Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Heliphyrin: An open porphryinoid with helical chirality.

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Supplementary Information

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General Information

Experimental

All reagents and starting materials were purchased from commercial vendors and used without further purification. 1,3-diiminoisoindoline (DII) was synthesized according to previously published procedures.[1] Deuterated solvents were purchased from Cambridge Isotope Laboratories and used as received.

NMR spectra were recorded on 300 MHz and 500 MHz spectrometers and chemical shifts were given in ppm relative to residual solvent resonances (^{1}H NMR and ^{13}C NMR spectra). High-resolution mass spectrometry experiments were performed on a Bruker MicroTOF-III and MicroTOF-qIII instruments. Infrared spectra were collected on Thermo Scientific Nicolet iS5 that was equipped with an iD5 ATR. UV-visible spectra were recorded on a Shimadzu UV-2600 UV-visible spectrometer.

X-ray intensity data were measured on a Bruker PHOTON II CPAD-based diffractometer with dual Cu/Mo ImuS microfocus optics (Cu Kα radiation, λ = 1.54178 Å, Mo Kα radiation, λ =0.71073 Å). Crystals were mounted on a cryoloop using Paratone oil and placed under a steam of nitrogen at 100 K (Oxford Cryosystems). The detector was placed at a distance of 5.00 cm from the crystal. The data were corrected for absorption with the SADABS program. The structures were refined using the Bruker SHELXTL Software Package (Version 6.1),[2] and were solved using direct methods until the final anisotropic full-matrix, least squares refinement of F^2 converged.

Electrochemistry measurements were conducted using a CHI 820D potentiostat in a standard three-electrode configuration. Platinum wire was used as the counter electrode. The working electrode used was a 2 mm diameter platinum disk. A nonaqueous Ag/Ag^+ reference electrode was used by immersing silver wire in a degassed DMF solution of 0.01 M $AgNO_3$ /0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$). All potentials were referenced to the

ferrocene/ferrocenium couple. The concentration of analyte was 1.0 mM, and the supporting electrolyte was 0.1 M $TBAPF_6$ dissolved in DMF.

Separation of Enantiomers

Enantiomeric separations of the three heliphyrin complexes were carried out by HPLC purification performed on a GE Äkta Purifier equipped with a UV900 detector and a 5 μm CHIRALPAK IE (Daicel) column. The solvent system used was 80%/20%/0.1% EtOH/hexane/DMF v/v/v. The detector was set to measure absorption at 254 nm.

Computational Details

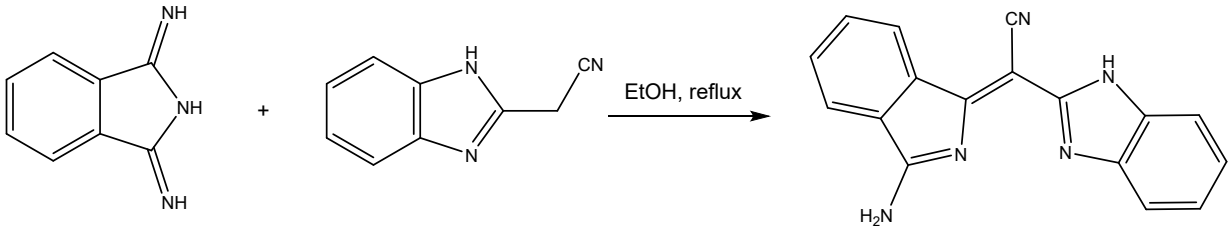
The starting geometries of compounds **1** and **M(Hlp)s** were optimized using a B3LYP exchange–correlation functional.[3] Energy minima in optimized geometry were confirmed by the frequency calculations (absence of the imaginary frequencies). The solvent effect was modeled using the polarized continuum model (PCM).[4] In all calculations, DMF was used as the solvent. In PCM-TDDFT calculation, the first 100 states were calculated. The Co, Ni, and Cu atoms were modeled using the 6-311+G basis set.[5] All other atoms were modeled using the 6-311G(d)[6] basis set. Gaussian 09 software was used in all calculations.[7] The QMForge program was used for molecular orbital analysis in all cases.[8]

Full citation for Gaussian

Gaussian 09, Revision D.01,. Frisch, M. J; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.;. Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.;. Cioslowski, J.; Stefanov, B. B.; Liu, G.;. Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2009.

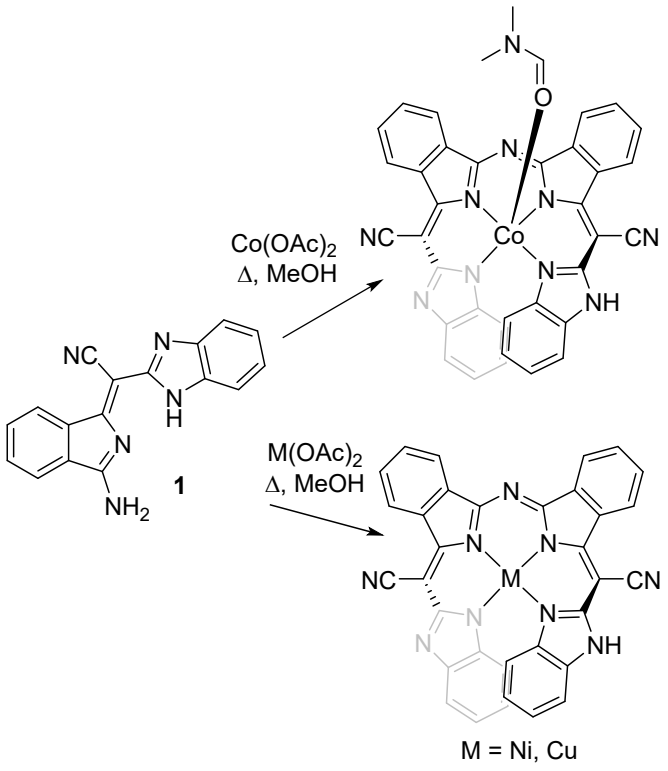
Syntheses.

DII (1.00 g, 6.9 mmol) and (2-benzimidazolyl)acetonitrile (1.08 g, 6.9 mmol) were dissolved in EtOH (10 mL) and refluxed for 1 hour. The resulting solution was cooled down to room temperature, filtered, and washed with cold EtOH to give orange powder. Crystals suitable for X-ray diffraction were grown from slow evaporation from DMF.



1: Yield: 1.94 g (98%). IR: 3546, 3378, 3011 cm^{-1} (ν_{NH}), 2210 cm^{-1} (ν_{CN}). ^1H NMR (300 MHz, $CDCl_3$): δ = 12.71 (s, 1H, N*H*), 9.35 (s, 1H, N*H*), 9.14 (s, 1H, N*H*), 8.37 (d, 1H, J = 7.58 Hz), 8.09 (d, 1H, J = 7.25 Hz), 7.75 (t, 1H, J = 7.58 Hz), 7.70-7.65 (m, 2H), 7.55 (d, 1H, J = 6.92 Hz), 7.22 (m, 2H). $^{13}C\{^1H\}$ NMR (125 MHz, d_6 - DMSO): δ = 168.6, 161.8, 149.0, 144.8, 143.2, 138.3, 133.9, 133.2, 131.8, 130.5, 123.2, 122.4, 121.9, 118.8, 117.6, 111.3, 84.4. HRMS (ESI-TOF, negative mode) m/z: calcd for $C_{17}H_{10}N_5$ 284.0942, found 284.0927 $[M-H]^-$.

Synthesis of Metal complexes. A solution of $M(OAc)_2$ hydrate (M = Co, Ni, Cu) (0.35 mmol), and two equivalents of **1** (0.20 g, 0.70 mmol) in MeOH (7.00 mL) were refluxed in an oil bath for 1 hour. The resultant precipitate was filtered and washed with hot MeOH. The compounds were isolated as dark blue solids. Crystals suitable for X-ray diffraction were grown by slow evaporation of DMF. The copper complex had one equivalent of disordered DMF in the unit cell that was removed by use of the SQUEEZE program.[9]



Co(Hlp)(DMF): Yield: 0.16 g (67%). IR: 3055, 2916 cm^{-1} (ν_{NH}), 2214 cm^{-1} (ν_{CN}). HRMS (ESI TOF, negative mode) m/z: calcd for $C_{34}H_{16}CoN_9$ 609.0866, found 609.0831 $[M-H]^-$.

Ni(Hlp): Yield: 0.18 g (84%). IR: 3059 cm^{-1} (ν_{NH}), 2219 cm^{-1} (ν_{CN}). ^1H NMR (300 MHz, DMSO): 9.24 (s, 2H), 8.90(s, 1H, N*H*), 8.05 (d, 1H), 7.74 (t, 2H), 7.58 (d, 1H), 6.68 (s, 8H). HRMS (ESI-TOF, negative mode) m/z: calcd for $C_{34}H_{16}N_9Ni$ 608.0888 found 608.0908 $[M-H]^-$.

Cu(Hlp): Yield: 0.14 g (65%). IR: 3077, 2919 cm^{-1} (ν_{NH}), 2213 cm^{-1} (ν_{CN}). HRMS (ESI-TOF, negative mode) m/z: calcd for $C_{34}H_{16}CuN_9$ 613.0825, found 613.0798 $[M-H]^-$.

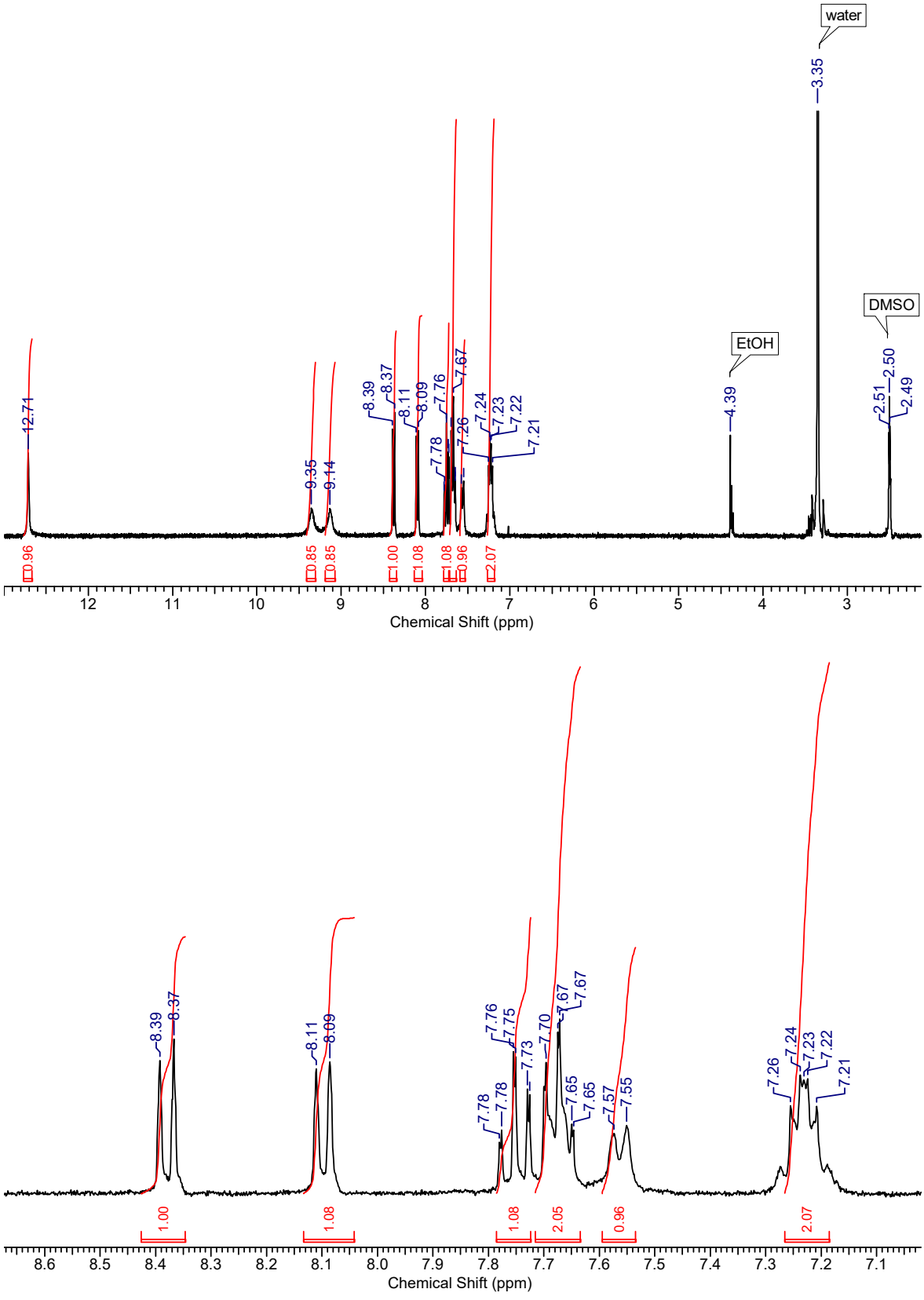


Figure S1: ^{1}H NMR (300 MHz) of **1** in d6-DMSO.

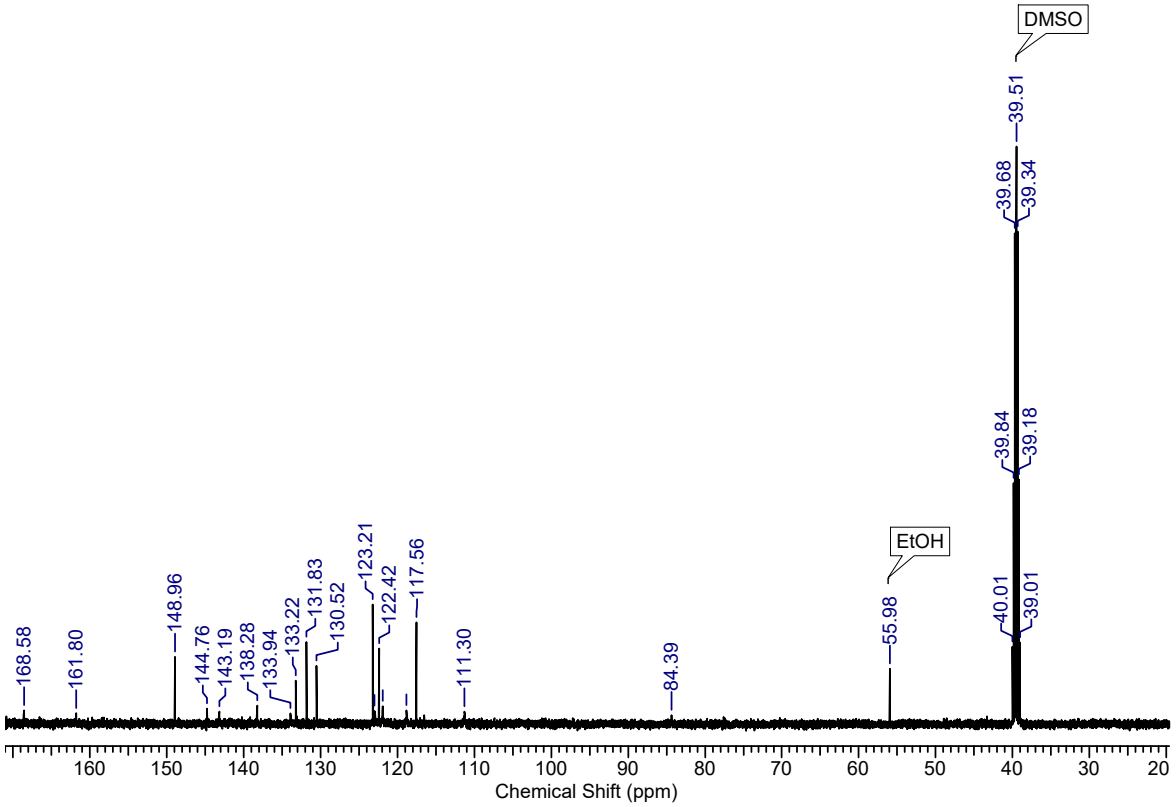


Figure S2: $^{13}C\{^{1}H\}$ NMR (125 MHz) of **1** in d6-DMSO.

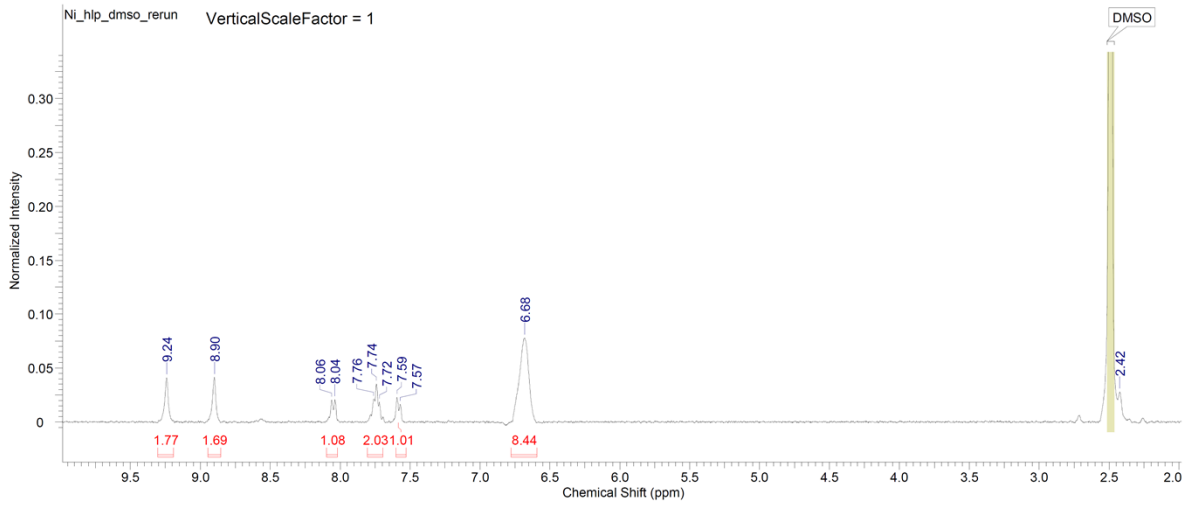


Figure S3: ^{1}H NMR (125 MHz) of **Ni(Hlp)** in d6-DMSO.

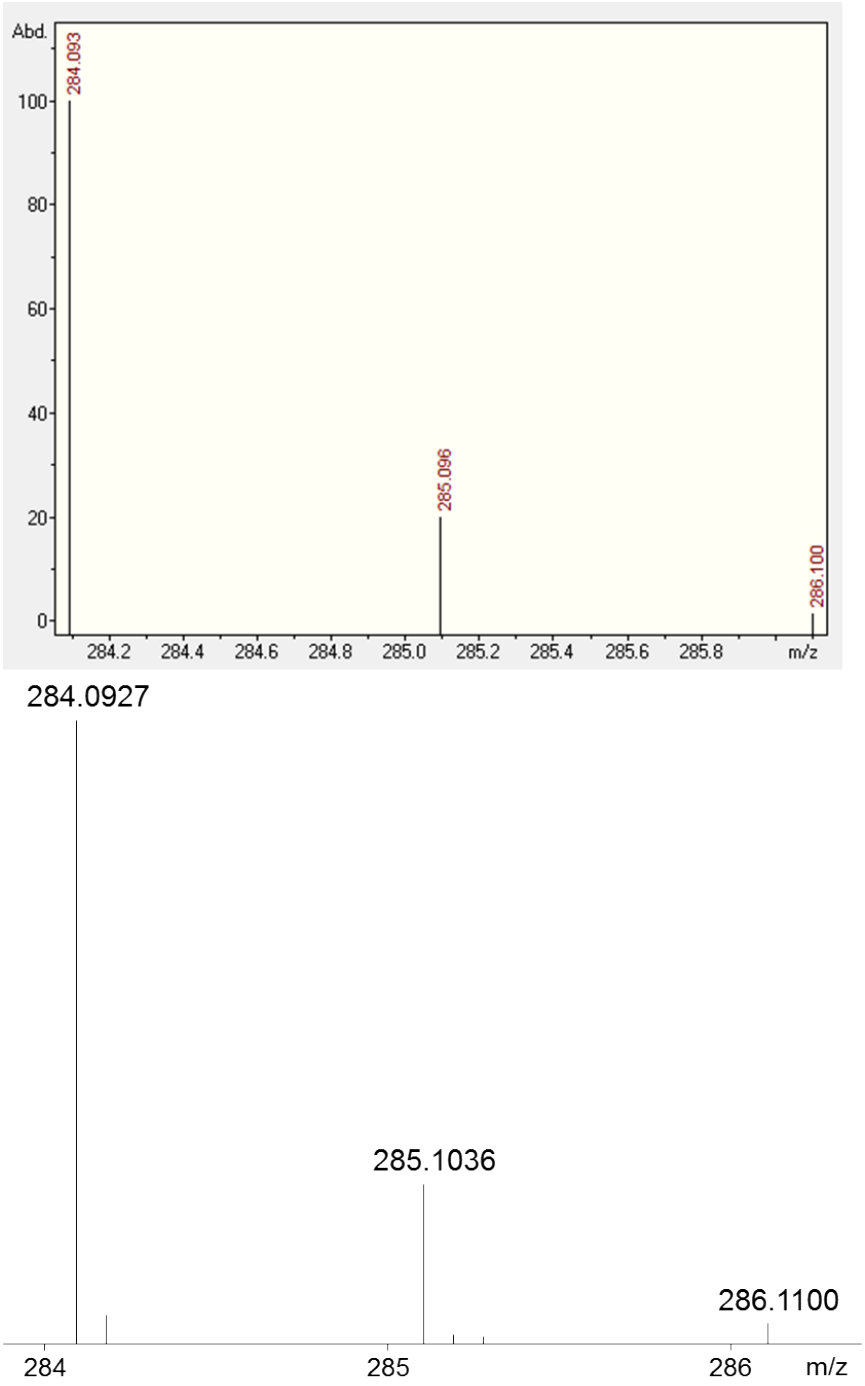


Figure S4: High-resolution ESI mass spectra of **1**. Top: calculated spectrum. Bottom: experimental spectrum.

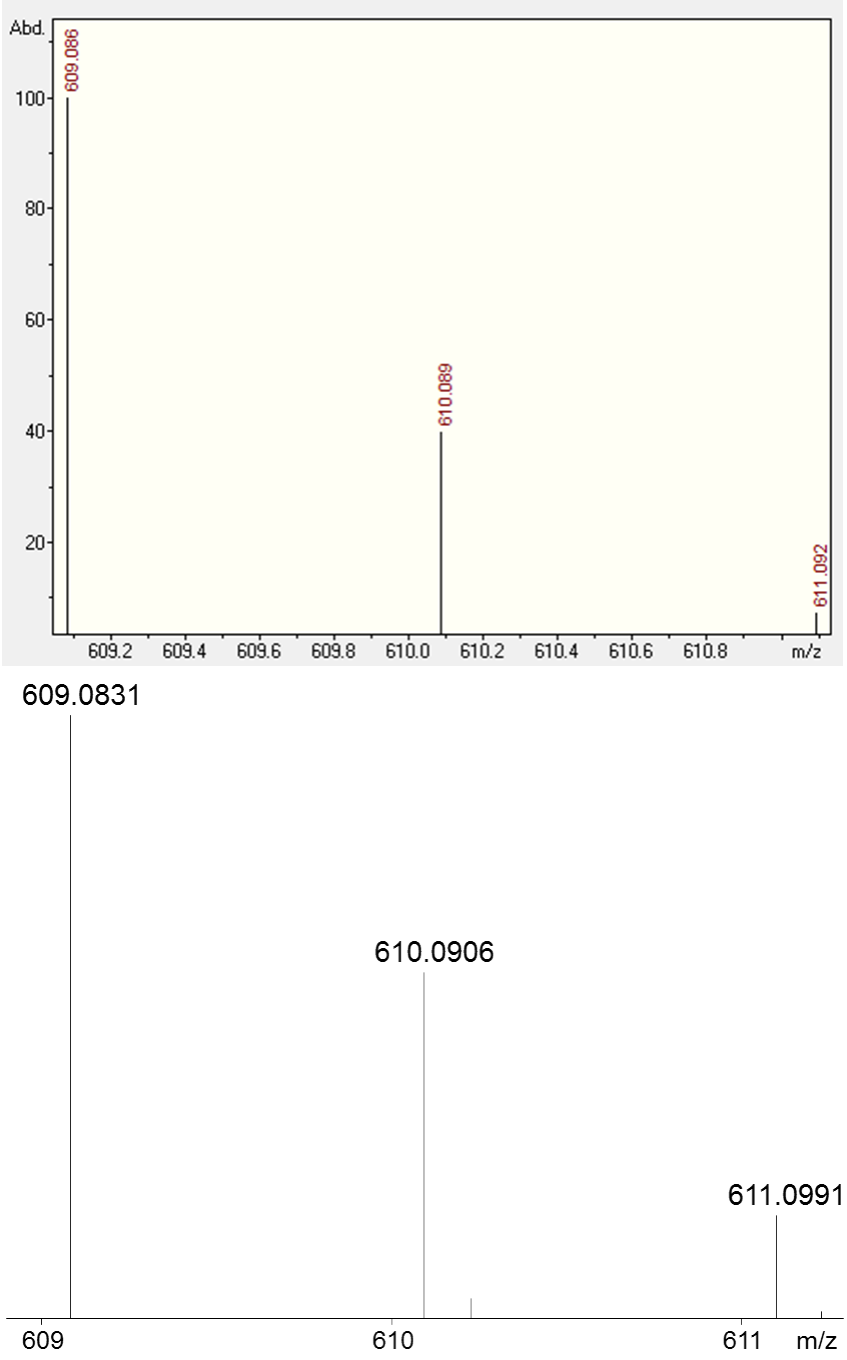


Figure S5: High-resolution ESI mass spectra of **Co(Hlp)(DMF)**. Top: calculated spectrum. Bottom: experimental spectrum.

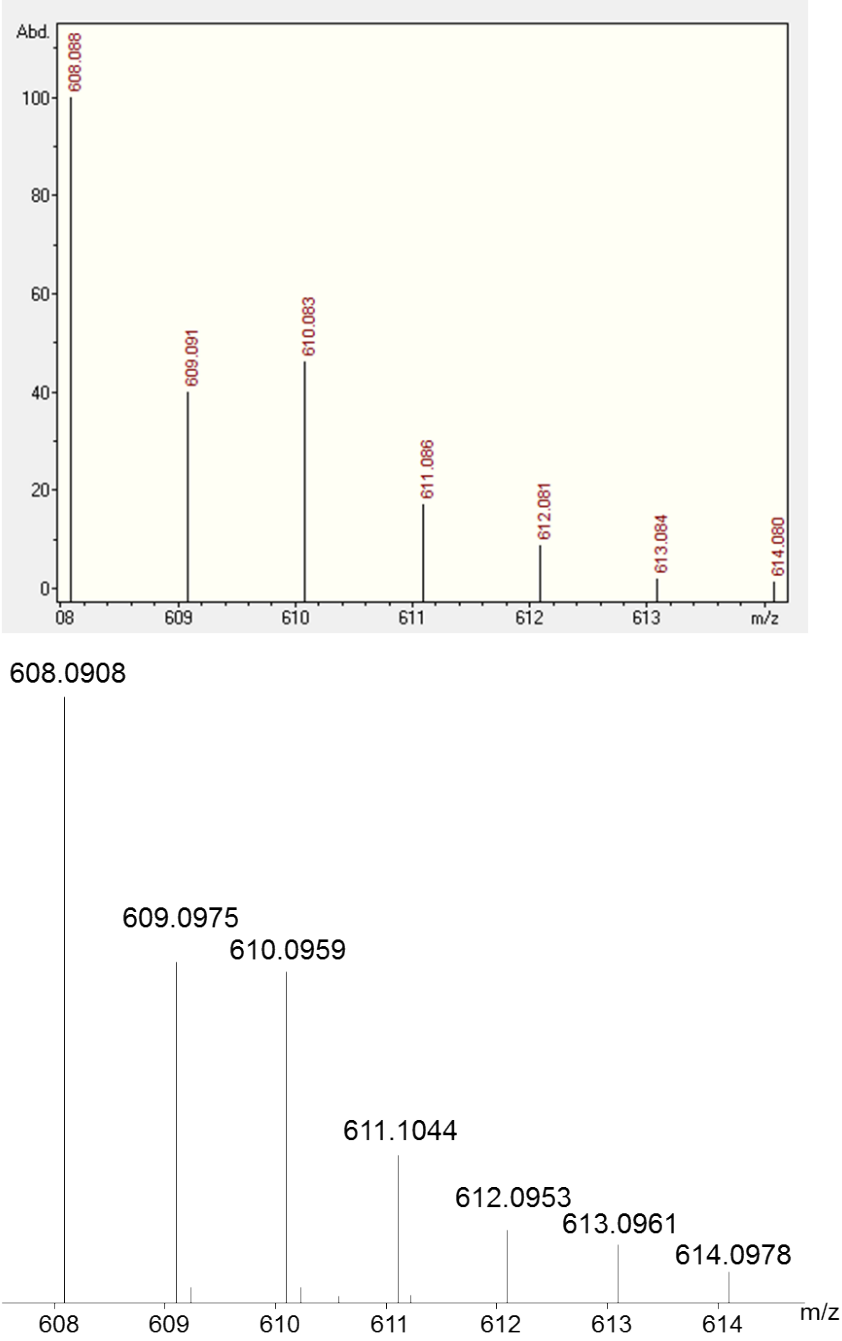


Figure S6: High-resolution ESI mass spectra of **Ni(Hlp)**. Top: calculated spectrum. Bottom: experimental spectrum.

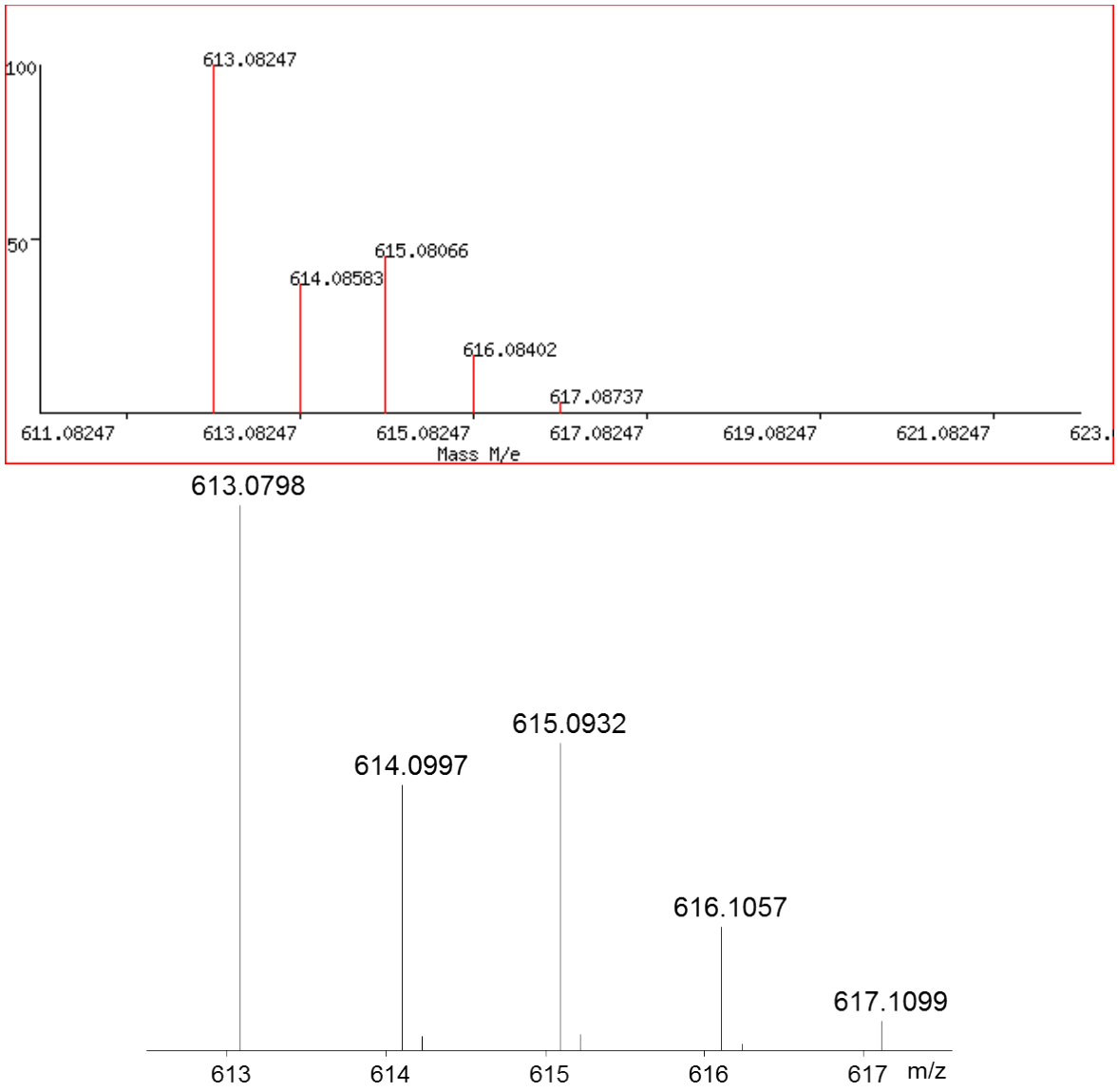


Figure S7: High-resolution ESI mass spectra of **Cu(Hlp)**. Top: calculated spectrum. Bottom: experimental spectrum.

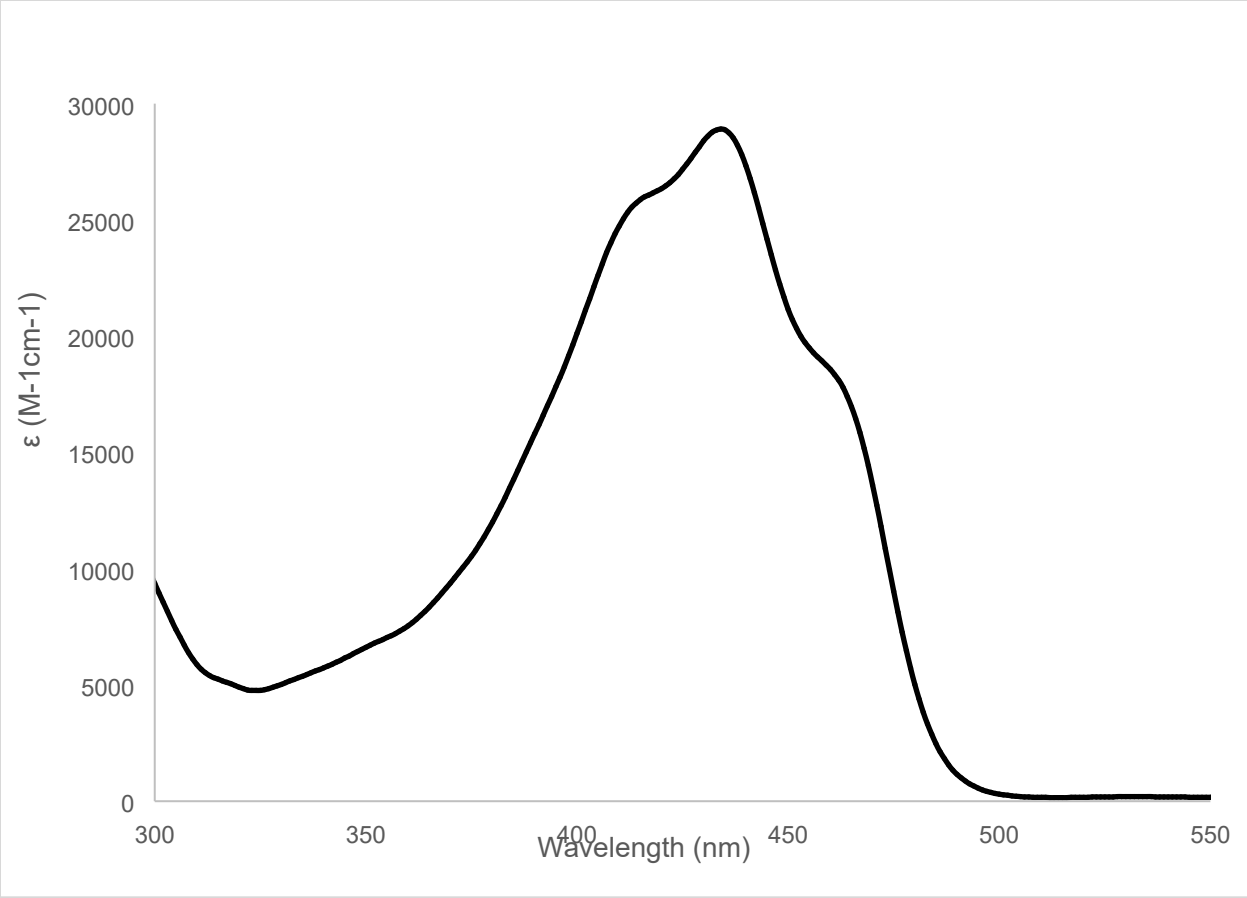
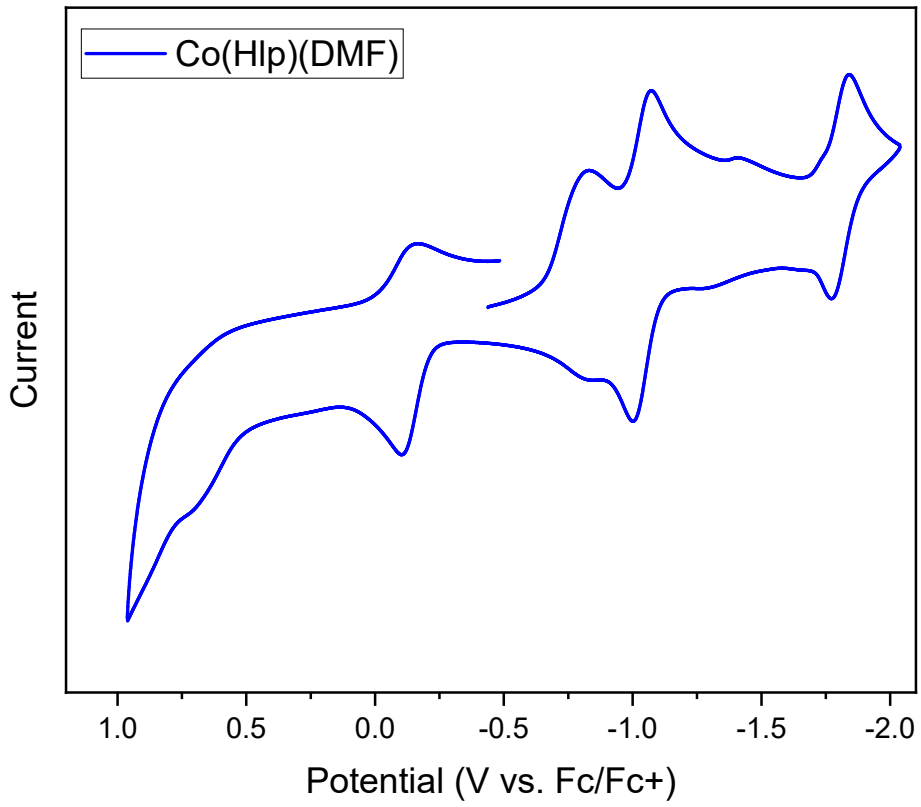
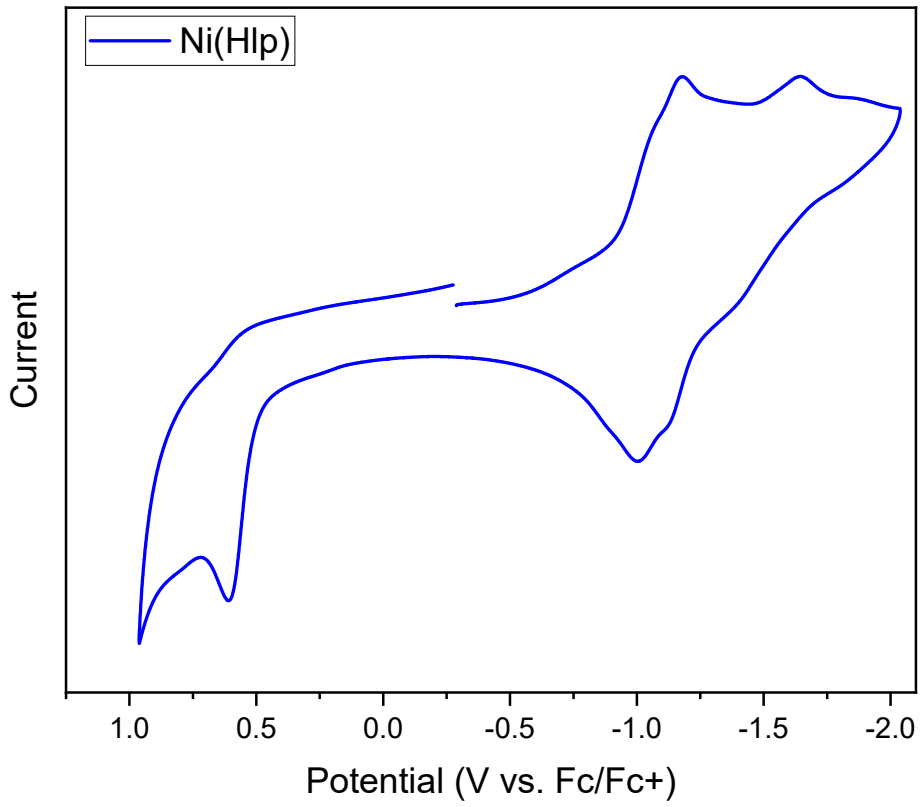


Figure S8: UV-visible spectrum for compound **1** in DMF.



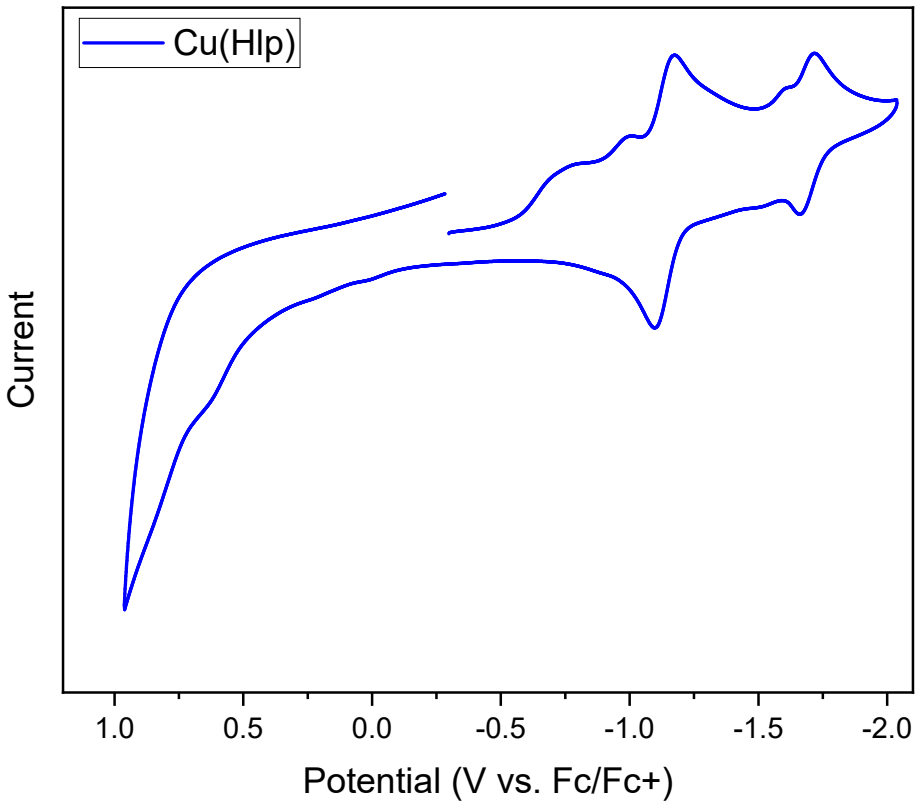
Compound	Potentials V
Co(Hlp)(DMF)(red)	-0.17, -0.83, -1.08, -1.42, -1.84
Co(Hlp)(DMF)(ox)	0.75, -0.066, -0.96, -1.74

Figure S9: Cyclic voltammograms for **Co(Hlp)(DMF)** recorded in the DMF/0.1 $TBAPF_6$ system at room temperature. Redox potentials (V) vs Fc/Fc^+ are displayed in the table.



Compound	Potentials V
Ni(Hlp)(red)	-1.18, -1.64
Ni(Hlp)(ox)	0.61, -1.00

Figure S10: Cyclic voltammograms for **Ni(Hlp)** recorded in the DMF/0.1 $TBAPF_6$ system at room temperature. Redox potentials (V) vs Fc/Fc^+ are displayed in the table.



Compound	Potentials V
Cu(Hlp)(red)	-0.72, -1.00, -1.18, -1.60, -1.72
Cu(Hlp)(ox)	0.65, -1.10, -1.66

Figure S11: Cyclic voltammograms for **Cu(Hlp)** recorded in the DMF/0.1 $TBAPF_6$ system at room temperature. Redox potentials (V) vs Fc/Fc^+ are displayed in the table.

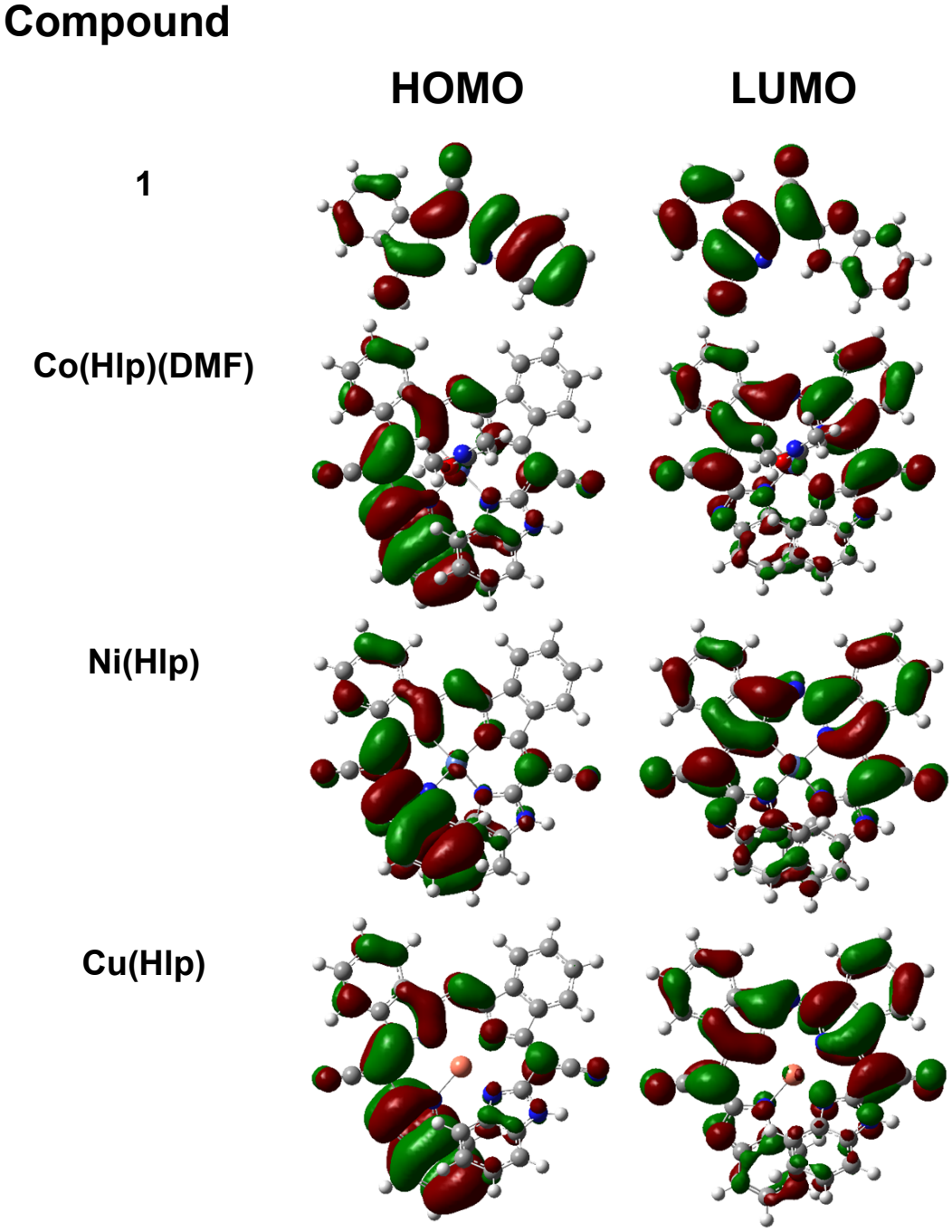


Figure S12: DFT-predicted frontier orbitals for **1** and **M(Hlp)** complexes**.**

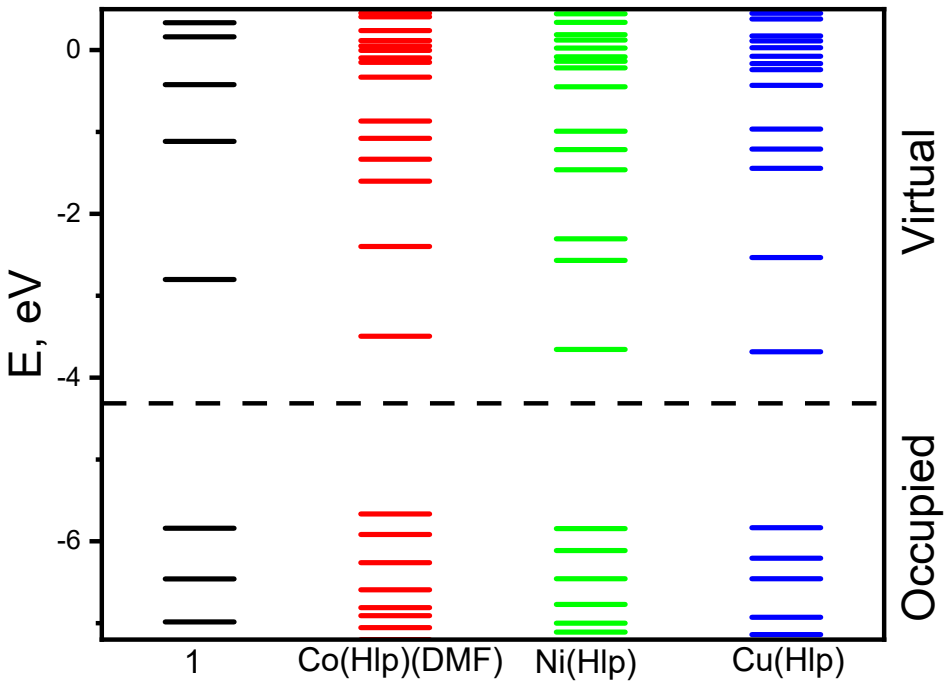


Figure S13: Relative energies of the frontier orbitals for **1** and **M(Hlp)** complexes (α-spin).

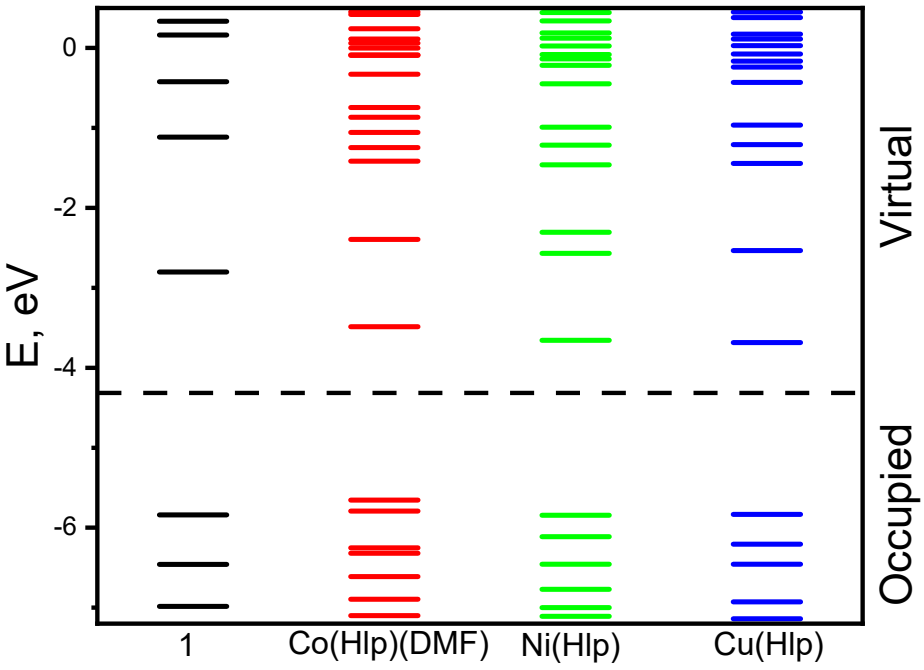


Figure S14: Relative energies of the frontier orbitals for **1** and **M(Hlp)** complexes (β-spin).

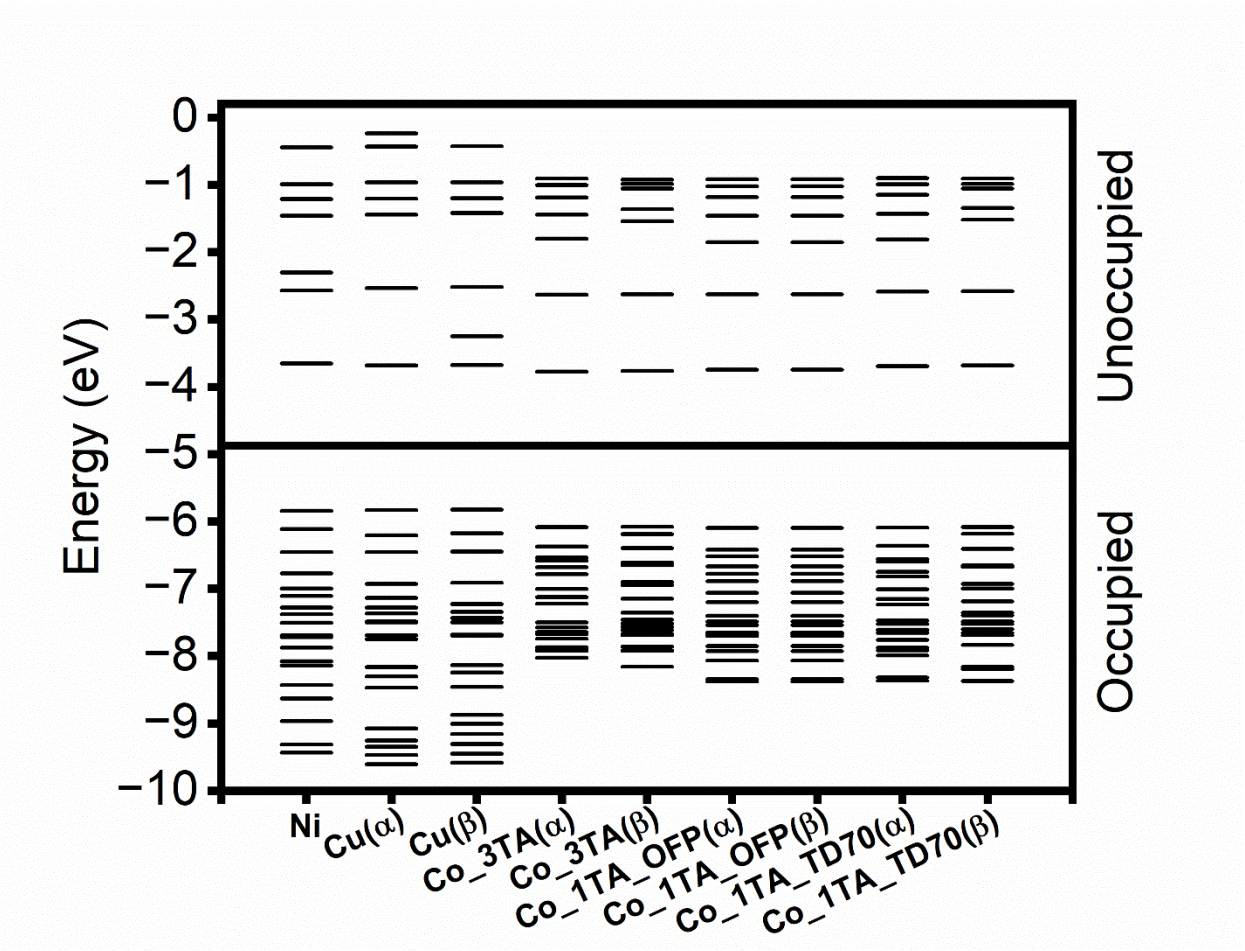


Figure S15: Relative energies of the frontier orbitals for **1** and **M(Hlp)** with and without tartaric acid.

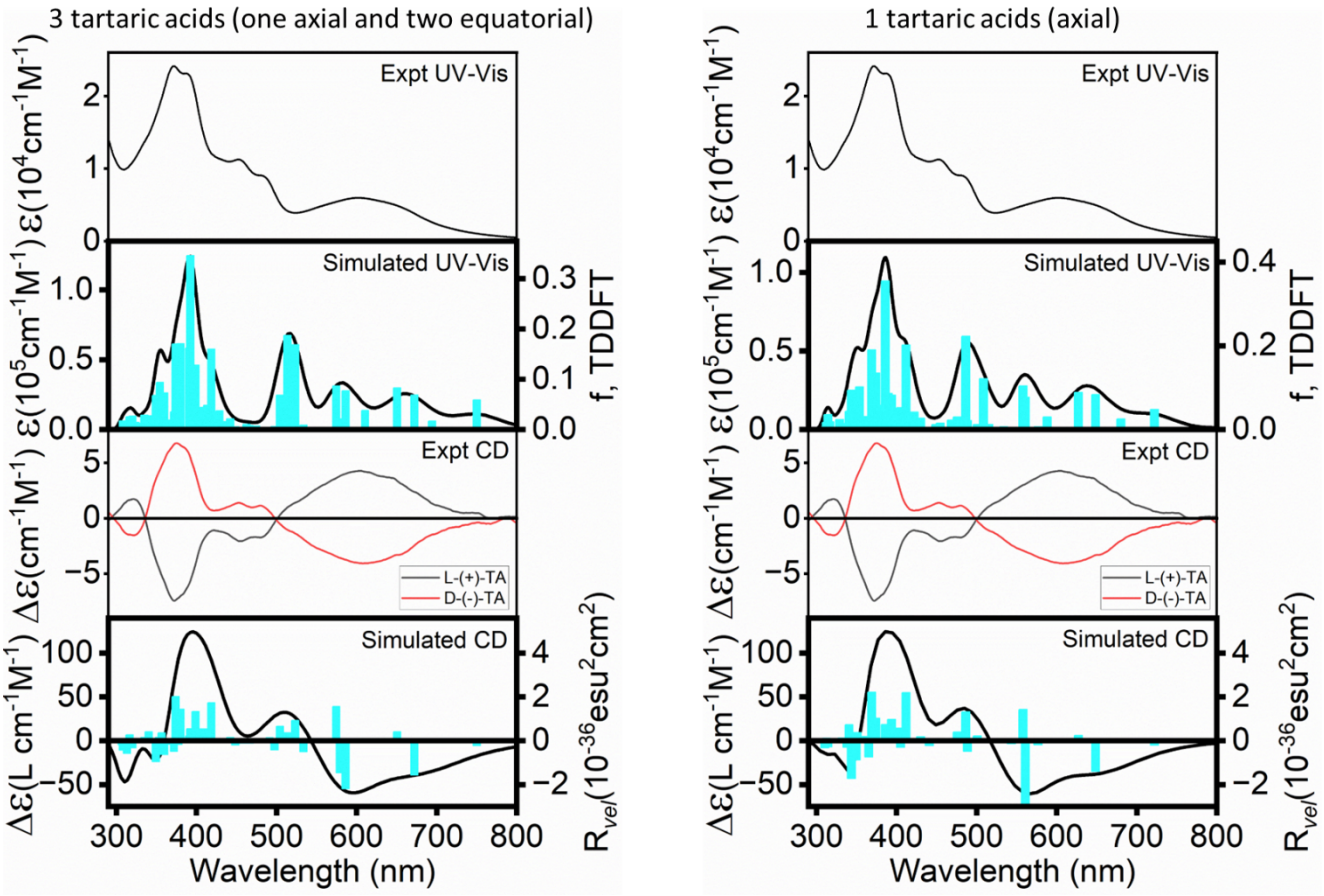


Figure S16: Experimental and calculated spectra of Co(Hlp) in the presence of one equivalent (right) and three equivalents (left) of D and L tartaric acid.

Table S1: X-ray crystal data and structure parameters for compounds **1** and **M(Hlp)** complexes.

Compound	**1**	**Co(Hlp)(DMF)**	**Ni(Hlp)**	**Cu(Hlp)**
CCDC				
Empirical formula	$C_{37}H_{29}N_{11}O$	$C_{37}H_{24}CoN_{10}O$	$C_{37}H_{24}N_{10}NiO$	$C_{34}H_{17}CuN_9$
Formula weight	643.71	683.59	683.37	615.10
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	Pn	P-1	$P2_1/n$	C2/c
a/ Å	6.029(4)	9.544(8)	9.2915(12)	10.247(13)
b/ Å	15.799(11)	12.116(10)	32.458(4)	33.06(5)
c/ Å	16.468(11)	14.974(14)	10.0812(12)	9.773(12)
α(°)	90	93.98(6)	90	90
β(°)	91.653(14)	99.20(8)	100.874(5)	104.16(6)
γ(°)	90	104.84(3)	90	90
Volume ($Å^3$)	1568.0(19)	1641(3)	2985.7(6)	3210(7)
Z	2	2	4	4
Dc (Mg/m^3)	1.363	1.383	1.520	1.273
μ (mm^{-1})	0.088	0.570	0.702	0.718
F(000)	672	702	1408	1252
reflns collected	35261	55759	65544	26202
indep. reflns	7788	5922	5245	2899
GOF on F^2	1.068	1.073	1.035	1.044
R1 (on F_o^2, I > 2σ(I))	0.0488	0.0696	0.0616	0.0712
wR2 (on F_o^2, I > 2σ(I))	0.1421	0.1468	0.1278	0.1717
R1 (all data)	0.0630	0.0985	0.1033	0.1034
wR2 (all data)	0.1502	0.1592	0.1447	0.1860

Table S2: B3LYP TDDFT-predicted energies and expansion coefficients for compound **1 (**only excited states with f > 0.05 and λ > 270 nm are listed).

Excited State 1: Singlet-A 2.6712 eV 464.15 nm f=1.0116 <S**2>=0.000
74 -> 75 0.70474
Excited State 4: Singlet-A 4.0381 eV 307.04 nm f=0.1384 <S**2>=0.000
70 -> 75 -0.25252
71 -> 75 0.61284
72 -> 75 -0.18974
Excited State 6: Singlet-A 4.2823 eV 289.53 nm f=0.2697 <S**2>=0.000
70 -> 75 0.55479
71 -> 75 0.23869
72 -> 75 -0.10676
74 -> 76 0.30876

Table S3: B3LYP TDDFT-predicted energies and expansion coefficients for compound **Co(Hlp)(DMF)** (only excited states with f > 0.05 and λ > 270 nm are listed).

Excited State 8: 2.194-A 1.7000 eV 729.30 nm f=0.2288 <S**2>=0.953
174A ->177A -0.17222
175A ->177A -0.33733
176A ->177A 0.64404
172B ->176B 0.13197
174B ->176B 0.13009
175B ->176B 0.61504

Excited State 9: 2.220-A 1.8012 eV 688.33 nm f=0.0879 <S**2>=0.982
175A ->177A 0.80712
176A ->177A 0.23508
172B ->176B -0.12427
174B ->176B 0.43928
175B ->176B 0.18336

Excited State 14: 2.658-A 2.2586 eV 548.95 nm f=0.1332 <S**2>=1.517
171A ->177A -0.11167
171A ->179A -0.10409
172A ->177A -0.11469
174A ->177A 0.39380
171B ->176B 0.52219
172B ->176B -0.19589
173B ->176B 0.55545
174B ->177B 0.14854
175B ->177B 0.10912

Excited State 16: 2.660-A 2.3173 eV 535.04 nm f=0.1716 <S**2>=1.519
160A ->179A -0.10573
163A ->179A -0.15844
170A ->177A 0.11886
171A ->177A 0.10650
172A ->177A 0.31153
172A ->179A 0.11886
174A ->177A 0.46491
174A ->179A 0.10123
175A ->179A 0.14481
176A ->178A 0.27563
168B ->182B 0.13293
169B ->182B -0.12561
171B ->176B -0.40394
173B ->176B 0.27263
174B ->177B -0.10500
174B ->182B 0.18920
175B ->177B -0.13315

Excited State 26: 2.706-A 2.8334 eV 437.59 nm f=0.4269 <S**2>=1.581
167A ->177A 0.12361
168A ->177A 0.36809

169A ->177A 0.12688
176A ->178A 0.42458
167B ->176B -0.36401
173B ->177B 0.13333
174B ->177B 0.23291
175B ->177B 0.56768
Excited State 27: 2.885-A 2.8388 eV 436.75 nm f=0.3779 <S**2>=1.830
168A ->177A -0.40696
168A ->178A 0.10612
169A ->177A -0.15430
170A ->177A -0.17014
172A ->177A 0.13482
175A ->178A -0.13813
176A ->178A 0.52922
167B ->176B 0.44310
168B ->176B 0.10550
170B ->176B -0.14133
173B ->177B -0.10649
174B ->177B 0.11738
175B ->177B 0.29171
Excited State 37: 2.503-A 3.2642 eV 379.83 nm f=0.1907 <S**2>=1.317
162A ->177A -0.12341
163A ->177A 0.24806
164A ->177A -0.11639
166A ->177A -0.44683
167A ->177A 0.13326
168A ->177A 0.43942
165B ->176B 0.33908
167B ->176B 0.48874
168B ->176B -0.22180
172B ->177B -0.11037
Excited State 38: 2.458-A 3.2833 eV 377.62 nm f=0.1750 <S**2>=1.261
163A ->177A -0.19060
165A ->177A 0.14942
166A ->177A 0.57544
167A ->177A 0.19208
168A ->177A 0.34775
174A ->178A 0.15770
164B ->176B -0.21698
165B ->176B -0.14622
166B ->176B 0.23291
167B ->176B 0.36577
173B ->177B 0.26231
Excited State 41: 2.227-A 3.3548 eV 369.57 nm f=0.2903 <S**2>=0.990
163A ->177A 0.19736
167A ->177A -0.33982

169A ->177A -0.10545
174A ->178A 0.49214
176A ->179A -0.13906
162B ->176B 0.13338
163B ->176B -0.13933
166B ->176B -0.40410
171B ->177B 0.10841
172B ->177B -0.13141
173B ->177B 0.51985
Excited State 42: 2.109-A 3.3878 eV 365.97 nm f=0.0591 <S**2>=0.862
163A ->177A 0.12885
164A ->177A -0.11106
166A ->177A -0.12770
167A ->177A 0.51117
168A ->177A -0.29799
173A ->178A 0.10002
174A ->178A 0.29162
166B ->176B 0.50657
167B ->176B -0.27215
169B ->176B -0.10016
172B ->177B -0.11187
173B ->177B 0.29848
Excited State 63: 2.953-A 3.9103 eV 317.07 nm f=0.0558 <S**2>=1.930
159A ->177A 0.16866
171A ->178A 0.11551
172A ->178A -0.12477
174A ->182A 0.13516
176A ->183A 0.11840
158B ->176B -0.20159
168B ->177B -0.29644
169B ->177B 0.45327
170B ->177B 0.50137
171B ->177B -0.19939
173B ->181B -0.13810
174B ->178B 0.13273
175B ->179B -0.13533
175B ->183B -0.13436
Excited State 83: 2.332-A 4.2591 eV 291.11 nm f=0.0561 <S**2>=1.110
159A ->177A 0.10893
176A ->182A 0.58260
166B ->177B 0.12760
167B ->177B -0.15352
168B ->177B 0.22248
172B ->179B -0.10376
174B ->181B -0.18835
175B ->181B 0.60351

175B ->182B -0.12109
Excited State 87: 2.283-A 4.3341 eV 286.06 nm f=0.0745 <S**2>=1.053
159A ->177A -0.25182
166A ->178A -0.10592
167A ->178A -0.11184
168A ->178A 0.56602
174A ->180A -0.16208
158B ->176B -0.24606
166B ->177B -0.12279
167B ->177B 0.52553
168B ->177B -0.15095
174B ->181B -0.11157
175B ->181B 0.19284
Excited State 94: 2.608-A 4.4335 eV 279.66 nm f=0.0575 <S**2>=1.451
158A ->177A -0.17374
159A ->177A 0.17184
163A ->178A -0.24027
167A ->178A 0.21127
169A ->178A 0.13100
170A ->180A 0.10263
171A ->180A 0.10954
173A ->180A 0.10780
174A ->180A -0.28911
175A ->182A -0.15806
158B ->176B 0.14938
164B ->177B 0.13831
165B ->177B 0.10082
167B ->177B 0.13371
171B ->178B -0.14217
172B ->178B 0.29949
172B ->179B -0.27634
172B ->180B 0.11526
173B ->178B -0.13535
173B ->179B 0.37912
174B ->181B -0.11565

Table S4: B3LYP TDDFT-predicted energies and expansion coefficients for compound **Ni(Hlp)** **(**only excited states with f > 0.05 and λ > 270 nm are listed).

Excited State 1: Singlet-A 1.7313 eV 716.13 nm f=0.2744 <S**2>=0.000
156 ->157 0.69899
Excited State 6: Singlet-A 2.3380 eV 530.30 nm f=0.4833 <S**2>=0.000
154 ->157 0.69191
Excited State 10: Singlet-A 2.7492 eV 450.98 nm f=0.1787 <S**2>=0.000
140 ->159 -0.17564
142 ->159 0.10677
153 ->159 0.10900
156 ->158 0.47398
156 ->159 0.39551
Excited State 12: Singlet-A 2.8937 eV 428.47 nm f=0.5544 <S**2>=0.000
151 ->157 -0.14449
156 ->158 -0.47032
156 ->159 0.47109
Excited State 15: Singlet-A 3.2283 eV 384.05 nm f=0.2304 <S**2>=0.000
148 ->157 0.23771
149 ->157 0.46631
154 ->158 0.28652
154 ->159 0.25082
155 ->159 -0.21182
Excited State 16: Singlet-A 3.2488 eV 381.63 nm f=0.3716 <S**2>=0.000
148 ->157 0.27287
149 ->157 0.34663
154 ->158 -0.25597
154 ->159 -0.32149
155 ->159 0.28752

Excited State 19: Singlet-A 3.4308 eV 361.38 nm f=0.2873 <S**2>=0.000
147 ->157 -0.14458
150 ->159 0.11390
151 ->159 -0.11264
154 ->158 0.54875
154 ->159 -0.18777
155 ->159 0.23830
Excited State 22: Singlet-A 3.5808 eV 346.25 nm f=0.0682 <S**2>=0.000
143 ->157 -0.17739
145 ->157 0.35465
146 ->157 -0.35288
147 ->157 0.41542
154 ->158 0.13679
154 ->159 -0.10118
Excited State 27: Singlet-A 3.8985 eV 318.03 nm f=0.1182 <S**2>=0.000
156 ->160 0.68213
Excited State 36: Singlet-A 4.3465 eV 285.25 nm f=0.0737 <S**2>=0.000

141 ->157 -0.19383
144 ->159 0.12165
145 ->159 0.11674
148 ->158 -0.15397
149 ->158 0.31245
149 ->159 -0.20725
150 ->159 -0.10133
151 ->159 -0.10990
156 ->162 0.44807

Excited State 37: Singlet-A 4.3831 eV 282.87 nm f=0.1011 <S**2>=0.000
140 ->157 0.18691
141 ->157 0.32677
142 ->157 0.14183
143 ->157 -0.11790
145 ->159 0.14377
148 ->158 0.27107
149 ->158 0.29691
154 ->160 -0.20511
156 ->161 -0.10005

Excited State 43: Singlet-A 4.5534 eV 272.29 nm f=0.0716 <S**2>=0.000
140 ->157 0.30282
141 ->157 -0.12669
144 ->159 0.15326
147 ->158 -0.10492
149 ->159 0.24757
155 ->162 0.46583

Table S5: B3LYP TDDFT-predicted energies and expansion coefficients for compound **Cu(Hlp) (**only excited states with f > 0.05 and λ > 270 nm are listed).

Excited State 2:	2.020-A	1.6990 eV	729.73 nm	f=0.0536	<S**2>=0.770
157A ->158A	0.30404				
121B ->158B	0.11636				
135B ->158B	0.18844				
141B ->158B	-0.13058				
143B ->158B	0.12191				
145B ->158B	-0.16166				
150B ->158B	0.15470				
151B ->158B	0.11593				
154B ->158B	-0.22729				
155B ->158B	-0.45105				
156B ->157B	0.32920				
156B ->158B	0.59313				
Excited State 3:	2.010-A	1.7153 eV	722.80 nm	f=0.2565	<S**2>=0.760
157A ->158A	0.63263				
155B ->158B	0.14722				
156B ->157B	0.61550				
156B ->158B	-0.36654				
Excited State 10:	2.007-A	2.3282 eV	532.52 nm	f=0.5117	<S**2>=0.757
155A ->158A	0.66213				
141B ->158B	0.17280				
142B ->158B	0.16104				
154B ->157B	0.66254				
154B ->158B	0.12312				
Excited State 11:	2.036-A	2.3619 eV	524.94 nm	f=0.0583	<S**2>=0.786
155A ->158A	-0.20336				
141B ->158B	0.38260				
142B ->158B	0.30984				
152B ->158B	-0.13982				
153B ->158B	-0.10743				
154B ->157B	-0.17559				
154B ->158B	0.65699				
155B ->158B	-0.36718				
156B ->158B	0.11721				
Excited State 21:	2.006-A	2.8738 eV	431.43 nm	f=0.8339	<S**2>=0.756
157A ->159A	0.68693				
156B ->159B	0.69214				
Excited State 26:	2.666-A	3.0807 eV	402.46 nm	f=0.0533	<S**2>=1.527
148A ->158A	0.25847				
149A ->158A	-0.24058				
150A ->158A	0.35311				
152A ->158A	0.23244				
155A ->159A	-0.26147				
147B ->157B	0.11609				

148B ->157B -0.13886
150B ->157B 0.44397
151B ->157B 0.34313
152B ->157B 0.26415
154B ->157B 0.11044
154B ->159B 0.32342
Excited State 30: 2.047-A 3.2068 eV 386.63 nm f=0.5147 <S**2>=0.797
149A ->158A 0.36847
150A ->158A -0.16312
151A ->158A 0.46121
152A ->158A 0.26985
149B ->157B -0.36207
150B ->157B -0.39482
151B ->157B 0.39652
152B ->157B 0.21929
154B ->159B 0.11912
Excited State 32: 2.247-A 3.2896 eV 376.89 nm f=0.0503 <S**2>=1.012
147A ->158A 0.21085
149A ->158A -0.46076
150A ->158A -0.35294
151A ->158A 0.14999
152A ->158A 0.21063
147B ->157B -0.20885
148B ->157B -0.19976
149B ->157B 0.56387
150B ->157B -0.25766
151B ->157B 0.13511
152B ->157B 0.16247
Excited State 35: 2.679-A 3.4403 eV 360.38 nm f=0.0919 <S**2>=1.544
146A ->158A -0.34066
148A ->158A -0.11672
155A ->159A 0.32008
143B ->158B 0.14413
145B ->157B 0.12176
146B ->157B 0.46245
147B ->158B -0.12103
151B ->158B -0.39710
152B ->158B 0.14064
154B ->159B 0.45561
Excited State 36: 2.956-A 3.4450 eV 359.90 nm f=0.0961 <S**2>=1.935
146A ->158A 0.53937
148A ->158A -0.11340
155A ->159A 0.43193
145B ->157B -0.12346
146B ->157B -0.46206
148B ->157B -0.11950

151B ->158B -0.21521
154B ->159B 0.31462
Excited State 37: 2.065-A 3.4558 eV 358.77 nm f=0.1561 <S**2>=0.816
148A ->158A -0.21066
155A ->159A 0.34685
143B ->158B -0.18218
145B ->158B 0.15098
146B ->157B 0.15602
146B ->158B -0.11181
147B ->157B 0.14146
147B ->158B 0.16456
148B ->157B -0.17564
151B ->158B 0.64412
152B ->158B -0.20324
154B ->159B 0.33435
Excited State 38: 2.014-A 3.5478 eV 349.47 nm f=0.1220 <S**2>=0.764
146A ->158A -0.12457
148A ->158A 0.60854
155A ->159A 0.24825
146B ->157B -0.12527
147B ->157B -0.46596
148B ->157B 0.41151
150B ->158B -0.11939
151B ->158B 0.12732
154B ->159B 0.25458
Excited State 52: 2.094-A 3.9233 eV 316.02 nm f=0.1279 <S**2>=0.846
157A ->160A 0.60793
157A ->161A -0.10977
153B ->159B 0.11787
156B ->160B 0.70227
156B ->161B -0.12767
Excited State 66: 2.035-A 4.2615 eV 290.94 nm f=0.0557 <S**2>=0.785
144A ->158A 0.50810
146A ->158A -0.14282
149A ->159A -0.11761
150A ->159A 0.11448
151A ->159A 0.37529
144B ->157B 0.51935
145B ->158B -0.17159
146B ->157B -0.11704
151B ->159B 0.38763
Excited State 71: 2.180-A 4.3684 eV 283.82 nm f=0.0546 <S**2>=0.938
144A ->158A -0.26964
146A ->158A 0.10371
149A ->159A -0.18072
151A ->159A 0.38675

152A ->159A 0.17440
157A ->162A 0.22393
143B ->157B -0.22552
144B ->157B -0.31144
145B ->158B 0.10274
149B ->159B 0.11828
150B ->159B -0.13718
151B ->159B 0.42662
152B ->159B 0.17006
154B ->160B 0.13066
156B ->162B 0.33541
Excited State 72: 2.032-A 4.3744 eV 283.43 nm f=0.2069 <S**2>=0.782
149A ->159A -0.13332
150A ->159A 0.34236
151A ->159A -0.23636
152A ->159A -0.15875
155A ->160A -0.14402
157A ->162A 0.46007
150B ->159B 0.41346
151B ->159B -0.16510
152B ->159B -0.10841
156B ->162B 0.53280

Table S6: B3LYP DFT optimized geometry of compound **1.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.134773	-1.884679	-0.000365
2	6	0	-3.239739	-0.911269	-0.000186
3	6	0	-4.619811	-1.052907	-0.000079
4	1	0	-5.097350	-2.026905	-0.000113
5	6	0	-5.395041	0.110072	0.000210
6	1	0	-6.476588	0.034774	0.000295
7	6	0	-4.788176	1.367282	0.000354
8	1	0	-5.407225	2.257699	0.000652
9	6	0	-3.395882	1.505624	0.000255
10	1	0	-2.953793	2.492506	0.000466
11	6	0	-2.618472	0.351218	-0.000032
12	6	0	-1.160242	0.073573	0.000017
13	6	0	-0.113130	0.970766	0.000121
14	6	0	-0.359645	2.371745	0.000128
15	6	0	1.294873	0.593058	0.000076
16	6	0	3.101261	-0.685176	0.000377
17	6	0	4.068611	-1.691551	0.000887
18	1	0	3.798865	-2.741968	0.001603
19	6	0	5.398022	-1.284396	0.000477
20	1	0	6.182025	-2.034365	0.000817
21	6	0	5.752337	0.080757	-0.000374
22	1	0	6.802815	0.352324	-0.000657
23	6	0	4.787011	1.078515	-0.000804
24	1	0	5.057920	2.128959	-0.001398
25	6	0	3.438944	0.692955	-0.000429
26	7	0	-2.283609	-3.205585	-0.000567
27	1	0	-1.473721	-3.806445	-0.001346
28	1	0	-3.191233	-3.640373	-0.001242
29	7	0	-0.948331	-1.293185	-0.000294
30	7	0	1.725711	-0.709616	0.001035
31	1	0	1.080753	-1.493031	0.000261
32	7	0	2.294218	1.463436	-0.000690
33	7	0	-0.562184	3.511137	0.000067

E_h = -928.243238 Hartree

Table S7: B3LYP DFT optimized geometry of compound **Co(Hlp)(DMF)**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.352835	-1.502719	-1.747728
2	6	0	3.202374	-0.469143	-2.174027
3	1	0	2.958263	0.571341	-1.999612
4	6	0	4.362267	-0.818679	-2.848731
5	1	0	5.031139	-0.036399	-3.193557
6	6	0	4.693286	-2.169307	-3.108664
7	1	0	5.612539	-2.395648	-3.639537
8	6	0	3.856490	-3.198029	-2.712008
9	1	0	4.092841	-4.235980	-2.924288
10	6	0	2.670471	-2.865030	-2.032766
11	6	0	0.780713	-2.814408	-1.057403
12	6	0	-0.529161	-3.258525	-0.629512
13	6	0	-0.678415	-4.668793	-0.483963
14	6	0	-1.616669	-2.431860	-0.475913
15	6	0	-3.022098	-2.796202	-0.236065
16	6	0	-3.700816	-3.997683	-0.021890
17	1	0	-3.186854	-4.947753	0.021981
18	6	0	-5.086230	-3.952455	0.144932
19	1	0	-5.626199	-4.877149	0.317751
20	6	0	-5.792255	-2.744317	0.093537
21	1	0	-6.868809	-2.746715	0.224004
22	6	0	-5.120976	-1.542330	-0.123090
23	1	0	-5.651207	-0.598052	-0.167649
24	6	0	-3.740720	-1.589995	-0.279816
25	6	0	-2.766671	-0.526669	-0.501110
26	6	0	-2.262770	1.735797	-0.634238
27	6	0	-2.649397	3.111964	-0.951631
28	6	0	-3.884998	3.659724	-1.265447
29	1	0	-4.774783	3.041803	-1.294943
30	6	0	-3.938025	5.026964	-1.541302
31	1	0	-4.885883	5.490256	-1.791761
32	6	0	-2.777962	5.806583	-1.499768
33	1	0	-2.839727	6.866554	-1.719989
34	6	0	-1.536239	5.250232	-1.180184
35	1	0	-0.658337	5.880726	-1.157157
36	6	0	-1.481002	3.884811	-0.903706
37	6	0	-0.402359	2.951660	-0.521597
38	6	0	0.926960	3.254453	-0.296679
39	6	0	1.420327	4.574456	-0.463867
40	6	0	1.874168	2.290097	0.211313
41	6	0	3.673781	1.522824	1.268978

42	6	0	4.875345	1.339901	1.953537
43	1	0	5.541758	2.169346	2.160113
44	6	0	5.168262	0.046962	2.364437
45	1	0	6.089272	-0.143803	2.904189
46	6	0	4.286798	-1.020503	2.102975
47	1	0	4.544952	-2.014650	2.451254
48	6	0	3.095857	-0.832533	1.415686
49	1	0	2.419194	-1.653419	1.227367
50	6	0	2.790609	0.462482	0.982695
51	6	0	-0.473186	0.138391	2.747668
52	1	0	-0.602445	1.208979	2.543765
53	6	0	-1.020717	0.805790	5.029406
54	1	0	-0.263575	0.835532	5.817004
55	1	0	-1.986513	0.567484	5.482025
56	1	0	-1.083574	1.789628	4.566278
57	6	0	-0.544635	-1.573907	4.483204
58	1	0	-0.279984	-2.203849	3.638780
59	1	0	-1.491074	-1.915685	4.909931
60	1	0	0.231260	-1.647093	5.249402
61	27	0	0.104409	-0.007964	-0.337586
62	7	0	1.144700	-1.498549	-1.081578
63	7	0	-1.529821	-1.041716	-0.607961
64	7	0	-3.135265	0.753797	-0.607519
65	7	0	-0.922967	1.680549	-0.377436
66	7	0	1.690491	0.971825	0.289073
67	7	0	1.666532	-3.674368	-1.580427
68	7	0	3.070386	2.653514	0.758050
69	1	0	3.406452	3.600902	0.847815
70	7	0	-0.796576	-5.811168	-0.347278
71	7	0	1.884344	5.629034	-0.579835
72	7	0	-0.670185	-0.194154	4.028594
73	8	0	-0.173834	-0.651587	1.842789

E_h = -3430.522905 Hartree

Table S8: B3LYP DFT optimized geometry of compound **Ni(Hlp)**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.529393	0.756656	1.427556
2	6	0	-2.995174	-0.475977	1.909270
3	1	0	-2.434981	-1.390842	1.761019
4	6	0	-4.195582	-0.485006	2.603080
5	1	0	-4.575749	-1.424406	2.991440
6	6	0	-4.934709	0.700127	2.827150
7	1	0	-5.869248	0.643782	3.375892
8	6	0	-4.477736	1.924214	2.371370
9	1	0	-5.029851	2.840684	2.552887
10	6	0	-3.259492	1.957481	1.669462
11	6	0	-1.474331	2.477284	0.633033
12	6	0	-0.390094	3.284024	0.121279
13	6	0	-0.681588	4.667268	-0.060671
14	6	0	0.881049	2.809226	-0.087689
15	6	0	2.102270	3.553863	-0.423393
16	6	0	2.381855	4.890978	-0.712022
17	1	0	1.607962	5.644980	-0.748779
18	6	0	3.708034	5.246125	-0.963969
19	1	0	3.941112	6.279983	-1.194327
20	6	0	4.741620	4.301757	-0.925699
21	1	0	5.760668	4.614765	-1.123930
22	6	0	4.469117	2.966410	-0.636576
23	1	0	5.256222	2.222313	-0.601651
24	6	0	3.146207	2.614463	-0.394081
25	6	0	2.546693	1.323735	-0.084459
26	6	0	2.714568	-0.970653	0.123587
27	6	0	3.475215	-2.187805	0.405524
28	6	0	4.828473	-2.377862	0.644548
29	1	0	5.517955	-1.541957	0.633374
30	6	0	5.264437	-3.678959	0.900859
31	1	0	6.314287	-3.866584	1.096128
32	6	0	4.359530	-4.744886	0.909899
33	1	0	4.718951	-5.747214	1.114322
34	6	0	2.998250	-4.549072	0.660469
35	1	0	2.324029	-5.394233	0.673777
36	6	0	2.560602	-3.250562	0.406595
37	6	0	1.251506	-2.653267	0.086229
38	6	0	0.052939	-3.304354	-0.120633
39	6	0	-0.066011	-4.710290	0.029868
40	6	0	-1.109898	-2.611940	-0.618579
41	6	0	-3.022947	-2.286832	-1.703732

42	6	0	-4.214289	-2.393729	-2.420353
43	1	0	-4.646803	-3.357852	-2.660437
44	6	0	-4.809843	-1.206275	-2.821728
45	1	0	-5.735410	-1.239791	-3.385459
46	6	0	-4.227972	0.040952	-2.523230
47	1	0	-4.714735	0.946570	-2.867732
48	6	0	-3.045228	0.141150	-1.804165
49	1	0	-2.602585	1.103661	-1.588657
50	6	0	-2.440847	-1.045685	-1.377028
51	7	0	-1.394712	1.116908	0.728869
52	7	0	1.215618	1.457663	0.079057
53	7	0	3.276351	0.213180	0.038013
54	7	0	1.397712	-1.284453	-0.048293
55	7	0	-1.262440	-1.287044	-0.665045
56	7	0	-2.577447	3.025427	1.153850
57	7	0	-2.165359	-3.244369	-1.198870
58	1	0	-2.252824	-4.243426	-1.315931
59	7	0	-0.920911	5.786591	-0.223364
60	7	0	-0.223541	-5.852020	0.136586
61	28	0	-0.022832	0.001822	0.034708

E_h = -3307.469552 Hartree

Table S9: B3LYP DFT optimized geometry of compound **Ni(Hlp)**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.544745	-1.155169	1.380400
2	6	0	-3.180262	0.012539	1.814051
3	1	0	-2.741417	0.986080	1.637961
4	6	0	-4.390342	-0.123632	2.479754
5	1	0	-4.905880	0.764183	2.828708
6	6	0	-4.966113	-1.387708	2.716309
7	1	0	-5.913379	-1.449059	3.240291
8	6	0	-4.342972	-2.556477	2.300219
9	1	0	-4.776501	-3.531580	2.488956
10	6	0	-3.125777	-2.413438	1.634818
11	6	0	-1.172943	-2.668568	0.595576
12	6	0	-0.009960	-3.351146	0.063852
13	6	0	-0.143147	-4.755012	-0.101442
14	6	0	1.197759	-2.722675	-0.173393
15	6	0	2.499374	-3.343363	-0.494481
16	6	0	2.916227	-4.645617	-0.762314
17	1	0	2.226233	-5.477341	-0.796610
18	6	0	4.276588	-4.864175	-0.999409
19	1	0	4.618734	-5.870038	-1.215899
20	6	0	5.201683	-3.816777	-0.962167
21	1	0	6.250139	-4.021703	-1.147262
22	6	0	4.787288	-2.511685	-0.689854
23	1	0	5.492800	-1.689893	-0.654880
24	6	0	3.435108	-2.297505	-0.466588
25	6	0	2.694720	-1.066752	-0.173138
26	29	0	-0.068530	0.007087	-0.051070
27	7	0	-1.338274	-1.349287	0.713448
28	7	0	1.369223	-1.361250	-0.046115
29	7	0	3.288265	0.098169	-0.030047
30	7	0	-2.239715	-3.337873	1.117169
31	1	0	-2.329873	-4.342137	1.170919
32	7	0	-0.311858	-5.894013	-0.220775
33	6	0	-2.587191	1.030651	-1.423818
34	6	0	-3.176296	-0.144953	-1.911718
35	1	0	-2.687504	-1.107196	-1.810974
36	6	0	-4.406493	-0.033526	-2.541841
37	1	0	-4.885463	-0.925425	-2.932936
38	6	0	-5.053293	1.215796	-2.694654
39	1	0	-6.014998	1.253498	-3.196043
40	6	0	-4.476705	2.383763	-2.226054
41	1	0	-4.962078	3.346378	-2.350692

42	6	0	-3.227826	2.293890	-1.585246
43	6	0	-1.359229	2.621357	-0.611269
44	6	0	-0.220024	3.344721	-0.074816
45	6	0	-0.431705	4.742540	0.118184
46	6	0	1.025596	2.811093	0.164192
47	6	0	2.285652	3.491644	0.505746
48	6	0	2.636725	4.808513	0.807721
49	1	0	1.902939	5.600939	0.856630
50	6	0	3.980826	5.091798	1.057489
51	1	0	4.267928	6.109438	1.298957
52	6	0	4.964170	4.096308	1.002608
53	1	0	5.998958	4.354033	1.198853
54	6	0	4.621519	2.780349	0.699012
55	1	0	5.369344	1.997453	0.649823
56	6	0	3.281198	2.498228	0.461233
57	6	0	2.613209	1.241817	0.138154
58	7	0	-1.392199	1.263438	-0.780950
59	7	0	1.292475	1.451132	0.002953
60	7	0	-2.437130	3.278140	-1.059305
61	7	0	-0.593408	5.873812	0.293985

E_h = -3439.636473 Hartree

Table S10: Major TDDFT-predicted excited state contributions for **Ni**, **Cu**, **Co_3TA**, **Co_1TA_OptFreqPlus**, and **Co_1TA_TD70** using the B3LYP exchange correlation functional.

Ni

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
1	716	13964	0.2744	H→L (98%)
4	648	15443	0.0321	H-1→L (70%), H-4→L+2 (10%), H-3→L+2 (5%), H-11→L+2 (5%), H-1→L+2 (3%)
6	530	18857	0.4833	H-2→L (96%)
8	491	20382	0.0282	H-3→L (63%), H-4→L (27%), H-5→L (3%)
10	451	22174	0.1787	H→L+1 (45%), H→L+2 (31%), H-16→L+2 (6%), H-3→L+2 (2%), H-14→L+2 (2%)
11	442	22636	0.0267	H-5→L (71%), H-6→L (16%), H-3→L (5%), H→L+2 (2%)
12	428	23339	0.5544	H→L+2 (44%), H→L+1 (44%), H-5→L (4%)
13	418	23930	0.0318	H-6→L (62%), H-5→L (12%), H-4→L (6%), H-1→L+1 (5%), H-7→L (5%), H→L+2 (2%), H→L+1 (2%)
14	409	24462	0.0353	H-1→L+1 (84%), H-6→L (7%), H-1→L+2 (5%)
15	384	26038	0.2304	H-7→L (44%), H-2→L+1 (16%), H-2→L+2 (13%), H-8→L (11%), H-1→L+2 (9%)
16	382	26203	0.3716	H-7→L (24%), H-2→L+2 (21%), H-1→L+2 (17%), H-8→L (15%), H-2→L+1 (13%)
17	374	26761	0.0381	H-8→L (71%), H-7→L (22%), H-6→L (3%)
19	361	27671	0.2873	H-2→L+1 (60%), H-1→L+2 (11%), H-2→L+2 (7%), H-9→L (4%), H-6→L+2 (3%), H-5→L+2 (3%)
22	346	28881	0.0682	H-9→L (35%), H-11→L (25%), H-10→L (25%), H-13→L (6%), H-2→L+1 (4%), H-2→L+2 (2%)
23	342	29223	0.0212	H-3→L+1 (58%), H-13→L (12%), H-4→L+1 (7%), H-3→L+2 (6%), H-5→L+1 (4%), H-2→L+2 (3%)
24	338	29550	0.0443	H-12→L (43%), H-13→L (22%), H-4→L+1 (17%), H-11→L (9%), H-15→L (3%)
25	335	29830	0.0304	H-4→L+1 (31%), H-13→L (29%), H-3→L+1 (20%), H-11→L (3%), H-4→L+2 (3%), H-6→L+1 (3%)
26	332	30129	0.0270	H-12→L (47%), H-4→L+1 (23%),

				H-13→L (13%), H-4→L+2 (4%), H-6→L+1 (4%), H-11→L (2%)
27	318	31444	0.1182	H→L+3 (93%)
28	315	31793	0.0483	H-5→L+1 (47%), H-3→L+2 (17%), H-6→L+2 (12%), H-4→L+2 (4%), H-6→L+1 (4%), H-3→L+1 (4%), H-5→L+2 (3%)
29	309	32345	0.0436	H-5→L+1 (35%), H-6→L+1 (22%), H-5→L+2 (19%), H-3→L+2 (13%)
32	298	33549	0.0368	H-1→L+3 (77%), H→L+4 (16%)
34	293	34132	0.0380	H-7→L+1 (38%), H-7→L+2 (22%), H-5→L+2 (10%), H-12→L+2 (6%), H-6→L+2 (6%), H-1→L+3 (3%), H-15→L (3%), H-11→L+2 (2%), H-3→L+2 (2%)
36	285	35057	0.0737	H→L+5 (40%), H-7→L+1 (20%), H-7→L+2 (9%), H-15→L (8%), H-8→L+1 (5%), H-12→L+2 (3%), H-11→L+2 (3%), H-5→L+2 (2%), H-6→L+2 (2%)
37	283	35352	0.1011	H-15→L (21%), H-7→L+1 (18%), H-8→L+1 (15%), H-2→L+3 (8%), H-16→L (7%), H-11→L+2 (4%), H-14→L (4%), H-13→L (3%), H→L+4 (2%)
41	275	36308	0.0271	H-2→L+3 (55%), H-16→L (13%), H-9→L+1 (10%), H-8→L+1 (5%), H-1→L+5 (3%), H-1→L+4 (3%), H-7→L+1 (2%)
43	272	36726	0.0716	H-1→L+5 (43%), H-16→L (18%), H-7→L+2 (12%), H-12→L+2 (5%), H-15→L (3%), H-9→L+1 (2%)
46	269	37228	0.0719	H-9→L+1 (33%), H-10→L+1 (18%), H-11→L+2 (8%), H-11→L+1 (6%), H-2→L+3 (5%), H-16→L (4%), H-10→L+2 (3%)
48	265	37685	0.0318	H-11→L+1 (41%), H-8→L+2 (10%), H-10→L+2 (10%), H-13→L+1 (10%), H-9→L+1 (6%), H-10→L+1 (5%), H-11→L+2 (4%), H-12→L+2 (2%)
49	262	38111	0.1098	H-9→L+2 (26%), H-3→L+3 (25%), H-13→L+1 (22%), H-10→L+2 (10%), H-11→L+1 (3%), H-8→L+2 (3%), H-11→L+2 (2%)
50	261	38358	0.0589	H-3→L+3 (28%), H-10→L+2 (20%), H-9→L+2 (20%), H-13→L+1 (10%),

				H-11→L+2 (3%), H-12→L+1 (3%), H-5→L+3 (2%)
51	260	38459	0.1135	H-3→L+3 (24%), H-13→L+1 (24%), H-10→L+2 (13%), H-9→L+2 (10%), H→L+6 (8%), H-12→L+1 (5%), H-2→L+4 (3%)
52	259	38586	0.0947	H→L+6 (64%), H-2→L+4 (10%), H-10→L+2 (7%), H-1→L+14 (3%), H-9→L+2 (2%)
53	259	38645	0.0227	H-9→L+2 (20%), H-2→L+4 (18%), H-13→L+1 (15%), H-11→L+1 (10%), H-11→L+2 (8%), H-10→L+2 (8%), H-3→L+3 (5%), H-4→L+3 (3%), H-2→L+5 (2%)
55	255	39152	0.0973	H-4→L+3 (76%), H-6→L+3 (7%), H-2→L+4 (3%), H-10→L+2 (3%)
56	255	39259	0.1158	H-2→L+5 (80%), H-3→L+7 (2%)
59	248	40314	0.0475	H-1→L+6 (71%), H→L+7 (11%), H→L+14 (5%), H-17→L (3%)
60	246	40569	0.2433	H-3→L+4 (60%), H-5→L+3 (10%), H-4→L+4 (7%), H-5→L+4 (3%), H-1→L+6 (3%), H-18→L (2%)

Cu

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
2	730	13703	0.0536	H(β)→L+1(β) (35%), H-1(β)→L+1(β) (20%), H(β)→L(β) (11%), H(α)→L(α) (9%), H-2(β)→L+1(β) (5%), H-21(β)→L+1(β) (4%), H-11(β)→L+1(β) (3%), H-6(β)→L+1(β) (2%), H-15(β)→L+1(β) (2%)
3	723	13835	0.2565	H(α)→L(α) (40%), H(β)→L(β) (38%), H(β)→L+1(β) (13%), H-1(β)→L+1(β) (2%)
10	533	18778	0.5117	H-2(β)→L(β) (44%), H-2(α)→L(α) (44%), H-15(β)→L+1(β) (3%), H-14(β)→L+1(β) (3%), H-2(β)→L+1(β) (2%)
11	525	19050	0.0583	H-2(β)→L+1(β) (43%), H-15(β)→L+1(β) (15%), H-1(β)→L+1(β) (14%), H-14(β)→L+1(β) (10%), H-2(α)→L(α) (4%), H-2(β)→L(β) (3%), H-4(β)→L+1(β) (2%)
19	448	22304	0.0367	H-3(α)→L(α) (49%), H-3(β)→L(β) (36%), H-4(α)→L(α) (8%)
21	431	23179	0.8339	H(β)→L+2(β) (48%), H(α)→L+1(α) (47%)
26	402	24848	0.0533	H-6(β)→L(β) (20%), H-7(α)→L(α) (13%),

				H-5(β)→L(β) (12%), H-2(β)→L+2(β) (11%), H-4(β)→L(β) (7%), H-2(α)→L+1(α) (7%), H-9(α)→L(α) (7%), H-8(α)→L(α) (6%), H-5(α)→L(α) (5%), H-8(β)→L(β) (2%)
27	401	24934	0.0363	H-7(α)→L(α) (30%), H-2(α)→L+1(α) (16%), H-2(β)→L+2(β) (12%), H-9(α)→L(α) (5%), H-6(α)→L(α) (4%), H-9(β)→L(β) (4%), H-7(β)→L(β) (4%), H-8(β)→L(β) (3%), H-4(β)→L(β) (3%), H-5(α)→L(α) (3%), H-6(β)→L(β) (2%), H-2(α)→L(α) (2%)
30	387	25865	0.5147	H-6(α)→L(α) (21%), H-5(β)→L(β) (16%), H-6(β)→L(β) (16%), H-8(α)→L(α) (14%), H-7(β)→L(β) (13%), H-5(α)→L(α) (7%), H-4(β)→L(β) (5%), H-7(α)→L(α) (3%)
32	377	26532	0.0503	H-7(β)→L(β) (32%), H-8(α)→L(α) (21%), H-7(α)→L(α) (13%), H-6(β)→L(β) (7%), H-10(α)→L(α) (4%), H-5(α)→L(α) (4%), H-9(β)→L(β) (4%), H-8(β)→L(β) (4%), H-4(β)→L(β) (3%), H-6(α)→L(α) (2%), H-5(β)→L(β) (2%)
33	375	26670	0.0272	H-4(β)→L+1(β) (56%), H-5(β)→L+1(β) (12%), H-15(β)→L+1(β) (4%), H-14(β)→L+1(β) (4%), H-3(β)→L+1(β) (4%), H-13(β)→L+1(β) (3%), H-6(β)→L+1(β) (3%), H-22(β)→L+1(β) (2%), H-9(β)→L+1(β) (2%)
35	360	27748	0.0919	H-10(β)→L(β) (21%), H-2(β)→L+2(β) (21%), H-5(β)→L+1(β) (16%), H-11(α)→L(α) (12%), H-2(α)→L+1(α) (10%), H-13(β)→L+1(β) (2%), H-4(β)→L+1(β) (2%)
36	360	27786	0.0961	H-11(α)→L(α) (29%), H-10(β)→L(β) (21%), H-2(α)→L+1(α) (19%), H-2(β)→L+2(β) (10%), H-5(β)→L+1(β) (5%), H-11(β)→L(β) (2%)
37	359	27873	0.1561	H-5(β)→L+1(β) (42%), H-2(α)→L+1(α) (12%), H-2(β)→L+2(β) (11%), H-9(α)→L(α) (4%), H-4(β)→L+1(β) (4%), H-13(β)→L+1(β) (3%), H-8(β)→L(β) (3%), H-9(β)→L+1(β) (3%), H-10(β)→L(β) (2%), H-11(β)→L+1(β) (2%), H-9(β)→L(β) (2%)
38	349	28615	0.1220	H-9(α)→L(α) (37%), H-9(β)→L(β) (22%), H-8(β)→L(β) (17%), H-2(β)→L+2(β) (6%), H-2(α)→L+1(α) (6%), H-5(β)→L+1(β) (2%), H-10(β)→L(β) (2%), H-11(α)→L(α) (2%)
41	345	29005	0.0216	H-6(β)→L+1(β) (50%), H-9(β)→L+1(β) (7%),

				H-3(β)→L+2(β) (4%), H-3(α)→L+1(α) (3%), H-15(β)→L+1(β) (3%), H-14(β)→L+1(β) (2%), H-5(β)→L+1(β) (2%), H(α)→L+2(α) (2%), H(β)→L+3(β) (2%), H-7(β)→L+1(β) (2%), H-8(β)→L+1(β) (2%), H-3(α)→L+4(α) (2%)
42	344	29089	0.0254	H-11(α)→L(α) (44%), H-10(β)→L(β) (36%), H-13(α)→L(α) (5%), H-12(β)→L(β) (3%), H-9(α)→L(α) (2%), H-8(β)→L(β) (2%)
52	316	31644	0.1279	H(β)→L+3(β) (49%), H(α)→L+2(α) (37%), H(β)→L+4(β) (2%)
58	305	32820	0.0386	H-10(β)→L+1(β) (81%), H-11(β)→L+1(β) (3%), H-21(β)→L+1(β) (2%), H-27(β)→L+1(β) (2%)
66	291	34371	0.0557	H-12(β)→L(β) (27%), H-13(α)→L(α) (26%), H-5(β)→L+2(β) (15%), H-6(α)→L+1(α) (14%), H-11(β)→L+1(β) (3%), H-11(α)→L(α) (2%)
71	284	35234	0.0546	H-5(β)→L+2(β) (18%), H-6(α)→L+1(α) (15%), H(β)→L+5(β) (11%), H-12(β)→L(β) (10%), H-13(α)→L(α) (7%), H-13(β)→L(β) (5%), H(α)→L+4(α) (5%), H-8(α)→L+1(α) (3%), H-5(α)→L+1(α) (3%), H-4(β)→L+2(β) (3%), H-6(β)→L+2(β) (2%), H-2(β)→L+3(β) (2%)
72	283	35282	0.2069	H(β)→L+5(β) (28%), H(α)→L+4(α) (21%), H-6(β)→L+2(β) (17%), H-7(α)→L+1(α) (12%), H-6(α)→L+1(α) (6%), H-5(β)→L+2(β) (3%), H-5(α)→L+1(α) (3%), H-2(α)→L+2(α) (2%), H-8(α)→L+1(α) (2%)
89	266	37652	0.0382	H-9(α)→L+1(α) (30%), H-9(β)→L+2(β) (25%), H-8(β)→L+2(β) (23%), H-2(β)→L+3(β) (2%), H-14(α)→L(α) (2%), H-2(β)→L+5(β) (2%)
96	260	38470	0.0350	H-10(β)→L+2(β) (29%), H-11(α)→L+1(α) (29%), H(β)→L+6(β) (9%), H(α)→L+5(α) (7%), H-2(α)→L+3(α) (2%), H-13(α)→L+1(α) (2%), H-2(β)→L+4(β) (2%), H-16(α)→L(α) (2%)
97	259	38644	0.1446	H(β)→L+6(β) (28%), H(α)→L+5(α) (25%), H-10(β)→L+2(β) (10%), H-11(α)→L+1(α) (8%), H-1(β)→L+14(β) (3%), H-13(β)→L+1(β) (2%),

98	258	38749	0.0222	H-13(α)→L+1(α) (2%), H-15(β)→L(β) (2%), H-2(α)→L+3(α) (26%), H-1(α)→L+13(α) (10%), H-16(α)→L(α) (7%), H-1(β)→L+14(β) (6%), H(α)→L+5(α) (4%), H-2(β)→L+4(β) (4%), H-16(β)→L(β) (3%), H-18(α)→L(α) (2%), H-19(β)→L(β) (2%), H-1(α)→L+10(α) (2%)
99	258	38789	0.0219	H-2(β)→L+4(β) (43%), H-2(α)→L+3(α) (23%), H-1(α)→L+13(α) (4%), H(α)→L+5(α) (3%), H-16(α)→L(α) (2%), H-16(β)→L(β) (2%), H-1(β)→L+14(β) (2%)
100	256	38990	0.0394	H-15(α)→L(α) (24%), H-16(α)→L(α) (13%), H-2(β)→L+4(β) (11%), H-4(α)→L+2(α) (9%), H-2(α)→L+3(α) (8%), H-13(β)→L+1(β) (3%), H-2(β)→L+5(β) (2%)

Co_3TA

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
8	750	13331	0.0591	H-2(β)→L(β) (36%), H-1(β)→L(β) (17%), H(α)→L(α) (16%), H-1(α)→L(α) (5%), H(β)→L(β) (5%), H(α)→L+2(α) (4%), H-2(α)→L+2(α) (4%), H-5(α)→L+2(α) (2%)
10	672	14875	0.0688	H-2(β)→L(β) (34%), H-1(β)→L(β) (19%), H(α)→L(α) (15%), H-2(α)→L(α) (13%), H-1(α)→L(α) (6%), H-5(α)→L(α) (3%), H-3(α)→L(α) (2%)
11	651	15371	0.0825	H-1(α)→L(α) (48%), H-3(β)→L(β) (13%), H-2(β)→L(β) (10%), H(β)→L(β) (10%), H-1(β)→L(β) (2%), H-3(α)→L(α) (2%)
12	611	16373	0.0380	H-3(α)→L(α) (40%), H-2(α)→L(α) (19%), H-3(β)→L(β) (14%), H-4(α)→L(α) (6%), H-6(α)→L(α) (5%), H-1(α)→L(α) (3%), H(α)→L+1(α) (2%), H-4(β)→L(β) (2%)
13	586	17052	0.0771	H-2(α)→L(α) (44%), H-3(β)→L(β) (8%), H-4(α)→L(α) (7%), H-1(β)→L(β) (6%), H-2(β)→L(β) (5%), H(α)→L(α) (2%), H-1(α)→L+2(α) (2%), H(β)→L+6(β) (2%), H-3(α)→L(α) (2%)
14	579	17260	0.0208	H-3(α)→L(α) (23%), H-2(α)→L(α) (14%), H(β)→L+6(β) (6%), H-4(α)→L(α) (5%), H-1(α)→L+2(α) (5%), H-2(β)→L(β) (4%), H-14(α)→L+2(α) (3%), H-21(α)→L+2(α) (2%),

				H-3(β)→L(β) (2%), H-8(β)→L+4(β) (2%), H-8(β)→L+6(β) (2%), H-15(α)→L+2(α) (2%), H-1(β)→L(β) (2%)
15	575	17405	0.0868	H-3(α)→L(α) (17%), H-4(α)→L(α) (13%), H-3(β)→L(β) (10%), H-1(α)→L(α) (8%), H-1(α)→L+2(α) (3%), H-7(α)→L(α) (2%), H-21(α)→L+2(α) (2%), H-2(β)→L(β) (2%), H-14(α)→L+2(α) (2%), H-15(α)→L+2(α) (2%), H-8(β)→L+6(β) (2%), H-8(β)→L+4(β) (2%), H(β)→L(β) (2%), H-8(β)→L+5(β) (2%), H(β)→L+6(β) (2%)
19	523	19108	0.1686	H-4(α)→L(α) (30%), H-5(β)→L(β) (20%), H-6(β)→L(β) (10%), H-3(β)→L(β) (5%), H(β)→L+6(β) (3%), H-1(α)→L(α) (2%), H-8(β)→L(β) (2%), H(α)→L+1(α) (2%), H-6(β)→L+2(β) (2%), H-2(α)→L+6(α) (2%) H-3(β)→L+2(β) (2%)
20	514	19472	0.1875	H-3(β)→L(β) (19%), H-5(β)→L(β) (17%), H-4(α)→L(α) (7%), H-6(β)→L(β) (6%), H-4(β)→L(β) (4%), H-6(α)→L(α) (4%), H-8(β)→L+3(β) (4%), H-1(α)→L(α) (4%), H-8(β)→L+4(β) (2%), H-8(β)→L+2(β) (2%), H-8(β)→L(β) (2%), H-7(α)→L(α) (2%), H-8(α)→L(α) (2%)
21	504	19834	0.0680	H-3(β)→L(β) (14%), H-4(α)→L(α) (14%), H-8(β)→L+3(β) (9%), H-8(β)→L+6(β) (4%), H-8(β)→L+4(β) (4%), H-2(β)→L+6(β) (3%), H-8(β)→L+2(β) (3%), H-5(β)→L+3(β) (3%), H-6(β)→L(β) (2%), H-3(α)→L+2(α) (2%), H-5(β)→L(β) (2%), H-1(β)→L+6(β) (2%), H-7(β)→L(β) (2%), H-5(β)→L+6(β) (2%)
30	442	22609	0.0214	H-8(β)→L(β) (56%), H-7(β)→L(β) (8%), H-11(β)→L(β) (5%), H-5(β)→L(β) (4%), H-12(β)→L(β) (4%), H-1(β)→L+1(β) (3%), H-6(β)→L(β) (2%), H-2(β)→L+1(β) (2%), H-6(α)→L(α) (2%)
32	429	23317	0.0371	H-9(β)→L(β) (18%), H-12(β)→L(β) (18%), H-2(β)→L+1(β) (8%), H-8(α)→L(α) (7%), H-8(β)→L(β) (6%), H-10(β)→L(β) (5%), H-11(α)→L(α) (5%), H(α)→L+1(α) (5%), H-13(α)→L(α) (3%), H-1(β)→L+1(β) (3%), H-1(α)→L+1(α) (3%), H-5(β)→L(β) (2%), H-11(β)→L(β) (2%)
33	419	23878	0.1601	H-1(β)→L+1(β) (27%), H(α)→L+1(α) (21%), H-9(β)→L(β) (11%), H-2(β)→L+1(β) (7%),

				H-2(α)→L+1(α) (4%), H-9(α)→L(α) (4%), H(β)→L+1(β) (3%), H-8(α)→L(α) (3%), H-13(β)→L(β) (3%), H-12(β)→L(β) (2%), H-13(β)→L(β) (2%)
34	413	24193	0.0480	H-1(α)→L+1(α) (22%), H-11(α)→L(α) (13%), H-9(β)→L(β) (12%), H-14(β)→L(β) (10%), H-1(β)→L+1(β) (7%), H-13(α)→L(α) (4%), H-3(β)→L+1(β) (4%), H-12(β)→L(β) (3%), H-10(β)→L(β) (3%), H-12(α)→L(α) (3%), H(β)→L+1(β) (2%)
35	409	24468	0.0442	H-2(β)→L+1(β) (24%), H-13(β)→L(β) (15%), H-12(α)→L(α) (13%), H-11(α)→L(α) (8%), H-12(β)→L(β) (6%), H-2(α)→L+1(α) (5%), H(α)→L+1(α) (5%), H-14(β)→L(β) (2%), H-8(α)→L(α) (2%)
37	400	24971	0.0321	H-11(β)→L(β) (24%), H-14(β)→L(β) (10%), H-15(β)→L(β) (9%), H-1(α)→L+1(α) (8%), H-12(α)→L(α) (7%), H-10(α)→L(α) (5%), H-9(β)→L(β) (4%), H-18(α)→L(α) (4%), H-1(β)→L+1(β) (3%), H-7(β)→L(β) (3%), H-8(α)→L(α) (3%), H-14(α)→L(α) (2%), H-2(β)→L+1(β) (2%), H-2(α)→L+1(α) (2%)
38	399	25065	0.1282	H-2(β)→L+1(β) (29%), H-13(β)→L(β) (19%), H-12(α)→L(α) (15%), H-11(β)→L(β) (6%), H-1(β)→L+1(β) (5%), H-3(α)→L+1(α) (3%), H-11(α)→L(α) (2%), H(α)→L+1(α) (2%)
39	392	25486	0.3458	H-10(β)→L(β) (38%), H-9(α)→L(α) (35%), H-9(β)→L(β) (6%), H-13(α)→L(α) (6%), H-10(α)→L(α) (5%), H-15(α)→L(α) (3%)
40	391	25586	0.1618	H-13(α)→L(α) (22%), H-15(α)→L(α) (13%), H-9(α)→L(α) (9%), H-9(β)→L(β) (9%), H-12(β)→L(β) (5%), H-17(α)→L(α) (5%), H-14(β)→L(β) (5%), H-10(α)→L(α) (5%), H-14(α)→L(α) (4%), H-11(β)→L(β) (4%), H-1(α)→L+1(α) (3%), H-8(β)→L(β) (2%), H-11(α)→L(α) (2%), H-16(α)→L(α) (2%)
42	380	26294	0.1705	H-2(α)→L+1(α) (52%), H-3(α)→L+1(α) (16%), H-1(β)→L+1(β) (7%), H-4(β)→L+1(β) (3%), H-13(β)→L(β) (2%), H-11(α)→L(α) (2%)
43	378	26472	0.0256	H-12(β)→L(β) (27%), H-14(α)→L(α) (21%), H-15(α)→L(α) (8%), H-13(α)→L(α) (7%), H-11(α)→L(α) (7%), H-12(α)→L(α) (3%), H-17(α)→L(α) (3%), H-2(α)→L+1(α) (3%), H-18(α)→L(α) (2%), H-14(β)→L(β) (2%), H-3(α)→L+1(α) (2%)

45	374	26730	0.1700	H-3(α)→L+1(α) (41%), H-2(α)→L+1(α) (21%), H-3(β)→L+1(β) (12%), H-2(β)→L+1(β) (6%), H-11(α)→L(α) (4%), H-4(α)→L+1(α) (3%)
46	372	26884	0.0354	H-3(β)→L+1(β) (32%), H-4(α)→L+1(α) (20%), H-3(α)→L+1(α) (18%), H-2(β)→L+1(β) (5%), H-11(β)→L(β) (3%), H-11(α)→L(α) (2%), H-1(α)→L+1(α) (2%), H-10(α)→L(α) (2%)
50	360	27791	0.0726	H-14(β)→L(β) (33%), H-4(α)→L+1(α) (15%), H-13(α)→L(α) (15%), H-12(α)→L(α) (12%), H-11(α)→L(α) (7%), H-5(α)→L+1(α) (4%), H-3(β)→L+1(β) (2%), H-5(β)→L+1(β) (2%), H-12(β)→L(β) (2%)
51	357	28043	0.0347	H-5(α)→L+1(α) (68%), H-14(β)→L(β) (3%), H(α)→L+2(α) (3%), H-5(β)→L+1(β) (2%), H-15(β)→L(β) (2%), H-12(α)→L(α) (2%), H-4(β)→L+1(β) (2%)
52	354	28220	0.0935	H-5(β)→L+1(β) (18%), H-4(α)→L+1(α) (15%), H-3(β)→L+1(β) (10%), H-6(β)→L+1(β) (6%), H-14(β)→L(β) (6%), H-5(α)→L+1(α) (6%), H-13(α)→L(α) (5%), H-6(α)→L(α) (4%), H-15(β)→L(β) (4%), H-1(α)→L+1(α) (3%)
53	353	28321	0.0650	H-18(α)→L(α) (45%), H-15(β)→L(β) (30%), H-10(α)→L(α) (3%), H-5(β)→L+1(β) (2%), H-7(α)→L+1(α) (2%), H-21(β)→L(β) (2%)
55	350	28610	0.0679	H-4(α)→L+1(α) (18%), H-6(α)→L+1(α) (17%), H-5(β)→L+1(β) (16%), H-3(β)→L+1(β) (14%), H-4(β)→L+1(β) (2%), H-12(α)→L(α) (2%), H-6(α)→L+5(α) (2%), H-14(β)→L(β) (2%)
58	341	29359	0.0277	H(α)→L+2(α) (54%), H-2(α)→L+2(α) (16%), H-5(α)→L+2(α) (7%), H-5(α)→L+1(α) (2%), H-3(α)→L+2(α) (2%), H-18(α)→L+2(α) (2%)
60	335	29855	0.0283	H-21(α)→L(α) (42%), H-21(β)→L(β) (16%), H-23(β)→L(β) (13%), H-22(α)→L(α) (4%), H-19(β)→L(β) (3%), H(β)→L+2(β) (3%), H-10(β)→L+1(β) (2%), H-9(β)→L+1(β) (2%)
70	320	31250	0.0266	H-7(α)→L+1(α) (43%), H-7(β)→L+1(β) (15%), H-6(β)→L+1(β) (12%), H-6(α)→L+1(α) (3%), H-4(α)→L+1(α) (2%), H-8(β)→L+1(β) (2%)
72	317	31585	0.0256	H-7(β)→L+1(β) (26%), H-8(β)→L+1(β) (9%), H(β)→L+2(β) (8%), H-7(α)→L+1(α) (5%),

				H(β)→L+3(β) (4%), H-2(β)→L+2(β) (3%), H-8(α)→L+1(α) (3%), H-11(β)→L+1(β) (3%), H-12(β)→L+1(β) (3%), H-6(α)→L+1(α) (2%)

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Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
8	727	13749	0.0486	H-2(β)→L(β) (28%), H(α)→L(α) (12%), H-1(β)→L(β) (12%), H(α)→L+2(α) (10%), H-5(α)→L+2(α) (7%), H(β)→L(β) (6%), H-2(α)→L+2(α) (5%), H-1(α)→L(α) (4%), H-20(α)→L+2(α) (3%), H-14(α)→L+2(α) (2%)
9	689	14518	0.0349	H-2(α)→L(α) (28%), H-5(α)→L+2(α) (12%), H-1(β)→L(β) (11%), H(α)→L(α) (11%), H-2(α)→L+2(α) (9%), H-2(β)→L(β) (7%), H(β)→L(β) (5%), H-20(α)→L+2(α) (4%), H-14(α)→L+2(α) (3%), H-3(α)→L(α) (2%), H-7(α)→L+2(α) (2%), H-2(α)→L(α) (2%)
10	657	15216	0.0486	H-2(β)→L(β) (35%), H-1(β)→L(β) (16%), H(α)→L(α) (15%), H-2(α)→L(α) (12%), H-1(α)→L(α) (9%), H-5(α)→L(α) (3%)
11	628	15920	0.0825	H-1(α)→L(α) (40%), H-4(β)→L(β) (16%), H-2(β)→L(β) (11%), H(β)→L(β) (9%), H-2(α)→L(α) (3%), H-1(β)→L(β) (3%)
12	592	16880	0.0710	H-3(α)→L(α) (32%), H-2(α)→L(α) (28%), H-4(β)→L(β) (11%), H-1(α)→L(α) (8%), H-1(α)→L(α) (4%), H(β)→L(β) (3%), H-4(α)→L(α) (2%), H-1(β)→L(β) (2%), H(α)→L+1(α) (2%)
14	569	17564	0.0736	H-2(α)→L(α) (44%), H-3(α)→L(α) (14%), H-1(β)→L(β) (9%), H-4(β)→L(β) (7%), H-2(β)→L(β) (6%), H-4(α)→L(α) (4%)
15	556	17976	0.0892	H-3(α)→L(α) (30%), H-4(α)→L(α) (14%), H-4(β)→L(β) (9%), H-1(α)→L(α) (6%), H-7(α)→L(α) (5%), H-3(β)→L(β) (3%), H-2(β)→L(β) (3%), H-5(β)→L(β) (3%), H-5(α)→L(α) (3%), H(β)→L+6(β) (2%), H-3(α)→L+2(α) (2%), H-2(β)→L+6(β) (2%)
18	511	19552	0.1012	H-5(α)→L(α) (23%), H-7(β)→L+3(β) (5%), H-9(β)→L+3(β) (5%), H-4(β)→L(β) (5%), H-1(α)→L(α) (4%), H-4(α)→L(α) (4%), H-15(α)→L+2(α) (3%), H-9(β)→L+6(β) (3%), H-3(α)→L(α) (3%), H-2(β)→L+6(β) (2%), H-7(β)→L+6(β) (2%), H-5(β)→L+3(β) (2%), H-18(α)→L+2(α) (2%), H-3(α)→L+2(α) (2%),

				H-5(β)→L(β) (2%), H-7(β)→L+4(β) (2%), H-7(β)→L+2(β) (2%), H-5(β)→L+6(β) (2%)
19	508	19672	0.0662	H-5(α)→L(α) (52%), H-4(α)→L(α) (14%), H-6(β)→L(β) (4%), H-5(β)→L(β) (3%), H-2(α)→L(α) (2%), H-2(β)→L(β) (2%), H(β)→L+1(β) (2%)
21	491	20378	0.0973	H-4(α)→L(α) (20%), H-4(β)→L(β) (8%), H-7(β)→L+6(β) (5%), H-18(α)→L+2(α) (5%), H-15(α)→L+2(α) (4%), H-16(α)→L+2(α) (4%), H-9(β)→L+6(β) (3%), H-7(α)→L+2(α) (3%), H-5(β)→L+6(β) (3%), H-6(β)→L+6(β) (2%), H-8(α)→L+2(α) (2%), H-4(α)→L+2(α) (2%), H-4(β)→L+6(β) (2%)
22	491	20383	0.1412	H-4(β)→L(β) (25%), H-7(α)→L(α) (14%), H-6(α)→L(α) (10%), H-5(β)→L(β) (10%), H-4(α)→L(α) (6%), H-6(β)→L(β) (6%), H-7(β)→L(β) (4%), H-2(β)→L+1(β) (2%)
24	471	21243	0.0202	H-6(α)→L(α) (26%), H-6(β)→L(β) (21%), H-7(β)→L(β) (14%), H-4(α)→L(α) (5%), H(β)→L+1(β) (5%), H-9(β)→L(β) (5%), H-1(β)→L+1(β) (3%), H-3(α)→L(α) (2%)
29	430	23236	0.0244	H-9(α)→L(α) (24%), H-10(β)→L(β) (16%), H(β)→L+1(β) (15%), H-8(β)→L(β) (11%), H-8(α)→L(α) (6%), H-9(β)→L(β) (6%), H(α)→L+1(α) (2%), H-10(α)→L(α) (2%), H-1(β)→L+1(β) (2%), H-7(β)→L(β) (2%)
32	416	24059	0.2310	H-1(β)→L+1(β) (25%), H(α)→L+1(α) (22%), H-9(β)→L(β) (14%), H-11(β)→L(β) (5%), H-2(α)→L+1(α) (4%), H-2(β)→L+1(β) (4%), H-8(α)→L(α) (3%), H(β)→L+1(β) (3%), H-9(α)→L(α) (3%), H-10(β)→L(β) (3%), H-6(β)→L(β) (2%), H-5(β)→L(β) (2%)
34	405	24670	0.0371	H-11(α)→L(α) (21%), H-8(β)→L(β) (20%), H-13(β)→L(β) (14%), H-1(α)→L+1(α) (10%), H-8(α)→L(α) (6%), H-12(β)→L(β) (4%), H-10(β)→L(β) (3%), H-4(β)→L+1(β) (3%), H-1(β)→L+1(β) (2%), H-14(α)→L(α) (2%)
37	395	25306	0.0964	H-2(β)→L+1(β) (33%), H-14(β)→L(β) (18%), H-12(α)→L(α) (16%), H-13(α)→L(α) (5%), H-1(β)→L+1(β) (4%), H-2(α)→L+1(α) (3%), H-3(α)→L+1(α) (2%), H(α)→L+1(α) (2%)
38	390	25631	0.3809	H-9(α)→L(α) (36%), H-8(β)→L(β) (27%), H-10(β)→L(β) (16%), H-13(β)→L(β) (8%), H-12(β)→L(β) (2%), H-10(α)→L(α) (2%)

39	388	25744	0.0589	H-10(β)→L(β) (30%), H-13(β)→L(β) (18%), H-8(β)→L(β) (9%), H-13(α)→L(α) (8%), H-14(α)→L(α) (7%), H-1(α)→L+1(α) (4%), H-9(α)→L(α) (4%), H-12(β)→L(β) (3%), H-12(α)→L(α) (3%), H-8(α)→L(α) (2%), H-11(α)→L(α) (2%), H-10(α)→L(α) (2%), H-15(α)→L(α) (2%)
40	383	26077	0.0643	H-15(α)→L(α) (36%), H-13(α)→L(α) (18%), H-12(β)→L(β) (14%), H-10(α)→L(α) (7%), H-10(β)→L(β) (4%), H-9(β)→L(β) (4%), H-15(β)→L(β) (3%), H-12(α)→L(α) (3%), H-14(β)→L(β) (2%)
41	379	26386	0.1384	H-2(α)→L+1(α) (34%), H-11(β)→L(β) (9%), H-9(β)→L(β) (7%), H-10(α)→L(α) (7%), H-15(β)→L(β) (7%), H-3(α)→L+1(α) (6%), H-4(β)→L+1(β) (3%), H-1(β)→L+1(β) (3%), H-16(α)→L(α) (2%), H-2(β)→L+1(β) (2%), H-7(β)→L(β) (2%), H-12(β)→L(β) (2%), H-3(β)→L+2(β) (2%)
43	377	26542	0.1567	H-2(α)→L+1(α) (28%), H-10(α)→L(α) (16%), H-11(β)→L(β) (16%), H-15(β)→L(β) (6%), H-1(β)→L+1(β) (6%), H-9(β)→L(β) (4%), H-9(α)→L(α) (3%), H-16(α)→L(α) (2%), H-13(α)→L(α) (2%), H-12(β)→L(β) (2%)
45	369	27112	0.0635	H-11(β)→L(β) (21%), H-4(β)→L+1(β) (13%), H-3(α)→L+1(α) (10%), H-15(β)→L(β) (7%), H-13(α)→L(α) (6%), H-15(α)→L(α) (6%), H-2(α)→L+1(α) (5%), H-11(α)→L(α) (4%), H-14(α)→L(α) (4%), H-12(β)→L(β) (4%), H-4(α)→L+1(α) (3%)
46	366	27303	0.0674	H-3(α)→L+1(α) (49%), H-2(β)→L+1(β) (10%), H-15(β)→L(β) (10%), H-11(β)→L(β) (4%), H-2(α)→L+1(α) (3%), H-15(α)→L(α) (2%)
48	362	27590	0.0286	H-3(β)→L+1(β) (86%), H-4(β)→L+1(β) (5%), H-4(α)→L+1(α) (2%)
49	359	27828	0.0230	H-14(β)→L(β) (26%), H-11(α)→L(α) (18%), H-13(α)→L(α) (15%), H-13(β)→L(β) (11%), H-12(α)→L(α) (9%), H-12(β)→L(β) (6%), H-3(β)→L+1(β) (3%), H-17(β)→L(β) (2%), H-4(α)→L+1(α) (2%)
50	358	27968	0.0530	H-12(α)→L(α) (33%), H-14(β)→L(β) (17%), H-13(β)→L(β) (11%), H-15(β)→L(β) (8%), H-4(α)→L+1(α) (7%), H-11(α)→L(α) (4%),

				H-3(α)→L+1(α) (4%), H-13(α)→L(α) (2%), H-15(α)→L(α) (2%)
51	354	28271	0.0739	H-14(α)→L(α) (31%), H-13(β)→L(β) (11%), H-13(α)→L(α) (10%), H-17(β)→L(β) (7%), H-15(β)→L(β) (6%), H-15(α)→L(α) (6%), H-16(α)→L(α) (6%), H-11(α)→L(α) (4%), H-4(α)→L+1(α) (4%), H-14(β)→L(β) (2%), H-18(α)→L(α) (2%)
53	349	28647	0.0680	H-5(β)→L+1(β) (24%), H-4(α)→L+1(α) (18%), H-6(α)→L+1(α) (7%), H-4(β)→L+1(β) (7%), H-16(α)→L(α) (5%), H-6(β)→L+1(β) (3%), H-1(α)→L+1(α) (3%), H-5(β)→L+7(β) (2%)
56	345	29012	0.0716	H-4(α)→L+1(α) (20%), H-4(β)→L+1(β) (17%), H-6(α)→L+1(α) (14%), H-5(β)→L+1(β) (6%), H-6(β)→L+1(β) (5%), H-3(α)→L+1(α) (2%), H-13(β)→L(β) (2%), H-13(α)→L(α) (2%), H-1(α)→L+1(α) (2%)
57	341	29304	0.0592	H(α)→L+2(α) (36%), H-5(α)→L+1(α) (21%), H-2(α)→L+2(α) (16%), H-5(α)→L+2(α) (6%), H-14(α)→L+2(α) (2%), H-3(α)→L+2(α) (2%), H-2(β)→L+1(β) (2%)
67	314	31884	0.0288	H-7(α)→L+1(α) (28%), H-6(β)→L+1(β) (26%), H-7(β)→L+1(β) (21%), H-16(β)→L(β) (4%), H-1(α)→L+2(α) (2%)
68	312	32089	0.0341	H(β)→L+2(β) (13%), H(β)→L+3(β) (9%), H-7(α)→L+1(α) (7%), H-2(β)→L+2(β) (6%), H-7(β)→L+1(β) (5%), H-9(β)→L+1(β) (4%), H-11(β)→L+1(β) (3%), H-8(β)→L+1(β) (3%), H-1(β)→L+2(β) (2%), H-12(β)→L+1(β) (2%), H-6(α)→L+1(α) (2%), H-11(α)→L+1(α) (2%), H(β)→L+5(β) (2%)
72	307	32521	0.0384	H-1(β)→L+2(β) (24%), H(α)→L+3(α) (19%), H(β)→L+2(β) (10%), H-1(α)→L+2(α) (7%), H-4(α)→L+2(α) (3%), H-10(β)→L+1(β) (3%), H-2(β)→L+3(β) (2%), H-7(β)→L+1(β) (2%), H-9(α)→L+1(α) (2%)

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Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
8	722	13847	0.0479	H-2(β)→L(β) (29%), H-1(β)→L(β) (14%), H(α)→L(α) (12%), H(α)→L+2(α) (8%),

				H-2(α)→L+2(α) (7%), H-1(α)→L(α) (5%), H(β)→L(β) (4%), H-5(α)→L+2(α) (4%), H-19(α)→L+2(α) (3%), H-15(α)→L+2(α) (2%)
9	680	14702	0.0252	H(α)→L+2(α) (19%), H-2(α)→L+2(α) (15%), H-2(β)→L(β) (10%), H-1(β)→L(β) (8%), H-5(α)→L+2(α) (8%), H(α)→L(α) (7%), H-19(α)→L+2(α) (5%), H-15(α)→L+2(α) (4%), H(β)→L(β) (3%), H-3(α)→L+2(α) (3%), H-3(α)→L(α) (2%)
10	649	15415	0.0831	H-2(β)→L(β) (23%), H-1(β)→L(β) (23%), H(α)→L(α) (18%), H-1(α)→L(α) (14%), H-2(α)→L(α) (11%), H-5(α)→L(α) (2%)
11	627	15946	0.0887	H-1(α)→L(α) (38%), H-2(β)→L(β) (18%), H(β)→L(β) (10%), H-3(β)→L(β) (7%), H-4(β)→L(β) (4%), H-2(α)→L(α) (3%), H-6(α)→L(α) (3%), H(α)→L+1(α) (2%)
12	588	17004	0.0299	H-3(α)→L(α) (47%), H-2(α)→L(α) (10%), H-3(β)→L(β) (9%), H-4(β)→L(β) (8%), H-4(α)→L(α) (6%), H-1(α)→L(α) (3%), H-6(α)→L(α) (3%), H(α)→L+1(α) (2%)
14	561	17822	0.0768	H-2(α)→L(α) (61%), H-3(α)→L(α) (11%), H-2(β)→L(β) (9%), H-1(β)→L(β) (6%), H(α)→L(α) (3%), H-3(β)→L(β) (2%)
15	558	17916	0.1041	H-3(α)→L(α) (26%), H-4(α)→L(α) (16%), H-3(β)→L(β) (15%), H-1(α)→L(α) (9%), H-7(α)→L(α) (5%), H-4(β)→L(β) (4%), H-2(α)→L(α) (4%), H-1(β)→L(β) (2%), H-5(β)→L(β) (2%), H-2(β)→L(β) (2%)
19	509	19665	0.1215	H-5(α)→L(α) (19%), H-4(α)→L(α) (11%), H-4(β)→L(β) (6%), H-5(β)→L(β) (5%), H-8(β)→L+3(β) (5%), H-8(β)→L+6(β) (4%), H-3(α)→L+2(α) (3%), H-17(α)→L+2(α) (3%), H-14(α)→L+2(α) (3%), H(β)→L+1(β) (3%), H-2(β)→L+6(β) (3%), H-1(α)→L(α) (2%), H-5(β)→L+6(β) (2%), H-5(β)→L+3(β) (2%), H(β)→L+6(β) (2%), H-6(α)→L+2(α) (2%), H(β)→L(β) (2%), H-2(α)→L(α) (2%)
21	489	20460	0.0210	H-4(α)→L(α) (12%), H-8(β)→L+6(β) (6%), H-7(α)→L(α) (5%), H-6(β)→L(β) (5%), H-5(β)→L(β) (4%), H-16(α)→L+2(α) (4%), H-14(α)→L+2(α) (3%), H-7(α)→L+2(α) (3%), H-5(β)→L+6(β) (3%), H-7(β)→L(β) (3%), H-17(α)→L+2(α) (3%), H-1(β)→L+6(β) (2%), H-6(α)→L(α) (2%), H-4(α)→L+2(α) (2%)
22	487	20544	0.2231	H-3(β)→L(β) (17%), H-4(β)→L(β) (15%),

				H-4(α)→L(α) (14%), H-7(α)→L(α) (11%), H-5(β)→L(β) (8%), H-6(α)→L(α) (6%), H-6(β)→L(β) (5%), H-7(β)→L(β) (4%), H-8(α)→L(α) (3%), H-1(α)→L(α) (2%)
23	476	21010	0.0300	H-5(β)→L(β) (23%), H-6(β)→L(β) (13%), H-7(β)→L(β) (9%), H-7(α)→L(α) (7%), H-4(α)→L(α) (7%), H-6(α)→L(α) (5%), H(β)→L+1(β) (4%), H-8(α)→L(α) (3%), H(α)→L+1(α) (2%), H-8(β)→L(β) (2%), H-5(α)→L(α) (2%)
24	469	21342	0.0225	H(β)→L+1(β) (28%), H-6(α)→L(α) (14%), H-6(β)→L(β) (11%), H-7(β)→L(β) (7%), H-8(β)→L(β) (4%), H(α)→L+1(α) (4%), H-5(β)→L(β) (4%), H-4(α)→L(α) (2%), H-10(β)→L(β) (2%), H-1(α)→L+1(α) (2%), H-3(β)→L(β) (2%), H-4(β)→L(β) (2%), H-8(α)→L(α) (2%), H-9(β)→L(β) (2%)
30	430	23255	0.0265	H-8(β)→L(β) (24%), H-9(α)→L(α) (11%), H-10(β)→L(β) (10%), H-7(β)→L(β) (8%), H(β)→L+1(β) (8%), H-8(α)→L(α) (5%), H-10(α)→L(α) (5%), H-6(β)→L(β) (3%), H-7(α)→L(α) (3%), H-11(β)→L(β) (2%), H-14(β)→L(β) (2%), H-11(α)→L(α) (2%)
32	422	23701	0.0419	H-9(β)→L(β) (17%), H-8(α)→L(α) (11%), H-2(β)→L+1(β) (9%), H-12(β)→L(β) (8%), H-1(α)→L+1(α) (7%), H-1(β)→L+1(β) (7%), H(α)→L+1(α) (6%), H-8(β)→L(β) (6%), H-14(β)→L(β) (3%), H-11(α)→L(α) (3%), H-10(β)→L(β) (3%), H-13(β)→L(β) (2%)
33	412	24276	0.2020	H-1(β)→L+1(β) (30%), H(α)→L+1(α) (22%), H-9(β)→L(β) (10%), H-2(β)→L+1(β) (4%), H-8(α)→L(α) (3%), H-7(β)→L(β) (3%), H-1(α)→L+1(α) (2%), H-2(α)→L+1(α) (2%), H-11(β)→L(β) (2%), H-9(α)→L(α) (2%), H-14(β)→L(β) (2%)
35	405	24680	0.0524	H-1(α)→L+1(α) (31%), H-9(β)→L(β) (21%), H-11(α)→L(α) (8%), H-14(β)→L(β) (4%), H-12(β)→L(β) (4%), H-12(α)→L(α) (4%), H-1(β)→L+1(β) (2%), H(β)→L+1(β) (2%), H-11(β)→L(β) (2%), H-8(β)→L(β) (2%), H-3(β)→L+1(β) (2%)
36	402	24905	0.0405	H-2(β)→L+1(β) (21%), H-12(β)→L(β) (19%), H-11(α)→L(α) (18%), H-13(β)→L(β) (5%), H(α)→L+1(α) (5%), H-2(α)→L+1(α) (5%), H-12(α)→L(α) (4%), H-1(α)→L+1(α) (4%), H-7(α)→L(α) (2%)

37	394	25381	0.0815	H-12(α)→L(α) (23%), H-2(β)→L+1(β) (19%), H-13(β)→L(β) (18%), H-1(β)→L+1(β) (5%), H-11(β)→L(β) (4%), H-2(α)→L+1(α) (2%), H-11(α)→L(α) (2%), H-15(β)→L(β) (2%), H-14(α)→L(α) (2%), H-12(α)→L(α) (2%), H-7(β)→L(β) (2%)
38	390	25654	0.0859	H-11(β)→L(β) (24%), H-14(β)→L(β) (11%), H-15(β)→L(β) (8%), H-9(α)→L(α) (8%), H-2(β)→L+1(β) (7%), H-7(β)→L(β) (4%), H-8(β)→L(β) (4%), H-3(α)→L+1(α) (3%), H-16(α)→L(α) (3%), H-13(β)→L(β) (2%), H-11(α)→L(α) (2%), H-13(α)→L(α) (2%), H-8(α)→L(α) (2%), H-10(α)→L(α) (2%)
39	386	25891	0.3548	H-10(β)→L(β) (43%), H-9(α)→L(α) (26%), H-10(α)→L(α) (14%), H-13(α)→L(α) (3%), H-9(β)→L(β) (3%), H-14(α)→L(α) (2%)
40	383	26094	0.0574	H-13(α)→L(α) (23%), H-9(β)→L(β) (13%), H-14(α)→L(α) (13%), H-15(α)→L(α) (11%), H-9(α)→L(α) (8%), H-14(β)→L(β) (4%), H-10(α)→L(α) (3%), H-12(β)→L(β) (3%), H-13(β)→L(β) (3%), H-15(β)→L(β) (2%), H-16(β)→L(β) (2%), H-11(β)→L(β) (2%)
42	374	26714	0.1343	H-2(α)→L+1(α) (40%), H-3(α)→L+1(α) (32%), H-1(β)→L+1(β) (6%), H-4(β)→L+1(β) (5%), H-11(β)→L(β) (3%)
44	369	27091	0.1903	H-3(α)→L+1(α) (42%), H-2(α)→L+1(α) (28%), H-2(β)→L+1(β) (11%), H-12(β)→L(β) (2%), H-13(α)→L(α) (2%), H-11(α)→L(α) (2%)
45	368	27138	0.0242	H-12(β)→L(β) (23%), H-14(β)→L(β) (10%), H-11(β)→L(β) (10%), H-11(α)→L(α) (9%), H-13(α)→L(α) (7%), H-14(α)→L(α) (7%), H-10(α)→L(α) (5%), H-16(α)→L(α) (5%), H-3(α)→L+1(α) (4%), H-9(β)→L(β) (4%), H-15(α)→L(α) (3%), H-13(β)→L(β) (2%), H-2(α)→L+1(α) (2%)
46	365	27361	0.0256	H-3(β)→L+1(β) (37%), H-4(α)→L+1(α) (14%), H-11(α)→L(α) (6%), H-4(β)→L+1(β) (6%), H-11(β)→L(β) (4%), H-10(α)→L(α) (4%), H-14(α)→L(α) (3%), H-2(α)→L+1(α) (3%), H-1(α)→L+1(α) (2%)
47	360	27753	0.0311	H-4(β)→L+1(β) (52%), H-3(β)→L+1(β) (27%), H-11(α)→L(α) (3%), H-5(α)→L+1(α) (2%),

				H-14(β)→L(β) (2%), H-3(α)→L+1(α) (2%)
49	358	27961	0.0284	H-13(β)→L(β) (21%), H-12(α)→L(α) (19%), H-11(α)→L(α) (18%), H-12(β)→L(β) (14%), H-14(β)→L(β) (7%), H-13(α)→L(α) (5%), H-4(β)→L+1(β) (4%), H-15(α)→L(α) (2%)
50	354	28256	0.1016	H-13(β)→L(β) (22%), H-12(α)→L(α) (19%), H-14(β)→L(β) (12%), H-4(α)→L+1(α) (9%), H-13(α)→L(α) (8%), H-5(α)→L+1(α) (7%), H-16(α)→L(α) (4%), H-12(β)→L(β) (4%), H-12(α)→L(α) (3%), H-15(α)→L(α) (2%)
51	351	28488	0.0526	H-5(α)→L+1(α) (42%), H-17(β)→L(β) (12%), H(α)→L+2(α) (5%), H-16(α)→L(α) (4%), H-16(β)→L(β) (2%), H-17(α)→L(α) (2%), H-14(α)→L(α) (2%), H-5(β)→L+1(β) (2%), H-14(β)→L(β) (2%)
53	349	28645	0.0337	H-17(β)→L(β) (23%), H-5(β)→L+1(β) (12%), H-17(α)→L(α) (6%), H-13(α)→L(α) (6%), H-15(β)→L(β) (6%), H-4(α)→L+1(α) (5%), H-16(β)→L(β) (4%), H-6(α)→L+1(α) (4%), H-12(α)→L(α) (3%), H-16(α)→L(α) (3%), H-5(α)→L+1(α) (3%), H-13(β)→L(β) (3%), H-2(α)→L+1(α) (2%)
55	344	29086	0.0936	H-4(α)→L+1(α) (26%), H-6(α)→L+1(α) (13%), H-4(β)→L+1(β) (10%), H-3(β)→L+1(β) (8%), H-6(β)→L+1(β) (6%), H-12(α)→L(α) (2%), H-14(β)→L(β) (2%), H-5(β)→L+1(β) (2%), H-1(α)→L+1(α) (2%)
56	341	29342	0.0435	H(α)→L+2(α) (48%), H-2(α)→L+2(α) (16%), H-5(α)→L+1(α) (7%), H-5(α)→L+2(α) (6%), H-15(β)→L(β) (2%), H-16(α)→L+2(α) (2%), H-15(α)→L+2(α) (2%)
61	329	30398	0.0239	H-17(α)→L(α) (26%), H(β)→L+2(β) (14%), H-5(β)→L+1(β) (5%), H-17(β)→L(β) (5%), H-1(α)→L+3(α) (4%), H-19(β)→L(β) (4%), H-8(β)→L+1(β) (3%), H(α)→L+3(α) (2%), H-18(α)→L(α) (2%), H(β)→L+4(β) (2%), H-5(α)→L+1(α) (2%), H-6(α)→L+1(α) (2%)
66	314	31798	0.0354	H-6(β)→L+1(β) (33%), H-7(α)→L+1(α) (29%), H-7(β)→L+1(β) (14%), H-1(α)→L+2(α) (3%), H-3(α)→L+2(α) (2%)

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