999398
N   -0.627956   2.040908  -0.135419
C   -1.726211   2.772763  -0.358829
C   -1.360892   4.078458  -0.739981
C    0.013719   4.092640  -0.732555
H   -2.012871   4.896930  -0.999534
H    0.707992   4.875445  -0.985662
N    1.338241   0.000012  -0.189732
C    2.160093   1.100255  -0.123202
C    3.527736   0.723694  -0.004887
C    1.798238   2.455286  -0.158352
C    4.524337   1.693593   0.095107
C    2.807547   3.409096  -0.023499
C    4.150838   3.032634   0.094076
H    5.569228   1.414979   0.186277
H    2.559156   4.462794   0.011638
H    4.903273   3.806967   0.195086
C    2.160111  -1.100219  -0.123177
C    1.798281  -2.455258  -0.158292
C    3.527751  -0.723631  -0.004895
C    2.807616  -3.409043  -0.023446
C    4.524374  -1.693505   0.095087
C    4.150902  -3.032554   0.094093
H    2.559256  -4.462747   0.011705
H    5.569260  -1.414868   0.186249
H    4.903353  -3.806871   0.195101
C   -3.110790   2.206186  -0.187797
H   -3.004984   1.125821  -0.041225
C   -3.110759  -2.206187  -0.187972
H   -3.004983  -1.125780  -0.041670
C   -3.784953   2.770910   1.075071
H   -4.785262   2.345034   1.192592
H   -3.210395   2.524939   1.969006
H   -3.888696   3.858538   1.013870
C   -3.970231   2.434571  -1.442164
H   -4.950235   1.965301  -1.322001
H   -4.138690   3.500370  -1.622113
H   -3.500928   2.015729  -2.336169
C   -3.784927  -2.770635   1.075021
H   -3.210388  -2.524461   1.968911
H   -4.785245  -2.344748   1.192429
H   -3.888654  -3.858277   1.014047
C   -3.970190  -2.434879  -1.442292
H   -4.138659  -3.500721  -1.621975
H   -4.950193  -1.965576  -1.322247
H   -3.500884  -2.016260  -2.336399
N    0.445810  -2.860955  -0.355491
N    0.445762   2.860944  -0.355584
C   -1.340564  -0.000063   2.111288
N   -1.919948  -0.000072   3.118401

----
1 S=0
----
Ni  -0.370891  -0.000109   0.353134
N   -0.565283  -1.935690  -0.009409
C   -1.695448  -2.625573  -0.264282
C   -0.001510  -4.012889  -0.622784
C   -1.370828  -3.942208  -0.640737
H    0.670255  -4.813452  -0.881612
H   -2.056639  -4.727613  -0.913522
N   -0.566011   1.935499  -0.009232
C   -1.696444   2.625048  -0.263875
C   -1.372285   3.941631  -0.640918
C   -0.002980   4.012648  -0.623526
```

H	-2.058397	4.726776	-0.913691
H	0.668496	4.813293	-0.882856
N	1.381145	0.000179	-0.326728
C	2.204061	1.094628	-0.213712
C	3.574133	0.721574	-0.110610
C	1.836926	2.439436	-0.127227
C	4.563059	1.697719	0.024635
C	2.830594	3.399070	0.050100
C	4.181700	3.031300	0.104451
H	5.610440	1.421969	0.093984
H	2.563723	4.441922	0.174064
H	4.930466	3.804432	0.236486
C	2.204448	-1.093962	-0.213443
C	1.837808	-2.438893	-0.126661
C	3.574387	-0.720392	-0.110418
C	2.831821	-3.398118	0.050932
C	4.563665	-1.696142	0.025102
C	4.182790	-3.029841	0.105250
H	2.565333	-4.441042	0.175114
H	5.610943	-1.419991	0.094401
H	4.931833	-3.802667	0.237499
Cl	-1.815673	-0.000614	2.094894
C	-3.093129	2.064809	-0.212918
H	-3.022519	1.012731	0.050179
C	-3.092234	-2.065513	-0.214208
H	-3.021862	-1.013296	0.048427
C	-3.921187	2.750006	0.887022
H	-4.927613	2.323293	0.921112
H	-3.459400	2.600542	1.863382
H	-4.021096	3.825053	0.707284
C	-3.773629	2.180898	-1.589216
H	-4.765095	1.720595	-1.557800
H	-3.905998	3.223858	-1.891815
H	-3.193921	1.679147	-2.368414
C	-3.920760	-2.750349	0.885599
H	-3.459478	-2.600429	1.862124
H	-4.927259	-2.323753	0.919004
H	-4.020446	-3.825480	0.706238
C	-3.772035	-2.182256	-1.590798
H	-3.904140	-3.225361	-1.893007
H	-4.763564	-1.722043	-1.560076
H	-3.191987	-1.680782	-2.369921
N	0.472857	-2.803834	-0.238778
N	0.471829	2.803844	-0.239297

---
2 S=0

Ni	0.262560	0.000003	0.189547
N	0.443893	1.932087	-0.189773
C	1.563025	2.616714	-0.499965
C	-0.141911	4.002762	-0.802934
C	1.225627	3.929241	-0.878424
H	-0.823362	4.801480	-1.041643
H	1.900511	4.710139	-1.188866
N	0.444341	-1.931901	-0.189874
C	1.563490	-2.616382	-0.500327
C	1.226208	-3.929044	-0.878411
C	-0.141295	-4.002770	-0.802513
H	1.901126	-4.709893	-1.188899
H	-0.822682	-4.801643	-1.040887
N	-1.515576	-0.000064	-0.437754
C	-2.332429	-1.093999	-0.283899
C	-3.696314	-0.721335	-0.116603
C	-1.960521	-2.438060	-0.210769
C	-4.676557	-1.698514	0.066273
C	-2.943149	-3.398745	0.014334
C	-4.290663	-3.031826	0.130305
H	-5.719846	-1.423891	0.184576
H	-2.668882	-4.440877	0.128484
H	-5.031909	-3.805131	0.298641
C	-2.332633	1.093746	-0.284040
C	-1.960993	2.437891	-0.211107
C	-3.696453	0.720853	-0.116718
C	-2.943803	3.398430	0.013836
C	-4.676887	1.697877	0.065974
C	-4.291250	3.031273	0.129816
H	-2.669736	4.440627	0.127867
H	-5.720126	1.423074	0.184302
H	-5.032647	3.804461	0.298022
Br	1.723570	-0.000187	2.100932
C	2.956637	-2.046622	-0.508310
H	2.898591	-1.016831	-0.163344
C	2.956302	2.047253	-0.507312
H	2.898352	1.017496	-0.162230
C	3.869959	-2.803696	0.469758
H	4.870301	-2.362056	0.469317
H	3.479092	-2.749069	1.486655
H	3.972470	-3.857588	0.193012
C	3.532445	-2.051549	-1.936727
H	4.522895	-1.588153	-1.945650
H	3.641050	-3.068291	-2.325572
H	2.894519	-1.496802	-2.629523
C	3.869043	2.804654	0.471051
H	3.477757	2.750065	1.487790
H	4.869481	2.363232	0.471090
H	3.971436	3.858534	0.194219
C	3.532713	2.052137	-1.935483
H	3.641261	3.068853	-2.324412
H	4.523273	1.588963	-1.943925
H	2.895212	1.497158	-2.628485
N	-0.601473	2.799477	-0.384823
N	-0.600949	-2.799470	-0.384533

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3 S=0

Ni	-0.162719	0.000179	-0.005806
N	-0.324632	-1.928434	-0.388755
C	-1.426337	-2.612324	-0.757846
C	0.291561	-3.997181	-0.976492
C	-1.070554	-3.923473	-1.122186
H	0.984543	-4.795349	-1.181531
H	-1.728512	-4.703556	-1.468818
N	-0.324266	1.928821	-0.387858
C	-1.425754	2.612818	-0.757435
C	-1.069634	3.923764	-1.122181
C	0.292476	3.997212	-0.976385
H	-1.727377	4.703867	-1.469181
H	0.985666	4.795128	-1.181708
N	1.650632	-0.000035	-0.547816
C	2.456902	1.093066	-0.344412
C	3.809246	0.720863	-0.099048
C	2.079315	2.436086	-0.285818
C	4.775971	1.698841	0.141905
C	3.045880	3.397521	-0.002404
C	4.385294	3.031698	0.187553
H	5.811092	1.425312	0.319653
H	2.763566	4.438619	0.101437
H	5.114827	3.805195	0.400272
C	2.456630	-1.093383	-0.344550
C	2.078752	-2.436344	-0.286086
C	3.809062	-0.721521	-0.099098
C	3.045075	-3.398003	-0.002619
C	4.775554	-1.699742	0.141809
C	4.384567	-3.032505	0.187395
H	2.762512	-4.439039	0.101172
H	5.810734	-1.426464	0.319603
H	5.113910	-3.806179	0.400122
I	-1.689697	-0.000284	2.116393
C	-2.814379	2.038366	-0.837926
H	-2.777509	1.021292	-0.451519

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C   -2.814797  -2.037481  -0.838352
H   -2.777556  -1.020314  -0.452212
C   -3.795372   2.828118   0.043664
H   -4.791433   2.379927  -0.006710
H   -3.475775   2.819575   1.086674
H   -3.883489   3.868746  -0.283232
C   -3.290045   1.986751  -2.302050
H   -4.276844   1.519651  -2.362958
H   -3.371768   2.988571  -2.733678
H   -2.604403   1.410080  -2.927872
C   -3.795982  -2.826678   0.043522
H   -3.476316  -2.817939   1.086511
H   -4.791913  -2.378203  -0.006920
H   -3.884443  -3.867371  -0.283066
C   -3.290538  -1.986075  -2.302460
H   -3.372623  -2.987981  -2.733819
H   -4.277177  -1.518648  -2.363431
H   -2.604731  -1.409803  -2.928470
N    0.729377  -2.795456  -0.532063
N    0.729999   2.795466  -0.531736

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1Me S=0
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Ni   0.000039  -0.967082   0.259528
N    1.925663  -1.137606  -0.103898
C    2.600029  -2.260675  -0.421448
C    4.002141  -0.565572  -0.707181
C    3.914205  -1.933809  -0.793165
H    4.807778   0.110030  -0.938715
H    4.684883  -2.620143  -1.105558
N   -1.925525  -1.137748  -0.104024
C   -2.599766  -2.260881  -0.421598
C   -3.914002  -1.934150  -0.793223
C   -4.002101  -0.565928  -0.707140
H   -4.684616  -2.620556  -1.105618
H   -4.807833   0.109589  -0.938591
N   -0.000033   0.814939  -0.327481
C   -1.094703   1.631665  -0.184319
C   -0.721500   2.996525  -0.025623
C   -2.440232   1.260604  -0.118924
C   -1.698949   3.978093   0.147379
C   -3.401000   2.245849   0.094319
C   -3.033056   3.593296   0.206463
H   -1.424552   5.021992   0.260705
H   -4.444545   1.973942   0.201085
H   -3.806596   4.336186   0.366226
C    1.094565   1.631761  -0.184332
C    2.440123   1.260812  -0.118946
C    0.721246   2.996588  -0.025633
C    3.400811   2.246138   0.094281
C    1.698615   3.978239   0.147352
C    3.032754   3.593555   0.206422
H    4.444380   1.974318   0.201040
H    1.424131   5.022115   0.260680
H    3.806234   4.336511   0.366173
Cl  -0.000027  -2.513873   1.910048
N    2.801341  -0.099397  -0.290306
N   -2.801338  -0.099635  -0.290287
C   -2.015632  -3.635411  -0.432768
H   -1.167874  -3.699991  -1.119492
H   -1.655845  -3.925424   0.552640
H   -2.773165  -4.345819  -0.768212
C    2.016089  -3.635289  -0.432534
H    1.656284  -3.925273   0.552873
H    1.168382  -3.700051  -1.119305
H    2.773746  -4.345613  -0.767878

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1H S=0
----
Ni   0.000001  -1.284669   0.178039
N    1.938085  -1.373046  -0.054873
C    2.629140  -2.492640  -0.307085
C    4.013523  -0.817077  -0.664495
C    3.939001  -2.192220  -0.690181
H    4.820367  -0.147217  -0.908009
H    4.719228  -2.885441  -0.959083
N   -1.938082  -1.373048  -0.054881
C   -2.629133  -2.492642  -0.307107
C   -3.938999  -2.192222  -0.690186
C   -4.013524  -0.817080  -0.664490
H   -4.719226  -2.885443  -0.959088
H   -4.820372  -0.147221  -0.907993
N    0.000000   0.556157  -0.180155
C   -1.094807   1.377073  -0.074612
C   -0.721018   2.742804   0.074711
C   -2.445479   1.018970  -0.083505
C   -1.697487   3.731645   0.204326
C   -3.407942   2.012193   0.079200
C   -3.035462   3.356431   0.210474
H   -1.420503   4.775230   0.313820
H   -4.458433   1.751117   0.126185
H   -3.810078   4.105401   0.331630
C    1.094805   1.377074  -0.074614
C    2.445478   1.018974  -0.083508
C    0.721014   2.742805   0.074709
C    3.407940   2.012198   0.079194
C    1.697483   3.731648   0.204321
C    3.035458   3.356436   0.210467
H    4.458430   1.751123   0.126178
H    1.420498   4.775232   0.313815
H    3.810074   4.105407   0.331620
Cl   0.000001  -3.359866   1.087666
N    2.804761  -0.338464  -0.275896
N   -2.804761  -0.338467  -0.275895
H   -2.141078  -3.443937  -0.189172
H    2.141089  -3.443936  -0.189136

----
4 S=0
----
Ni  -0.577640   0.000524   0.168296
N   -0.716397  -1.940149   0.007217
C   -1.829246  -2.688174  -0.165938
C   -0.102894  -4.022136  -0.559467
C   -1.474593  -4.000725  -0.520224
H    0.581940  -4.810692  -0.819472
H   -2.138114  -4.819205  -0.744226
N   -0.713859   1.941278   0.006774
C   -1.825538   2.690549  -0.168239
C   -1.468731   4.003445  -0.519098
C   -0.096927   4.023628  -0.554697
H   -2.130897   4.822952  -0.743374
H    0.589305   4.811949  -0.811701
N    1.289312  -0.000486  -0.223923
C    2.105115   1.085589  -0.116453
C    3.478236   0.719495   0.019564
C    1.719325   2.428857  -0.075563
C    4.454506   1.705696   0.164929
C    2.705679   3.396737   0.109071
C    4.057481   3.037738   0.210192
H    5.503434   1.443878   0.263660
H    2.437232   4.442079   0.203829
H    4.795998   3.820022   0.347904
C    2.103683  -1.087812  -0.118549
C    1.716050  -2.430606  -0.079950
C    3.477294  -0.723805   0.018069
C    2.701166  -3.400185   0.102407
C    4.452276  -1.711600   0.161220
C    4.053485  -3.043207   0.203773
H    2.431331  -4.445331   0.195342
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H    5.501571  -1.451388   0.260298
H    4.790996  -3.826758   0.339666
C   -3.235904   2.189996   0.019873
H   -3.248243   1.138427  -0.266845
C   -3.238615  -2.186899   0.027734
H   -3.251841  -1.135537  -0.259723
C   -3.648447   2.278578   1.500845
H   -4.662268   1.891162   1.640041
H   -2.973117   1.696996   2.130110
H   -3.634185   3.315423   1.850630
C   -4.233953   2.940032  -0.875150
H   -5.225986   2.490004  -0.783978
H   -4.332517   3.992071  -0.590910
H   -3.943743   2.900427  -1.928140
C   -3.644794  -2.274110   1.510558
H   -2.966529  -1.692283   2.136418
H   -4.657847  -1.886169   1.653802
H   -3.629418  -3.310687   1.861094
C   -4.240854  -2.937256  -0.862290
H   -4.338704  -3.988984  -0.576652
H   -5.232258  -2.486662  -0.767217
H   -3.955225  -2.898740  -1.916577
N    0.347151  -2.788969  -0.229750
N    0.351095   2.789427  -0.226001
H   -1.940904   0.001718   0.677805

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5 S=0
----
Ni  -0.401823   0.001223   0.353019
N   -0.588279  -1.934578   0.016140
C   -1.717132  -2.634779  -0.227411
C   -0.016326  -4.013546  -0.583992
C   -1.386122  -3.951285  -0.594507
H    0.657666  -4.812260  -0.842507
H   -2.068281  -4.742430  -0.859278
N   -0.580216   1.936837   0.014297
C   -1.706147   2.640711  -0.231577
C   -1.370117   3.957766  -0.592063
C   -0.000181   4.016234  -0.575742
H   -2.049015   4.751765  -0.856690
H    0.676961   4.814017  -0.828814
N    1.374077  -0.001915  -0.302404
C    2.200105   1.088580  -0.192233
C    3.570552   0.714591  -0.090015
C    1.832357   2.432818  -0.096856
C    4.559108   1.689695   0.053465
C    2.826184   3.391186   0.088558
C    4.177193   3.022839   0.141495
H    5.606464   1.414067   0.123977
H    2.560471   4.433279   0.220818
H    4.925590   3.795148   0.280166
C    2.195848  -1.095789  -0.195170
C    1.822628  -2.438686  -0.103064
C    3.567741  -0.727497  -0.092029
C    2.812632  -3.401571   0.079468
C    4.552401  -1.706964   0.048495
C    4.165146  -3.038813   0.132857
H    2.542702  -4.442883   0.209317
H    5.600875  -1.435763   0.119565
H    4.910474  -3.814498   0.269206
C   -3.110404   2.096871  -0.191800
H   -3.051936   1.029336   0.006274
C   -3.120277  -2.088830  -0.177774
H   -3.059267  -1.021738   0.021507
C   -3.920998   2.734562   0.949102
H   -4.937490   2.331589   0.957310
H   -3.469752   2.515923   1.917149
H   -3.993058   3.820230   0.830778
C   -3.803340   2.290880  -1.553480
H   -4.797364   1.835844  -1.535157
H   -3.932852   3.349269  -1.797503
H   -3.235276   1.828366  -2.364860
C   -3.923801  -2.726777   0.968020
H   -3.465354  -2.510193   1.933155
H   -4.939477  -2.322031   0.984088
H   -3.998455  -3.812177   0.848830
C   -3.822991  -2.280320  -1.534758
H   -3.955860  -3.338213  -1.779135
H   -4.816188  -1.823851  -1.508912
H   -3.259997  -1.817698  -2.349607
N    0.455317  -2.800477  -0.211897
N    0.466646   2.800496  -0.206088
C   -1.739634   0.006123   1.676572
N   -2.422841   0.010015   2.616011
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Table S13. Frequencies (cm^{-1}) of all optimized species.

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1 S=1
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  17.3807    31.4124    33.7020
  36.6809    47.9852    55.3072
  62.3636    85.5406    86.2105
 100.2522   116.9773   142.6210
 157.2140   163.8936   171.1269
 182.7435   201.0234   224.5962
 232.4304   233.3338   238.5362
 238.8842   251.9250   263.4213
 273.8641   274.0736   295.5094
 313.3786   321.5631   337.7042
 342.4528   351.9381   378.3304
 396.5531   399.2691   409.5339
 410.1482   498.8108   524.1761
 541.3263   544.1397   582.1718
 583.9448   599.5703   605.1635
 634.8941   638.3930   643.6765
 649.3898   649.8048   715.5232
 722.0149   733.7384   734.8251
 737.3834   749.4286   772.5585
 772.9520   784.4314   801.5105
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 733.2342   734.0644   736.9954
 748.4890   768.4808   768.6714
 784.7950   801.4266   851.3454
 854.6603   854.6739   874.6639
 876.8891   888.2686   889.3444
 897.7361   925.2391   929.7361
 938.6104   938.6208   940.2621
 968.5465   969.7826   976.0325
1010.1617  1027.0335  1039.1407
1067.5322  1070.3293  1073.6319
1091.2828  1093.3524  1098.2190
1109.8794  1125.3027  1126.8801
1141.8038  1170.8655  1193.5360
1194.6792  1208.0562  1217.2663
1255.0956  1257.6750  1284.5681
1291.6479  1310.4537  1324.9601
1329.9408  1334.3632  1337.2324
1343.8911  1347.8684  1375.6474
1378.9935  1405.4198  1407.0698
1413.2373  1414.4956  1431.0330
1433.0185  1434.9832  1436.5189
1462.2703  1470.3554  1501.4532
1502.9796  1504.3454  1505.8643
1506.4284  1509.5457  1519.2749
1522.1647  1525.3689  1528.5712
1531.6445  1533.3841  1566.2803
1568.1297  1604.6075  1621.2724
1629.4066  1662.7896  1696.9774
3025.6534  3027.2946  3027.7446
3029.6975  3032.7474  3035.1141
3086.2023  3086.8729  3093.4918
3095.1359  3097.2092  3098.4789
3109.4633  3109.6437  3164.7074
3166.3988  3180.2082  3181.2776
3195.9907  3196.2637  3255.9019
3255.9171  3285.9748  3285.9811

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5 S=1
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  20.4581    33.3488    38.1137
  38.8621    46.3341    52.2736
  63.6557    65.3715    79.9265
  96.6695   115.0092   142.4135
 147.3729   162.2659   171.7151
 177.6806   197.7211   222.4259
 230.8870   231.7525   238.1210
 240.1797   249.6065   256.1755
 269.5473   272.9414   278.7296
 293.6879   316.4808   317.9765
 327.9029   341.9689   352.6001
 370.3182   386.7439   399.7971
 409.2590   409.7064   417.5397
 498.6507   524.9231   541.6561
 543.2058   582.9514   584.0636
 598.8697   605.6309   634.4272
 637.5344   642.9507   649.0164
 649.7274   714.7600   722.0866
 733.3507   734.3111   737.7065
 749.8003   771.4767   771.9514
 785.2425   803.1624   852.4399
 859.1765   859.2118   876.7991
 879.1987   889.0775   890.0394
 898.6559   931.2866   935.4046
 940.1647   942.3897   944.0793
 969.8686   971.4235   976.6106
1009.4308  1029.3187  1043.4918
1069.2454  1072.5114  1075.5908
1092.4594  1094.5536  1099.8745
1111.3851  1125.5358  1127.4573
1143.5616  1172.7447  1195.5329
1196.6091  1209.1362  1219.5082
1256.8725  1259.3484  1286.9600
1290.7832  1308.3975  1324.4258
1324.9285  1328.7078  1330.6073
1339.5726  1342.6859  1374.6895
1380.0159  1405.8495  1406.8916
1415.5949  1416.5921  1429.2056
1430.2004  1437.7915  1438.7825
1462.4930  1471.1307  1502.3113
1502.9531  1503.5755  1506.0960
1508.0895  1510.9558  1520.9992
1523.0425  1527.4590  1528.7823
1533.2534  1533.7711  1566.8721
1569.1444  1608.9438  1624.4886
1631.9923  1663.0664  2238.2311
3027.2357  3029.5009  3030.0323
3031.9626  3034.8112  3038.4626
3088.9253  3089.4011  3095.5888
3096.9685  3098.6747  3099.4187
3125.0531  3125.1803  3168.9310
3170.5050  3184.1046  3185.2156
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3260.5417  3288.8439  3288.8507

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   6.7156    35.7144    38.7736
  44.4866    59.1976    73.2095
  77.1932   108.9110   124.0285
 132.1320   139.9560   156.8294
 159.3922   180.0702   195.2455
 202.4184   217.7154   231.6029
 232.9887   236.6149   247.3115
 249.0310   259.4231   264.6751
 272.8119   293.1978   302.2499
 314.8365   322.4861   340.9533
 346.2102   350.9628   391.4558
 403.4922   407.5842   410.6528
 420.3165   499.0743   527.2373
 540.0726   546.3159   577.0879
 584.6852   601.3335   606.4431
 632.1447   634.4785   644.1323
 654.9651   656.9334   722.7111
 722.9217   730.2026   731.7203
 733.7292   743.7406   775.1256
 775.1701   778.4085   795.0102
 856.5573   861.1365   861.2999
 875.5311   877.3272   886.2420
 888.0553   906.1261   928.7542
 932.7402   936.2545   939.5083
 941.6721   968.1438   971.5672
 972.2436  1007.0277  1029.7377
1047.7966  1071.0352  1073.1644
1078.8971  1092.2227  1095.1587
1100.0679  1112.5887  1123.5539
1127.4702  1146.4582  1172.3471
1191.1107  1193.9850  1208.2674
1219.3425  1261.7468  1263.1223
1290.2307  1296.4862  1315.9091
1320.2497  1327.7711  1332.6960
1333.9824  1336.6756  1342.3760
1382.9856  1385.1199  1411.5000
1413.0121  1413.1328  1416.4713
1424.3785  1430.6679  1435.3015
1436.6672  1467.5968  1474.2159
1501.7926  1503.4307  1504.8655
1508.3196  1510.2053  1513.2168
1519.9020  1523.1068  1528.8175
1531.4044  1536.2141  1537.5883
1569.2061  1572.1448  1610.3347
1629.1356  1637.4294  1673.1136
3027.2648  3027.7126  3031.6249
3032.1839  3084.9920  3085.5805
3086.1512  3088.2415  3095.6379
3096.9037  3125.3775  3125.8453
3138.5064  3150.6165  3168.3273
3170.0335  3182.8373  3183.9046
3197.4528  3197.7481  3263.2368
3263.2500  3288.4501  3288.4604

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2 S=0
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  46.2017    59.7758    63.7510
  75.7977    86.0430   111.4285
 112.8427   124.1666   150.7928
 158.3051   170.3183   176.6543
 198.0552   211.7614   217.1586
 231.9097   233.9588   241.1173
 248.1758   259.5829   262.3504
 273.1065   292.2253   300.0873
 301.3639   322.5376   326.1003
 345.3750   350.1222   389.5767
 402.0813   403.9545   412.0068
 417.6870   498.6917   526.4897
 539.7720   546.5906   576.7936
 584.4370   601.0343   606.3623
 632.3182   634.9150   644.3979
 655.2537   657.1328   721.6110
 722.9990   730.3867   731.6120
 734.0908   744.0209   775.1988
 775.3331   778.7221   796.0290
 856.2145   861.6189   861.7566
 876.1816   878.0615   885.7746
 887.6218   905.7796   929.3054
 932.8761   936.4486   937.4729
 941.5564   967.6556   971.0246
 972.4721  1007.1673  1029.8348
1047.7587  1070.8703  1073.0999
1078.5251  1091.7431  1094.9270
1099.6613  1112.0887  1122.8464
1126.6075  1146.2819  1172.2145
1191.0370  1193.9470  1207.7561
1219.0331  1261.3818  1262.9266
1289.7197  1296.3924  1315.0400
1321.8725  1329.5265  1332.1513
1333.8943  1335.7104  1344.1697
1382.5717  1384.8158  1411.7256
1413.5218  1413.9904  1416.3712
1424.9324  1430.3684  1435.7304
1437.3123  1467.1580  1474.2969
1501.6344  1504.3453  1504.6336
1507.3816  1510.8100  1512.5958
1519.2739  1523.0246  1528.0548
1531.3502  1536.3714  1537.3567
1568.7011  1571.6026  1609.9808
1628.9277  1637.2716  1672.8055
3027.7456  3028.4541  3032.3728
3032.9473  3086.0558  3086.4090
3086.9355  3088.8166  3096.6199
3098.6222  3120.5438  3121.2653
3129.0762  3140.9783  3168.4359
3170.1381  3182.7357  3183.7716
3197.2117  3197.5163  3263.3250
3263.3378  3288.0108  3288.0178

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3 S=0
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  51.0246    57.2316    59.7029
  70.2215    77.5422   102.8320
 110.2851   122.5498   138.3233
 153.5283   157.6233   176.2239
 195.1970   206.9956   216.9430
 232.3373   235.4951   241.4076
 248.0870   259.7378   262.9692
 274.3173   292.4008   293.0629
 301.2644   323.0420   323.5314
 345.2705   350.1154   389.1012
 401.4190   401.6388   413.2494
 418.0969   498.5153   525.9179
 539.6455   546.8190   576.7139
 584.3374   600.6418   606.4644
 632.8061   635.5147   644.7359
 655.6195   657.6101   720.7168
 722.8920   730.4313   731.5619
 734.2812   744.2552   775.2688
 775.4692   779.1457   796.4937
 855.8326   861.9204   862.0341
 876.5419   878.4747   885.5063
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 932.3307   935.8873   936.5173
 941.6542   967.3794   970.8832
 972.5834  1007.0514  1029.9463
1047.9101  1070.5512  1073.2271
1078.4534  1091.4315  1094.7844
1099.2017  1111.5512  1122.4891
1126.2115  1145.9843  1172.0163
1191.2780  1194.2390  1207.3702
1218.7617  1260.7967  1262.4360
1289.2720  1296.5761  1314.0833
1321.7881  1329.2850  1331.0065
1332.8984  1334.8041  1344.0873
1382.2865  1384.5197  1411.5489
1413.5878  1414.4809  1415.9886
1424.7507  1429.4947  1436.2670
1437.9709  1466.9250  1474.3239
1500.9730  1504.5892  1504.8522
1507.4541  1511.2726  1512.8013
1519.3666  1523.3842  1527.6323
1531.2591  1536.4992  1537.0605
1568.0128  1570.8444  1609.4509
1628.6190  1636.9451  1672.4565
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3033.8600  3084.8868  3087.4814
3087.7787  3089.0166  3097.8299
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3170.1411  3182.6426  3183.6555
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3263.7111  3287.8691  3287.8757

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1Me S=0
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  74.3409    77.0488    77.6902
 125.6063   129.9568   139.2329
 179.8879   182.4256   191.4449
 203.8978   235.5040   252.0820
 264.9693   270.4897   279.6237
 283.5911   289.4412   320.1222
 324.0196   340.7899   343.4635
 344.5808   357.0442   406.6617
 440.6322   467.0154   536.4740
 541.9796   568.3304   583.9185
 587.5085   601.8782   629.8650
 632.0919   639.5359   667.2437
 671.0259   679.2976   691.3369
 724.5764   731.1561   733.6449
 743.8299   761.5916   762.3236
 778.1035   795.5577   853.6006
 854.0304   856.9936   876.5672
 878.3853   906.7228   929.3500
 933.3274   940.7637   975.2404
1004.0450  1008.5228  1036.4269
1063.2508  1064.6064  1071.4085
1076.9516  1077.5635  1093.0370
1093.5713  1095.0947  1107.6031
1150.7173  1174.8077  1209.1053
1221.0548  1256.9117  1257.8787
1293.5712  1303.2520  1320.4376
1332.5242  1336.2334  1381.6088
1383.2249  1389.9884  1393.4758
1412.4209  1417.0413  1435.4684
1440.0596  1467.9690  1474.1811
1489.7356  1495.7751  1497.2692
1508.2840  1529.2943  1533.0776
1539.6901  1541.5424  1564.7311
1567.9054  1609.9320  1628.4129
1636.8163  1672.2749  3049.2038
3052.1526  3106.6224  3109.2747
3144.1558  3144.5483  3168.4800
3170.1755  3182.7116  3183.7462
3197.1585  3197.4694  3260.3175
3260.3322  3288.5627  3288.5680

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1H S=0
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 108.9922   110.2368   127.7058
 157.4515   191.4933   199.9003
 222.8052   236.4776   239.3683
 257.3510   271.9099   292.3814
 307.7971   327.8005   336.8131
 346.0348   350.9891   398.2859
 414.5545   434.7742   537.5028
 540.3244   571.5930   584.6253
 587.0607   604.0158   624.3602
 624.8212   640.3303   654.3569
 655.3478   717.4051   722.2580
 733.4488   744.0731   756.2431
 757.4340   780.1076   797.8665
 846.2355   846.5344   856.5500
 875.6094   877.7353   907.9927
 915.9806   917.9161   930.1961
 933.7830   934.0786   935.4666
 949.1233   985.1456  1018.0882
1056.7523  1089.8271  1091.4459
1093.8664  1098.3227  1119.0620
1145.7679  1166.5863  1175.5874
1215.2803  1223.1188  1241.2388
1244.2572  1295.0246  1302.1613
1323.7517  1333.8596  1339.8790
1350.1170  1351.7927  1386.8669
1388.9686  1447.9576  1448.8973
1465.2660  1467.4092  1490.1776
1493.8158  1532.9192  1533.8159
1558.1664  1560.2067  1611.0587
1629.4859  1638.4183  1674.6050
3169.2671  3170.9979  3183.9241
3184.9612  3198.6282  3198.9071
3265.2728  3265.2913  3289.0826
3289.1130  3297.4233  3297.9547

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4 S=0
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   8.2595    34.4644    42.2238
  56.0645    59.9635    70.9018
  82.0311   118.3442   128.6436
 149.7520   162.7946   170.3441
 192.1254   215.5988   217.8548
 240.3613   240.7363   256.0548
 262.8069   267.8459   270.4629
 276.8138   296.3230   296.7471
 309.2343   319.4112   324.4917
 342.2984   361.9991   384.4410
 394.1015   394.9516   422.9932
 423.2713   497.6590   523.0123
 538.8382   545.9796   574.0536
 584.8752   602.1446   603.0882
 626.2442   633.0497   638.2269
 640.9034   650.1692   650.2707
 719.6685   724.4879   729.4098
 732.0182   733.4038   744.9477
 769.4610   770.2674   782.9676
 794.6953   854.7501   855.8006
 855.9411   871.2015   873.3109
 886.2629   887.8841   905.3452
 922.4374   926.7252   934.1021
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 938.1045   942.4536   963.5805
 969.1890   971.9219   998.9316
1023.0057  1044.0470  1053.3128
1067.3386  1081.9497  1082.8125
1089.6662  1092.3819  1093.3469
1114.0722  1130.5371  1131.7668
1142.1121  1169.0503  1192.0107
1192.3028  1208.4982  1217.8295
1254.8825  1257.9681  1284.9124
1300.4260  1315.0141  1317.2172
1324.3094  1335.3378  1338.3414
1341.0405  1344.0780  1383.3614
1386.4238  1401.1703  1404.2668
1410.5375  1412.3879  1418.4436
1421.9280  1434.5888  1435.4765
1472.3361  1473.9779  1504.6014
1505.3754  1506.3558  1508.4144
1511.8965  1516.8163  1524.1120
1525.9150  1529.1062  1529.8222
1534.7726  1535.0539  1562.8005
1564.3694  1604.6190  1625.9888
1632.5675  1674.9453  2081.6712
3026.3763  3026.7398  3031.4245
3031.8158  3076.9420  3079.0020
3083.7808  3084.3887  3099.1622
3099.5310  3104.4352  3107.6058
3115.9146  3116.6691  3163.8954
3165.5599  3179.7701  3180.8211
3196.0538  3196.3151  3268.5061
3268.5561  3291.0899  3291.0973

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5 S=0
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  13.5934    35.1702    50.1550
  58.8463    61.4759    73.1275
  81.1381   102.5508   124.5278
 128.5148   129.0721   153.0052
 159.9807   171.5012   195.4921
 206.0145   214.3912   227.2532
 229.8448   242.9983   249.4236
 256.0891   257.3385   268.8827
 275.5553   289.0662   299.5164
 318.3342   320.0926   339.0040
 351.8722   361.4238   390.4213
 399.7163   402.8179   407.7529
 414.4688   447.0381   466.4263
 501.4448   531.5160   540.4291
 549.0145   579.9244   584.9429
 602.0335   607.3657   632.3987
 634.1768   644.3303   655.2163
 656.9716   722.3300   723.3074
 730.9900   732.4395   734.4354
 744.9702   776.7791   777.1831
 780.1229   795.9251   856.3432
 863.7785   863.9257   875.8587
 877.7958   887.1874   888.6736
 906.8207   929.2476   933.0909
 940.1156   940.6969   944.2630
 969.2996   971.4121   971.8096
1005.0711  1029.2655  1047.9379
1069.7157  1072.7384  1078.3466
1092.4071  1095.2173  1098.2305
1112.5219  1124.3210  1127.1184
1145.3810  1171.7876  1192.4622
1194.8784  1208.5058  1219.2922
1260.2892  1262.0213  1289.5049
1297.5002  1314.5200  1321.1751
1330.3070  1330.6019  1332.2693
1337.4096  1341.7726  1383.3618
1384.9997  1410.4354  1414.0642
1414.2590  1415.4200  1421.3416
1426.6041  1437.6820  1438.7511
1468.5069  1474.5087  1501.3677
1502.7976  1505.7350  1509.3666
1510.0171  1513.8134  1520.7246
1523.3660  1528.3325  1530.8420
1535.6176  1537.1943  1568.0492
1570.6672  1609.3348  1628.5913
1636.9233  1673.8480  2237.0363
3028.7581  3029.0316  3033.0516
3033.4984  3087.2016  3087.7292
3087.7699  3089.5306  3097.2258
3098.0476  3128.2375  3129.0636
3133.5539  3143.3150  3168.3147
3170.0072  3182.9018  3183.9330
3197.5902  3197.8788  3264.6834
3264.7185  3289.3794  3289.4468
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Table S14. Energies (E_h) of all optimized species.

Species	E(SCF)	H(gas)	G(gas)	$E(TZ)_{B3LYP}$	$E(TZ)_{OPBE}$
1 S=1	–1834.281586	–1833.814052	–1833.904368	–3171.927346	–3171.679469
2 S=1	–1387.475817	–1387.008435	–1387.099782	–5285.885866	–5286.390575
3 S=1	–1385.511086	–1385.043799	–1385.136372	–3009.502881	–3009.617938
1 THF S=1	–2066.794682	–2066.202118	–2066.307516	–	–
2 THF S=1	–1619.986696	–1619.394211	–1619.500374	–	–
3 THF S=1	–1618.020421	–1617.427977	–1617.535134	–	–
$\mathbf{1_{Me}}$ S=1	–1676.996655	–1676.647799	–1676.724629	–3014.617719	–3014.448431
$\mathbf{1_{H}}$ S=1	–1598.342455	–1598.052046	–1598.121115	–2935.951165	–2935.818653
$\mathbf{1_{tri}}$ S=1	–1630.387749	–1630.122214	–1630.191945	–	–

4 S=1	–1374.606534	–1374.136027	–1374.224755	–2712.215913	–2711.834134
5 S=1	–1466.913180	–1466.438311	–1466.530045	–2804.533787	–2804.275951
1 S=0	–1834.260343	–1833.791994	–1833.879306	–3171.914047	–3171.675539
2 S=0	–1387.452434	–1386.984278	–1387.072385	–5285.870706	–5286.384654
3 S=0	–1385.486421	–1385.018374	–1385.107387	–3009.486112	–3009.610211
$\mathbf{1}_{Me}$ S=0	–1676.977608	–1676.628030	–1676.702041	–3014.606591	–3014.446662
$\mathbf{1}_{H}$ S=0	–1598.335960	–1598.044749	–1598.110669	–2935.953685	–2935.832427
4 S=0	–1374.616641	–1374.143100	–1374.226241	–2712.234068	–2712.041128
5 S=0	–1466.904931	–1466.428817	–1466.515766	–2804.532470	–2804.286272

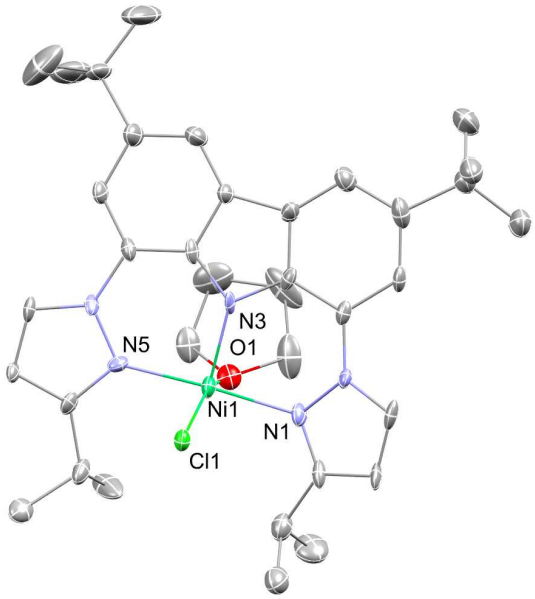


Figure S1. Molecular structure of **1**·THF with thermal ellipsoids at the 50% probability level. One of two crystallographically independent molecules is shown. Non-coordinated solvent molecules and hydrogen atoms are omitted for clarity. Color key: turquoise = Ni, blue = N, gray = C, red = O, green = Cl.

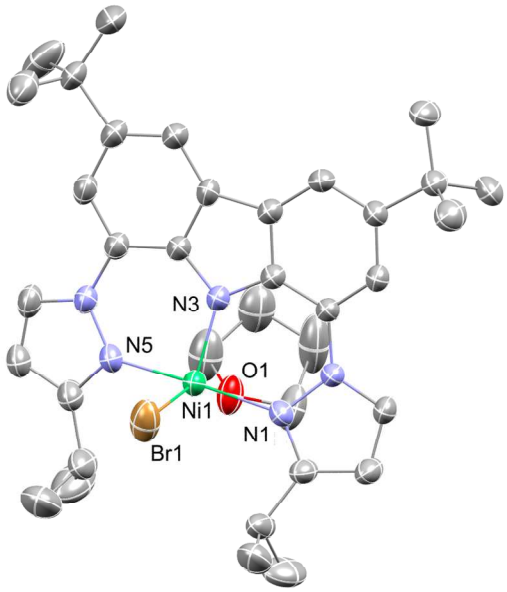


Figure S2. Molecular structure of **2**·THF with thermal ellipsoids at the 50% probability level. One of two crystallographically independent molecules is shown. Non-coordinated solvent molecules and hydrogen atoms are omitted for clarity. Color key: turquoise = Ni, blue = N, gray = C, red = O, brown = Br.

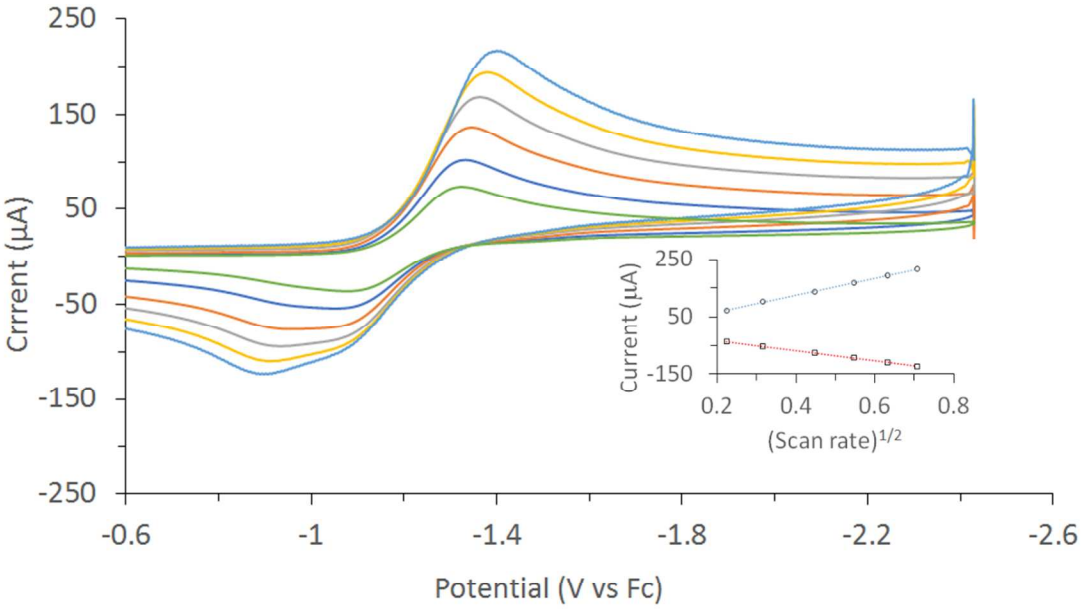


Figure S3. Cyclic voltammograms of 0.1 mM **3**·THF in THF (0.1 M nBu_4PF_6) at scan rates of 0.05, 0.1, 0.2, 0.3, 0.4, and 0.5 $V \cdot s^{-1}$. Inset: Plot of peak current versus square root of scan rate (i_{pc}, △; $R^2 = 0.9993$, and i_{pa}, □; $R^2 = 0.9997$).

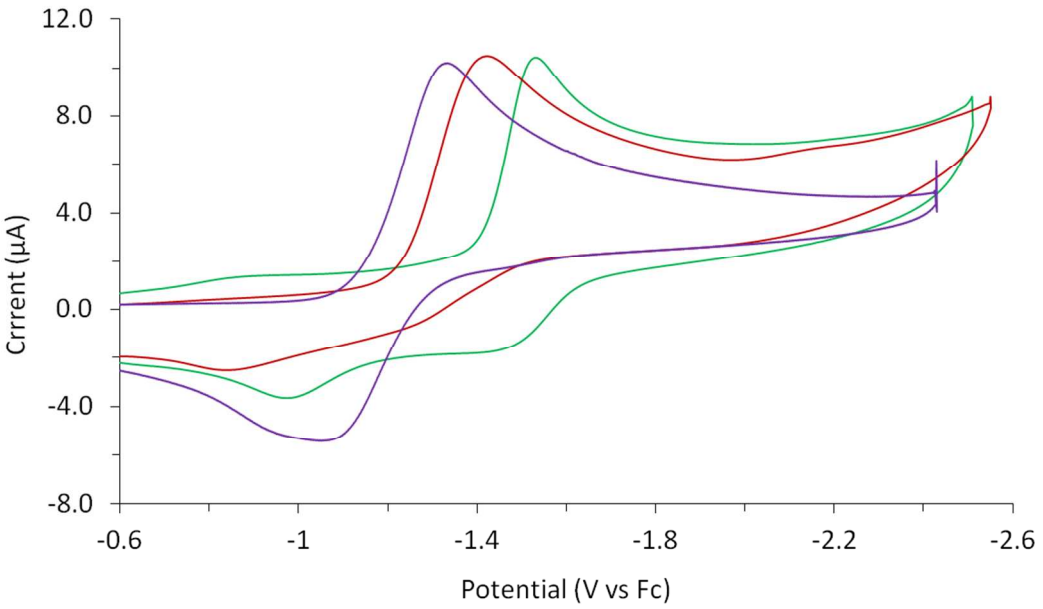


Figure S4. Cyclic voltammograms of **1**·THF (–), **2**·THF (–), and **3**·THF (–) in THF (0.1 M nBu_4PF_6) at scan rate of $0.1V \cdot s^{-1}$.

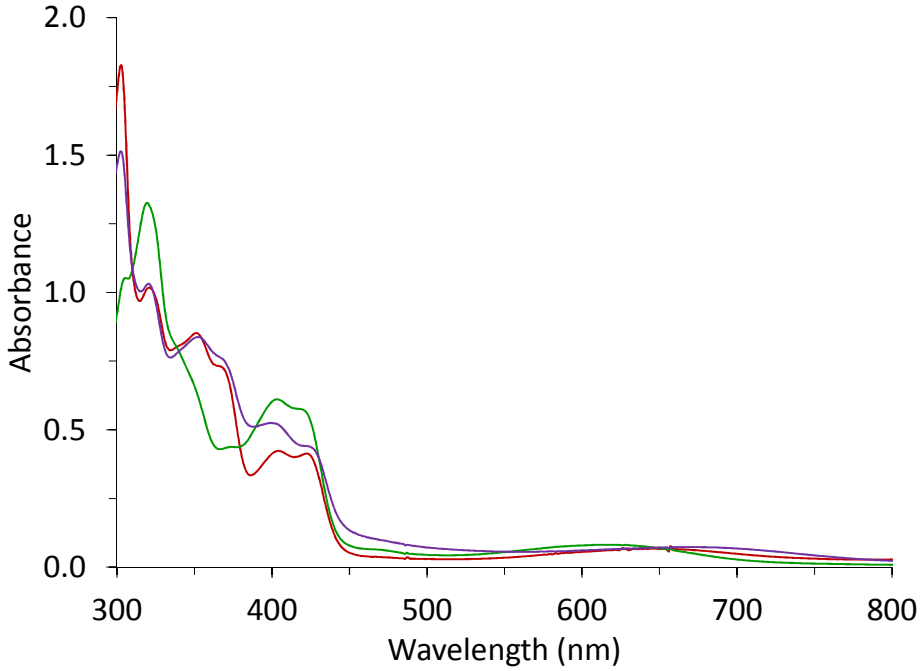


Figure S5. Electronic absorption spectra of 0.09 mM of **1**·THF (–), **2**·THF (–), and **3**·THF (–) in THF at 40 °C.

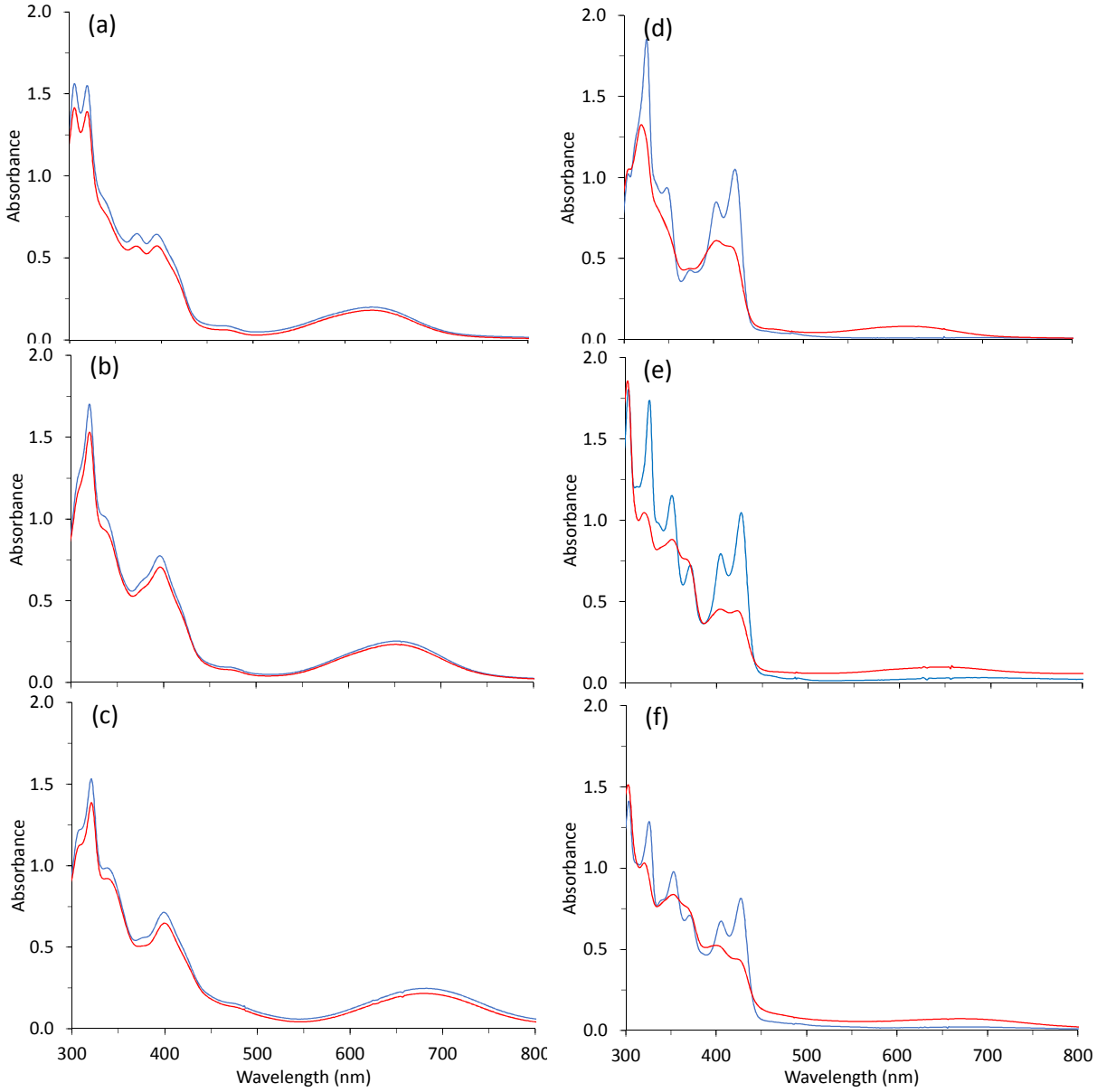


Figure S6. Temperature-dependent electronic absorption spectra of 0.09 mM of (a) **1**, (b) **2**, (c), **3**, (d) **1**·THF, (e) **2**·THF, (f) **3**·THF. 40 °C (–), −80 °C (–).

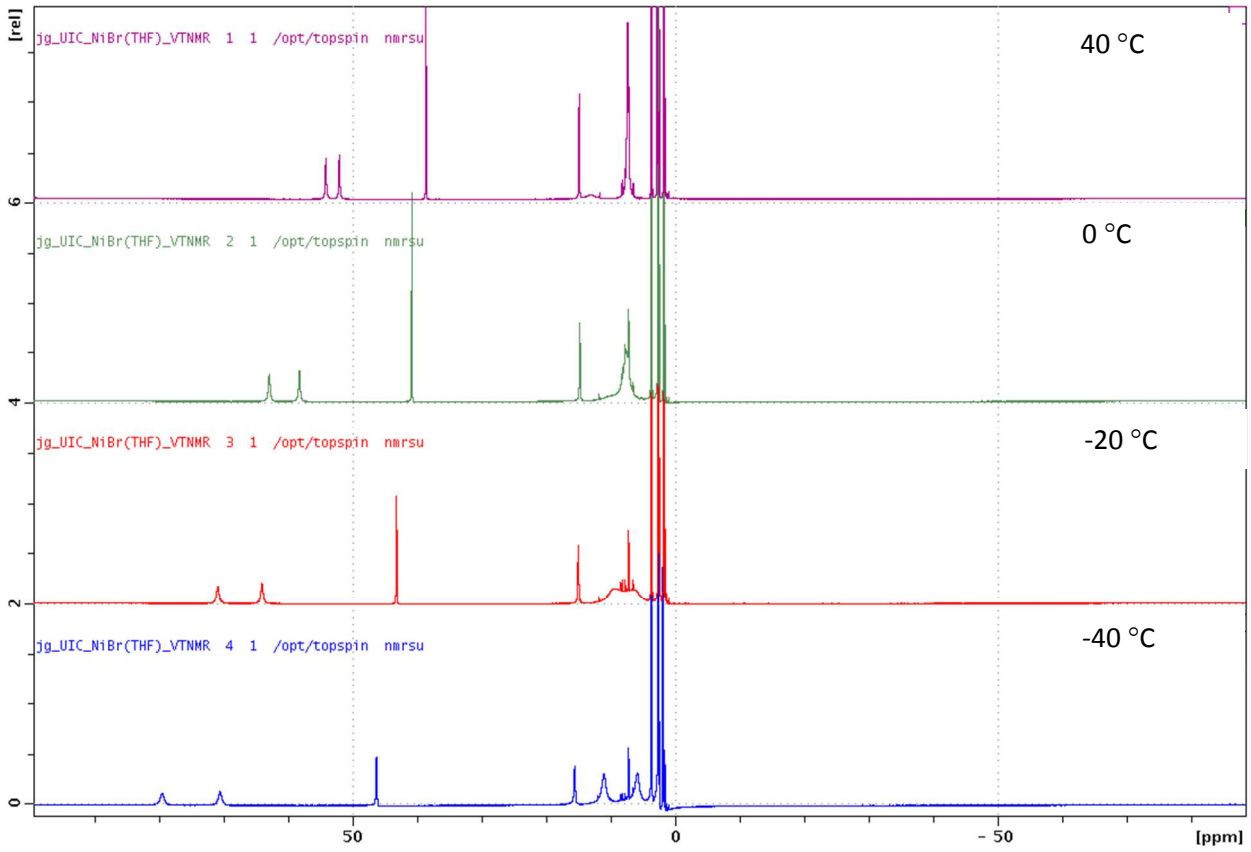


Figure S7. Various temperature NMR spectra of **2**·THF from 40 °C to −40 °C.

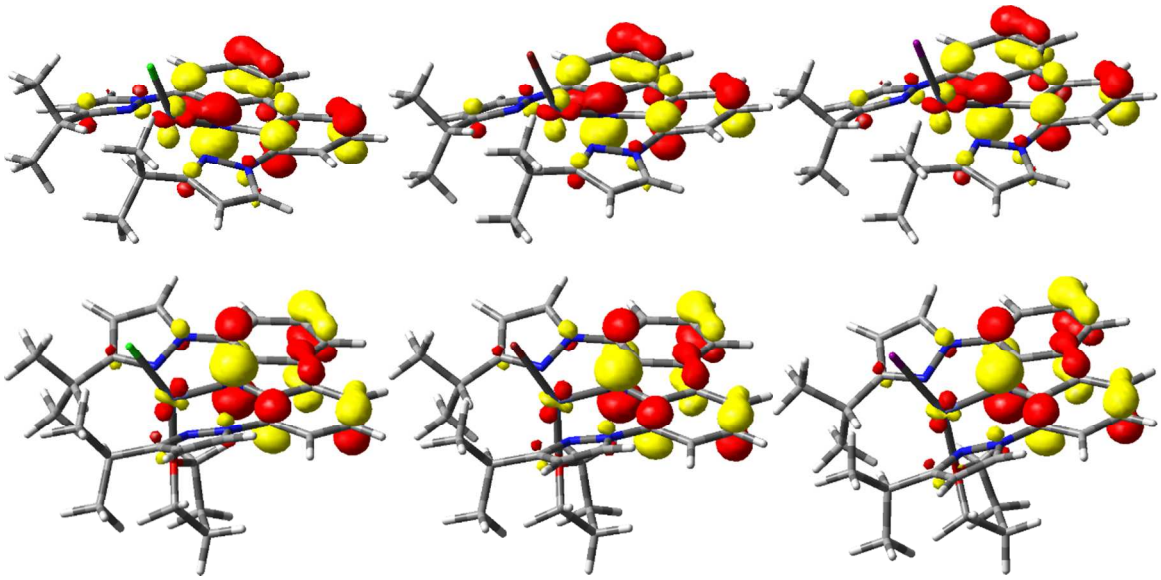


Figure S8. Isosurface plots (iso = 0.05 au) of the HOMO for **1** (top left), **2** (top middle), **3** (top right), **1**·THF (bottom left), **2**·THF (bottom middle), and **3**·THF (bottom right).

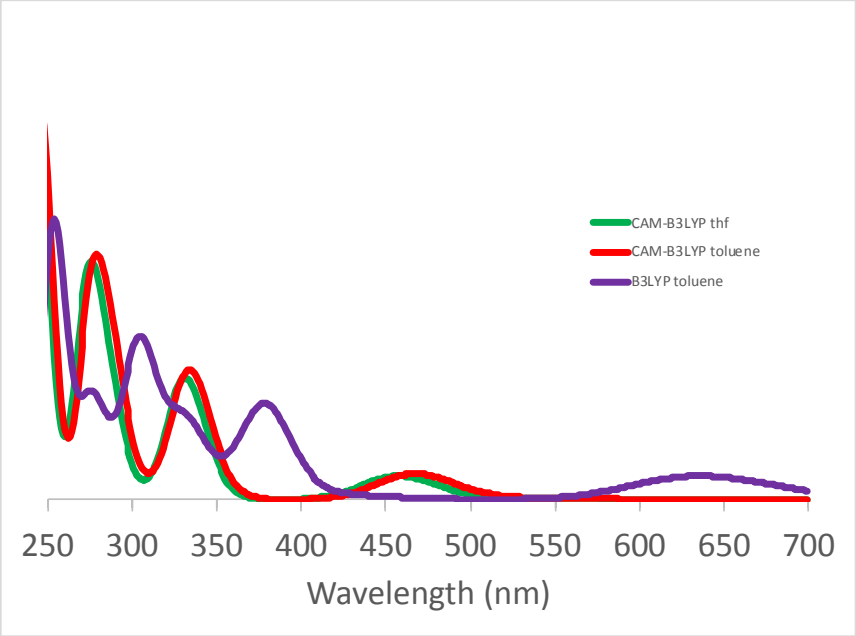


Figure S9. Comparison of CAM-B3LYP results with solvent = THF (green), solvent = red (toluene), and B3LYP with solvent = toluene (purple) for **1**. Only B3LYP reproduces the experimental spectrum qualitatively correct. Similar plots were seen for the other species (not shown).