

Supplementary Material

nickel(II) and copper(II) complexes of new unsymmetrically-substituted tetradentate Schiff base ligands: Spectral, structural, electrochemical and computational studies

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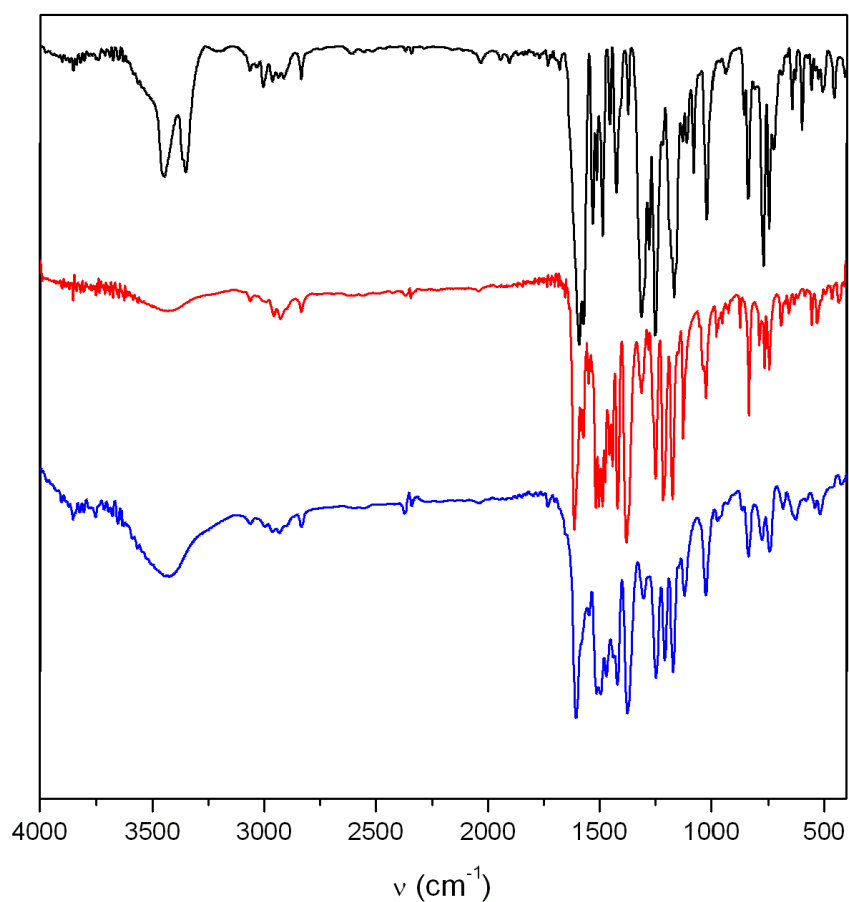


Fig. S1 Solid-state FT-IR spectra of compounds **1** (top), **4** (middle) and **5**(bottom)

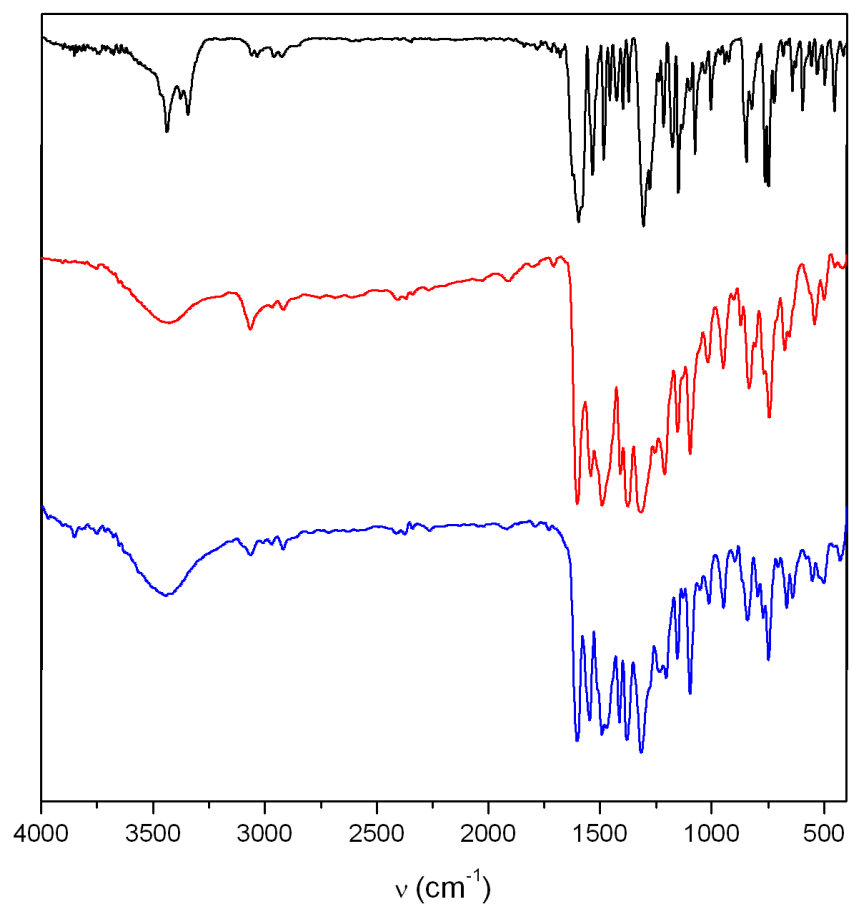


Fig. S2 Solid-state FT-IR spectra of compounds **2**(top), **10** (middle) and **11** (bottom).

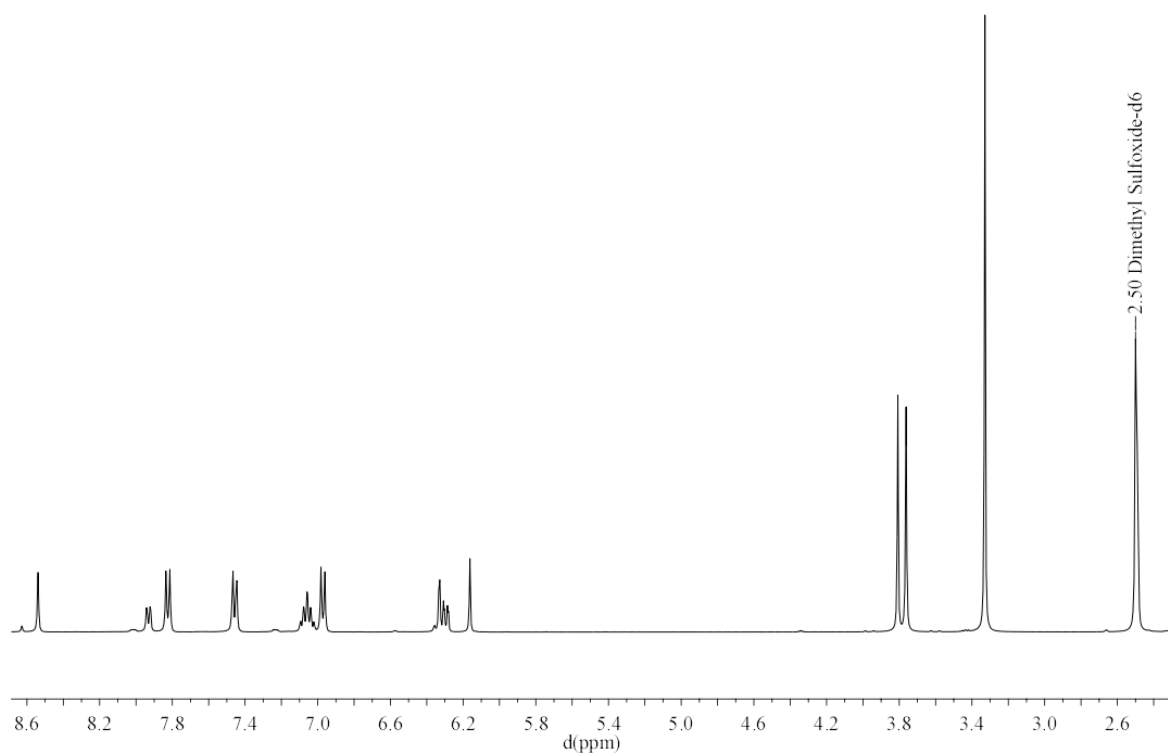
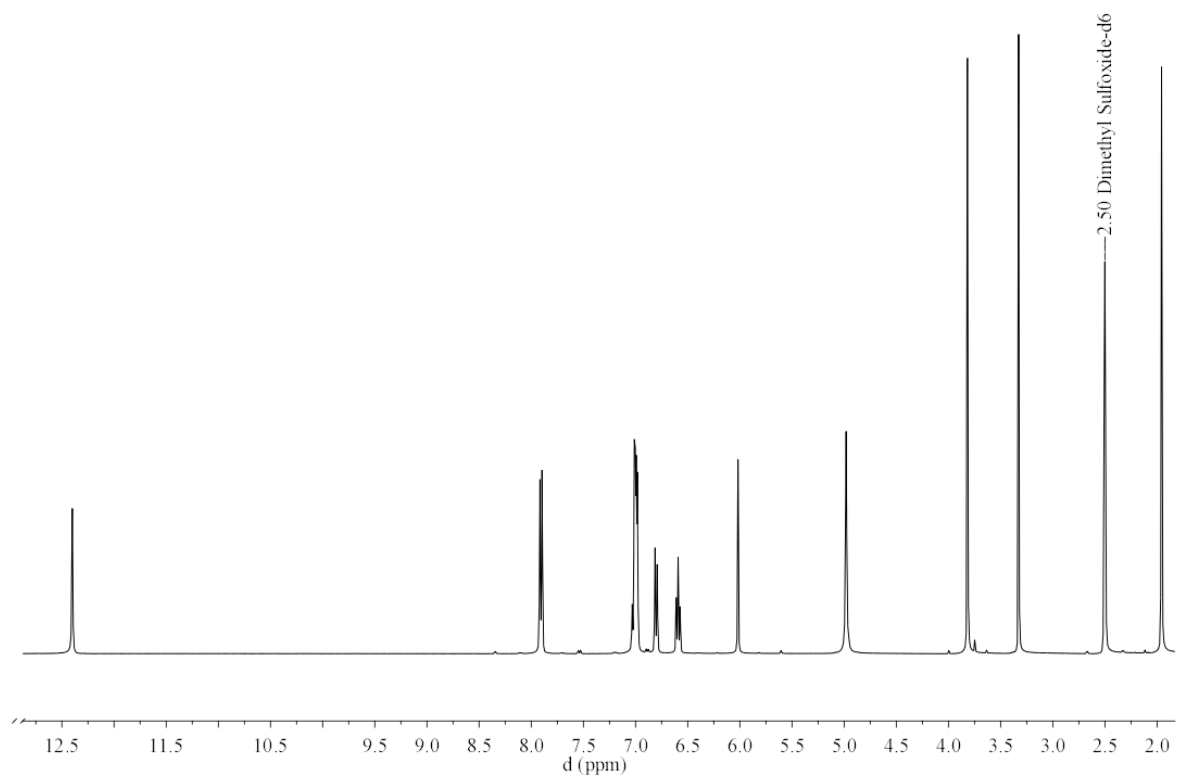


Fig. S3 ^1H NMR spectra of compounds **1** (top) and **4** (bottom) recorded in $\text{DMSO-}d_6$ at 298 K

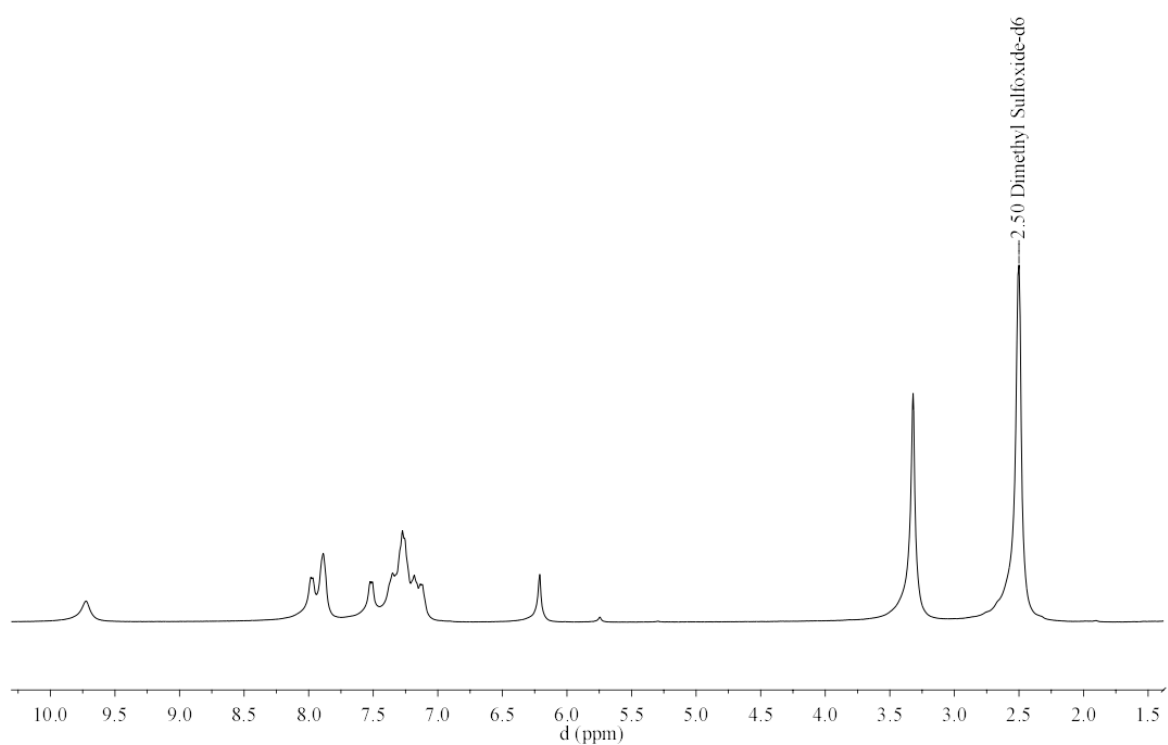
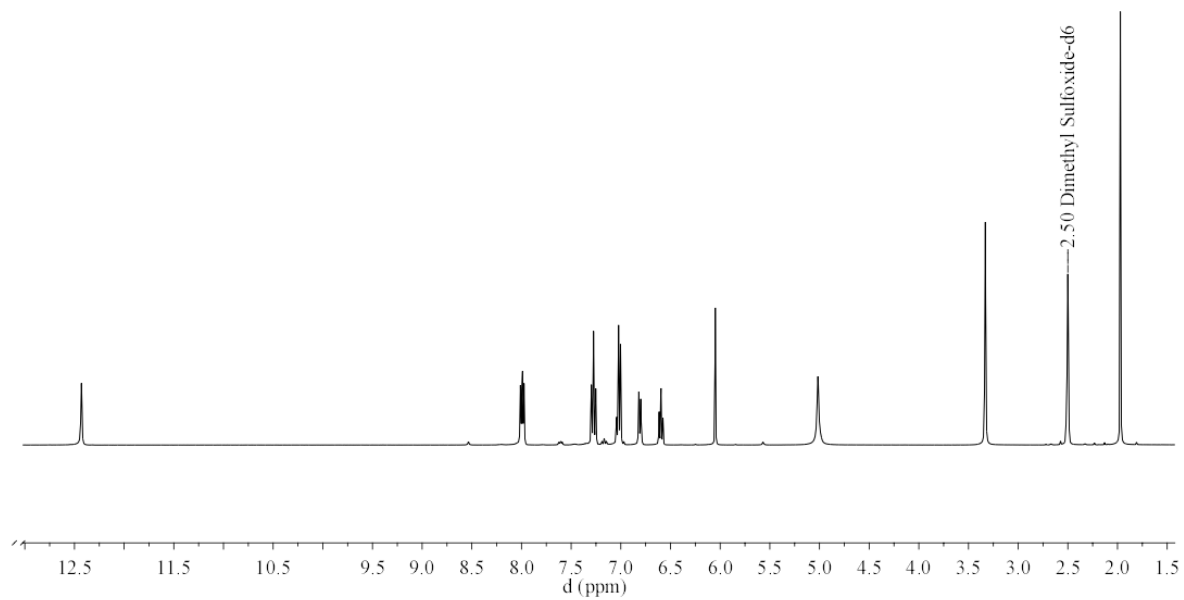


Fig. S4 ^1H NMR spectra of compounds **2** (top) and **8** (bottom) recorded in $\text{DMSO-}d_6$ at 298 K

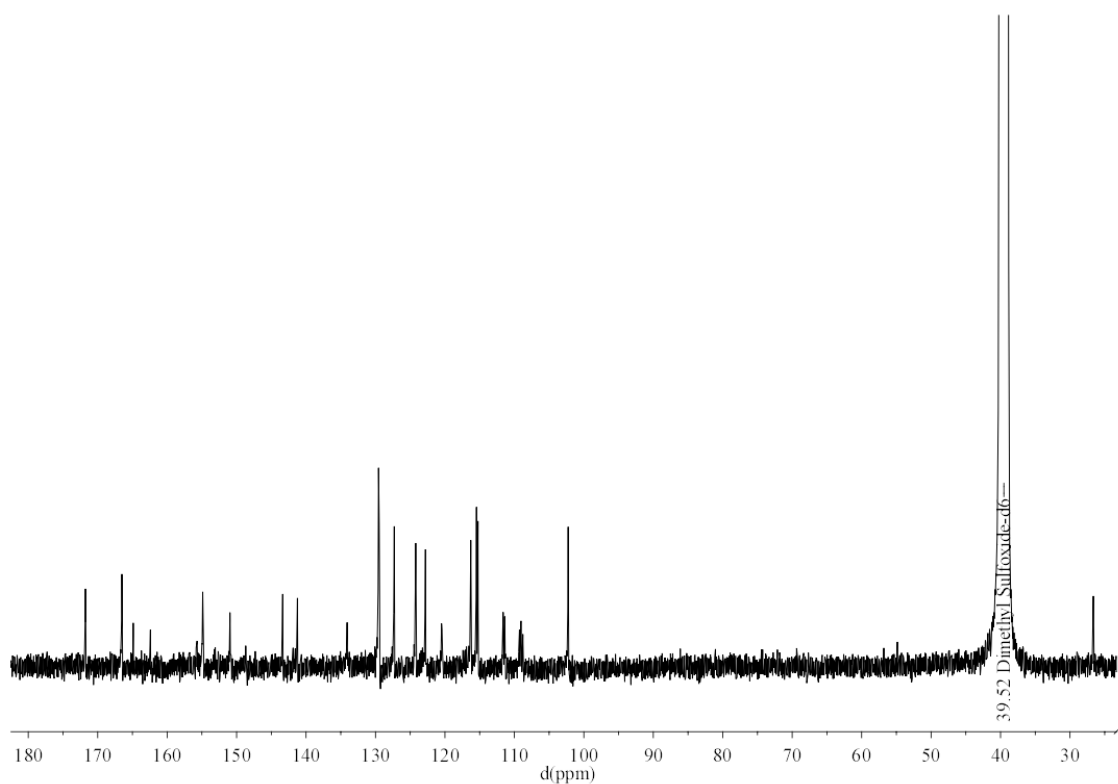
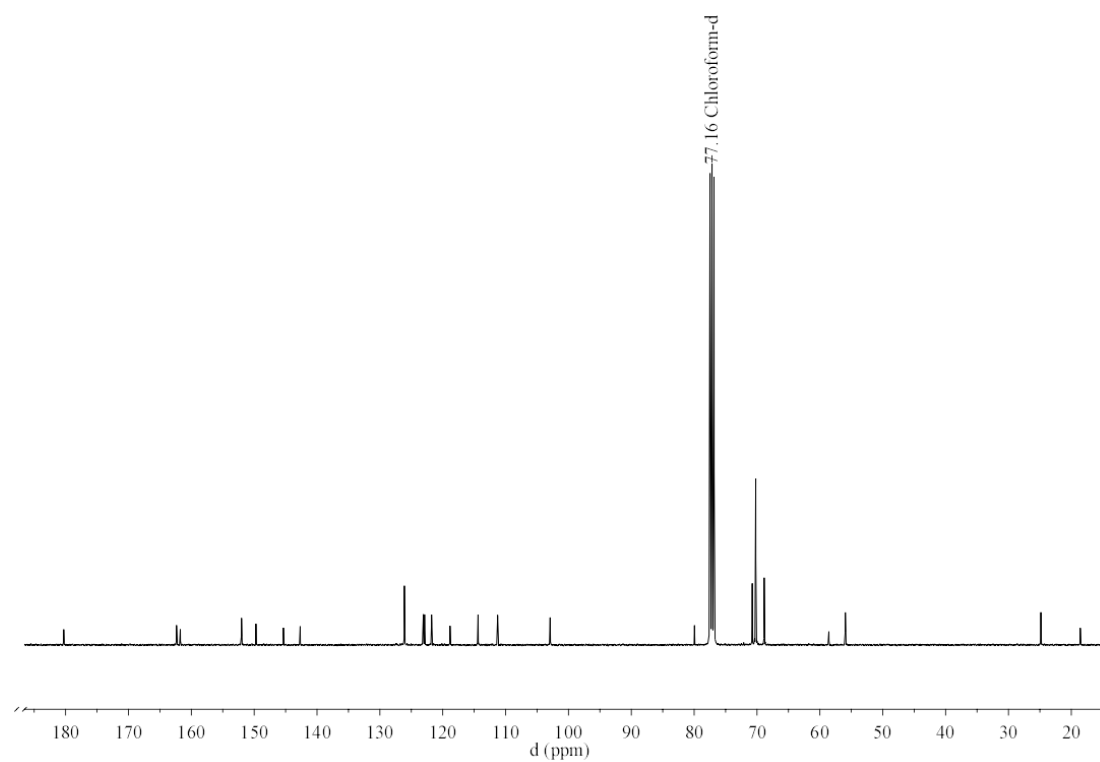


Fig. S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compounds **6** (top) recorded in CDCl_3 and **8** (bottom) recorded in $\text{DMSO}-d_6$, both at 298 K

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info
Analysis Name D:\Data\CRMPO\ESI_4888_MS_01.d
Method CRMPO_tune_low.m
Sample Name JC 013
Comment J-R. HAMON JC 013 Solvant : CH3OH/CH2Cl2 (90/10)

Acquisition Date 02/08/2016 5:16:16 PM
Operator Fabian LAMBERT
Instrument maXis

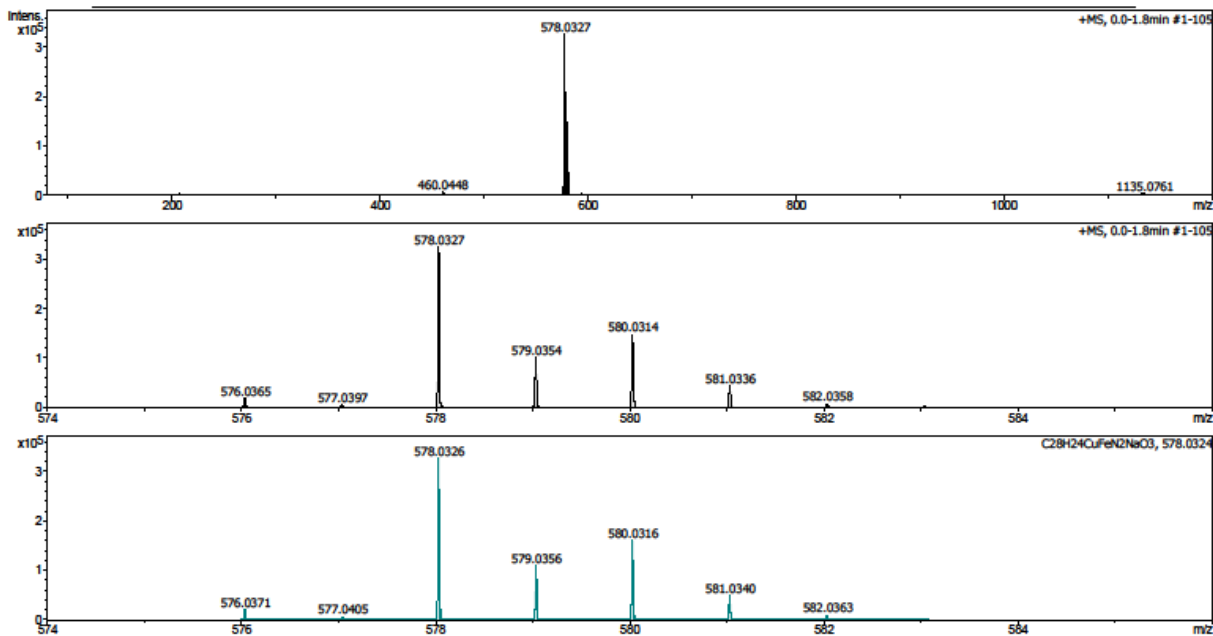


Fig. S6 Mass spectral data of **7**: full spectrum (top), experimental molecular ion peak (middle) and simulated molecular ion peak (bottom)

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info		Acquisition Date	10/13/2015 3:38:59 PM
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Sample Name	JC 010		
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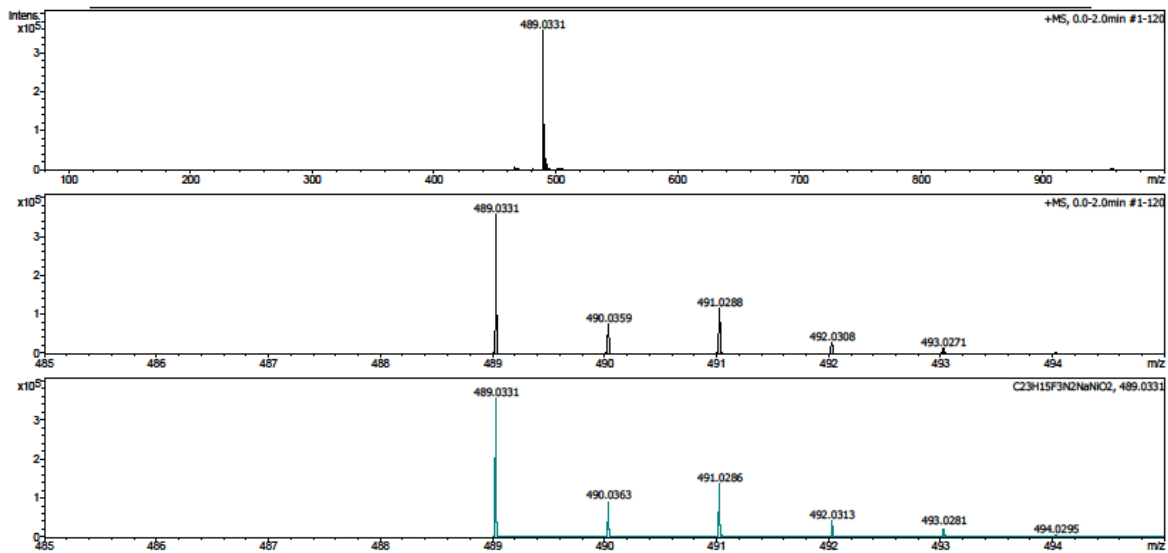


Fig. S7 Mass spectral data of **8**: full spectrum (top), experimental molecular ion peak (middle) and simulated molecular ion peak (bottom)

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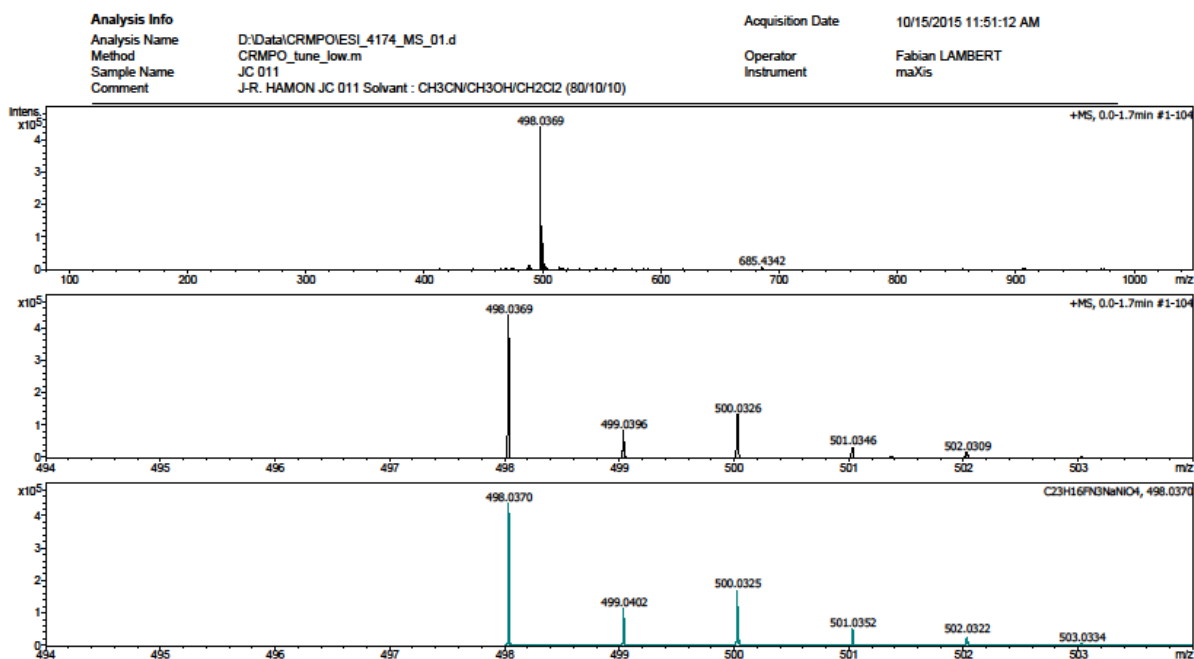


Fig. S8 Mass spectral data of **10**: full spectrum (top), experimental molecular ion peak (middle) and simulated molecular ion peak (bottom)

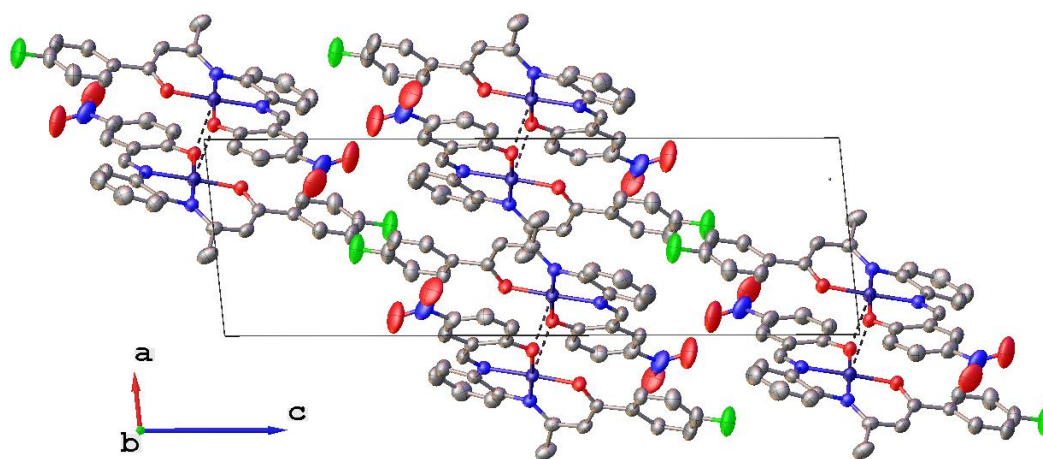


Fig. S9 Packing diagram of **11** showing the arrangement of the dimeric units in the lattice. Hydrogen atoms have been omitted for clarity.

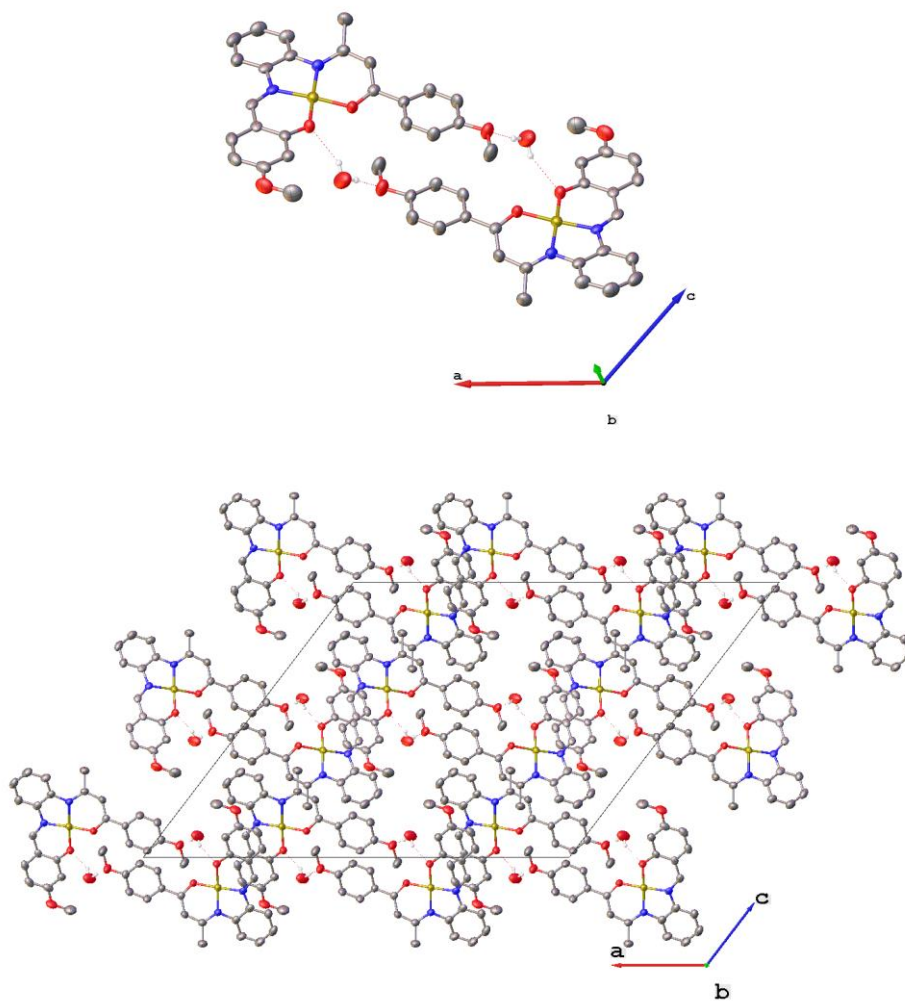


Fig. S10 Packing diagram of $4 \cdot \text{H}_2\text{O}$ showing the hydrogen bonding interactions implying the water crystallization molecules. All other hydrogen atoms have been omitted for clarity.

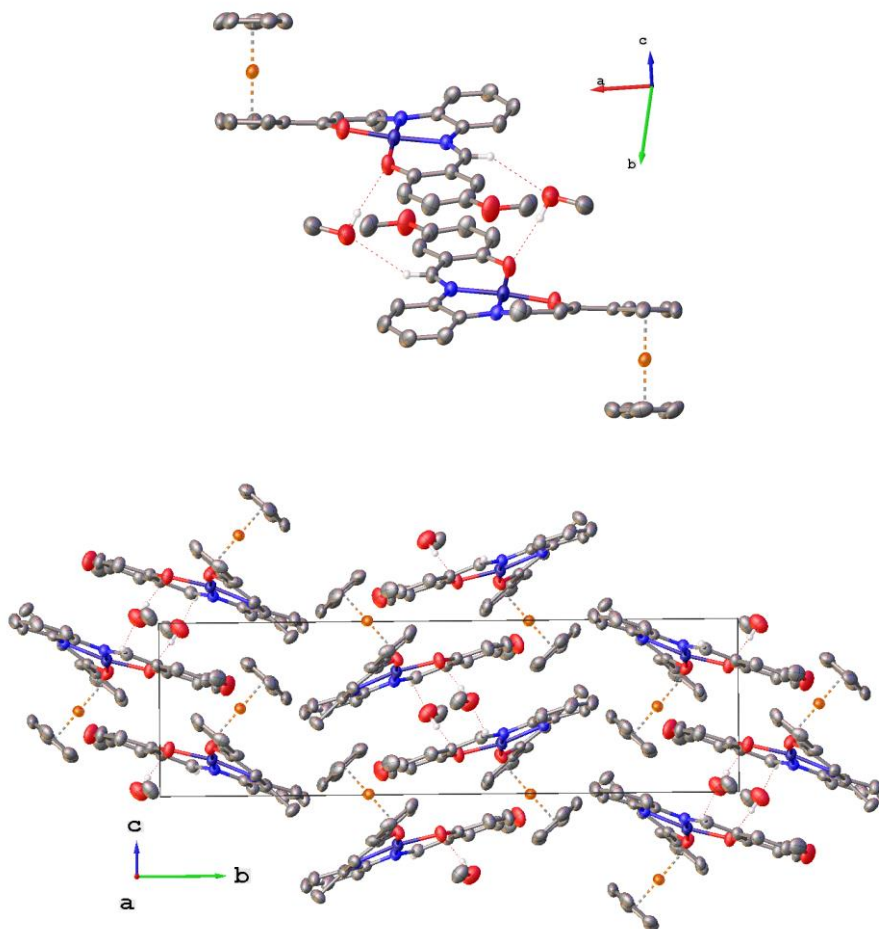


Fig. S11 Packing diagram of $7 \cdot \text{CH}_3\text{OH}$ showing the hydrogen bonds between the methanol crystallization solvent and phenolato oxygens of the Schiff base complexes. All other hydrogen atoms have been omitted for clarity.

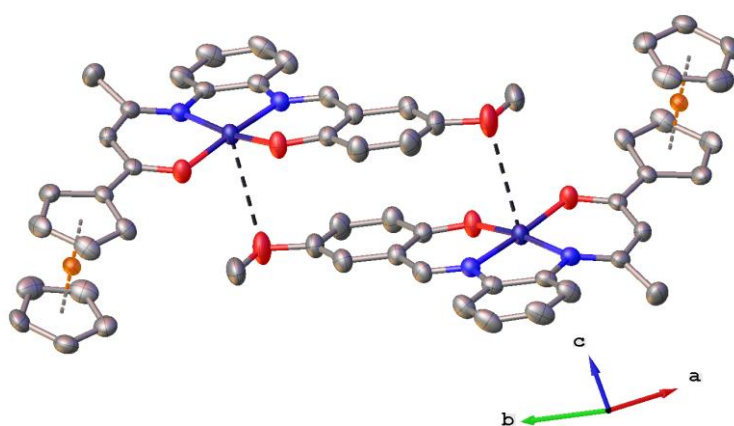


Fig. S12 Packing diagram of $7 \cdot \text{CH}_3\text{OH}$ showing the apical interaction (dashed line) between the Cu(II) center and the methoxy oxygen atom of the 5-substituted salicylidene ring of a neighboring molecule. Hydrogen atoms and crystallization solvent molecules have been omitted for clarity.

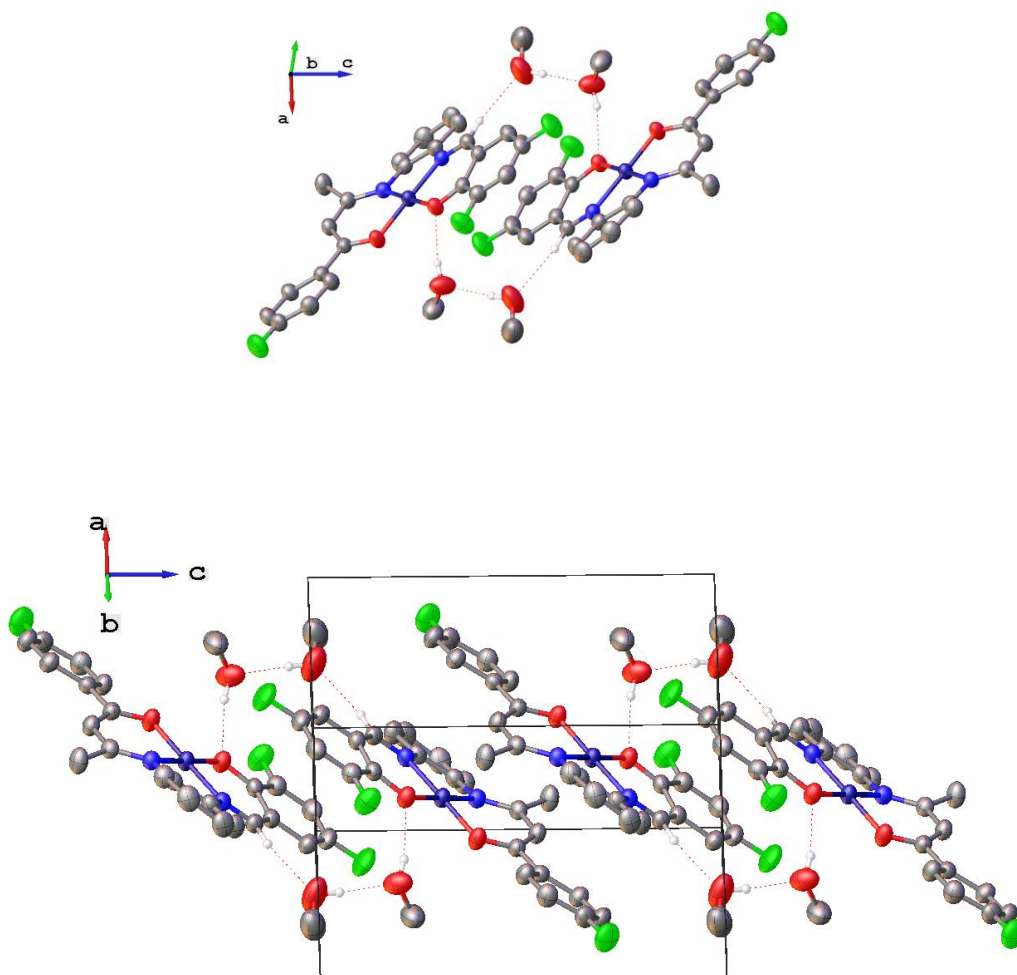


Fig. S13 Packing diagram of $9 \cdot 2\text{CH}_3\text{OH}$ showing the hydrogen bonding interactions between one methanol crystallization molecule and the phenolato oxygen of the complex and between the two methanol molecules. All other hydrogen atoms have been omitted for clarity.

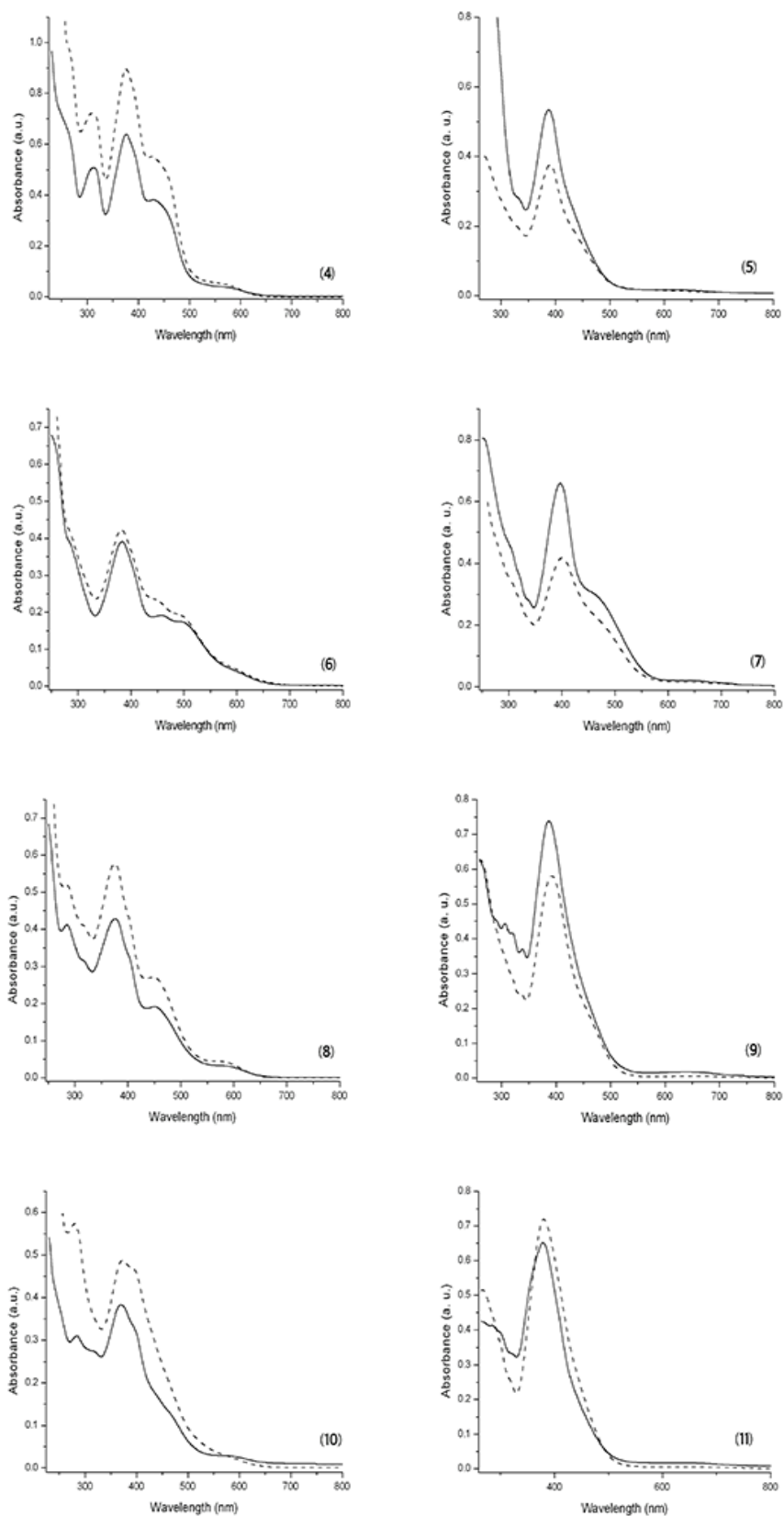


Fig. S14 Electronic absorption spectra of the Schiff base complexes **4-11** recorded in CH_2Cl_2 (solid line) and in DMSO (dashed line)

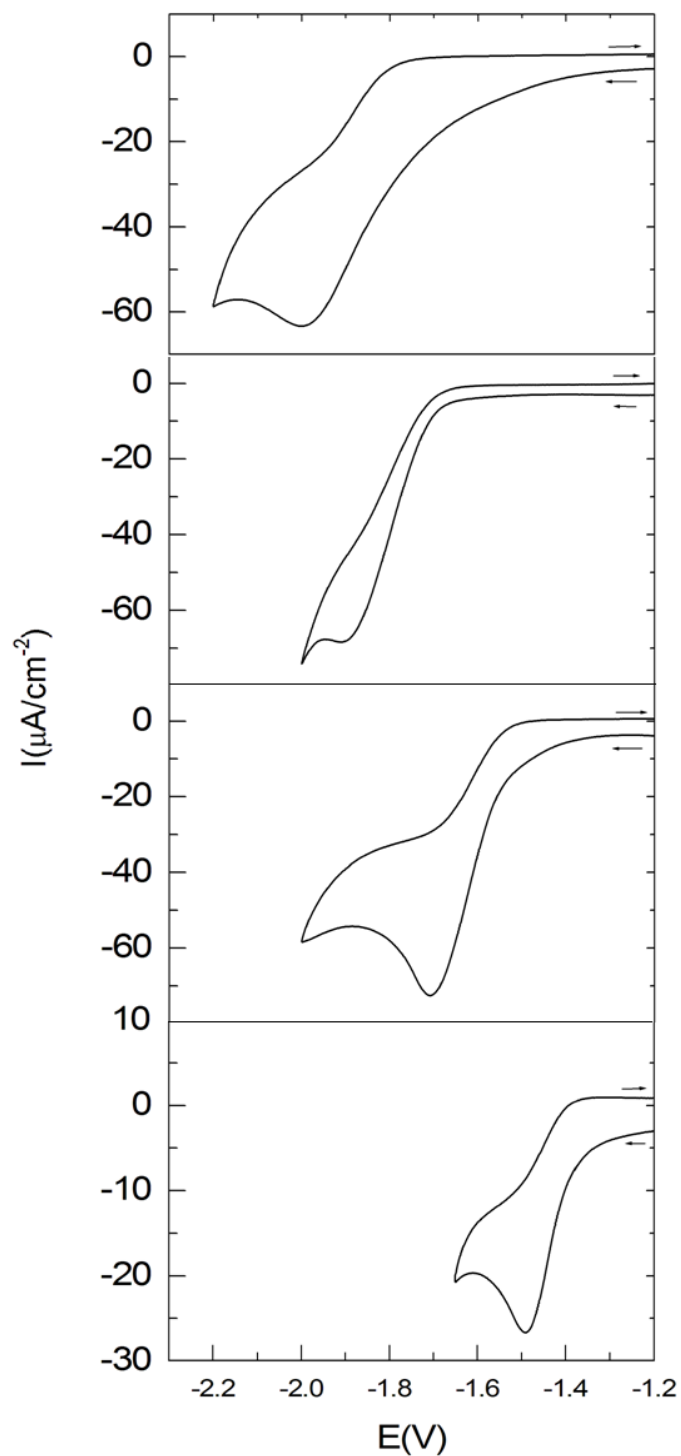


Fig. S15 Cyclic voltammograms of the Ni(II) Complexes **4**, **6**, **8** and **10** (from top to bottom), recorded in CH_2Cl_2 containing 0.1 M $n\text{-Bu}_4\text{N}^+\text{PF}_6^-$ at 293 K with a vitreous carbon working electrode, $\nu = 100\text{mV s}^{-1}$, reference electrode Ag/Ag^+ .

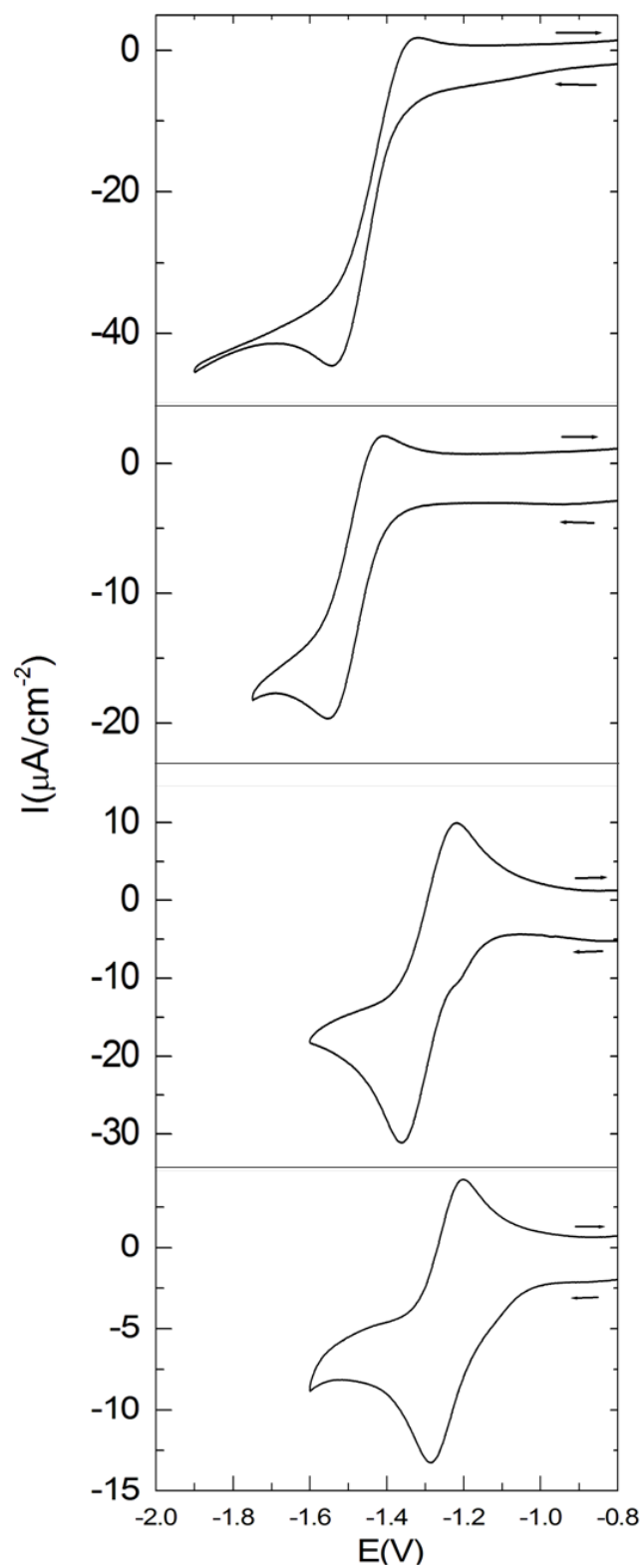


Fig. S16 Cyclic voltammograms of the Cu(II) Complexes **5**, **7**, **9** and **11** (from top to bottom), recorded in CH_2Cl_2 containing 0.1 M $n\text{-Bu}_4\text{N}^+\text{PF}_6^-$ at 293 K with a vitreous carbon working electrode, $\nu = 100\text{mV s}^{-1}$, reference electrode Ag/Ag^+ .

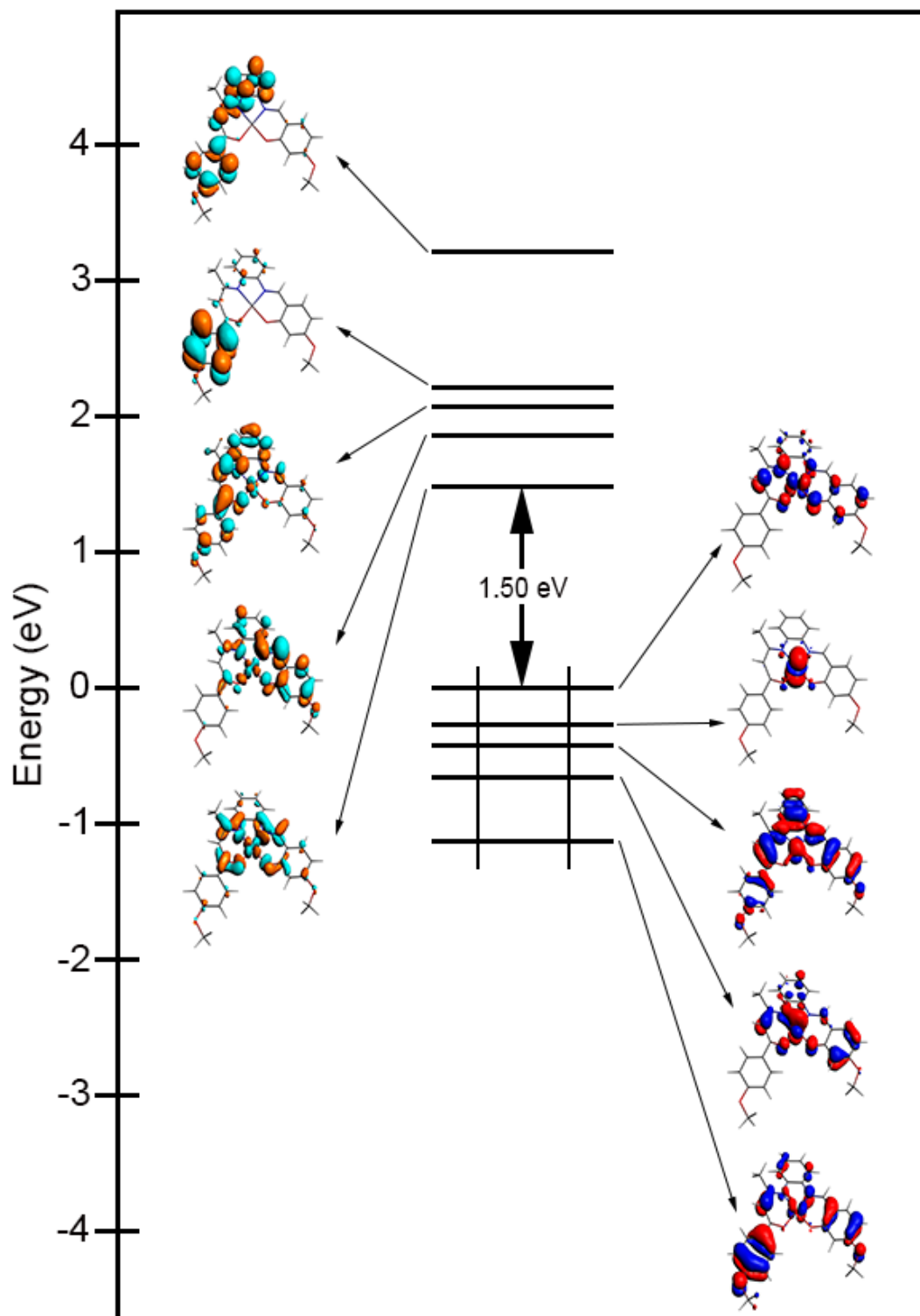


Fig. S17 MO diagram of compound **4**. The HOMO energy has been arbitrarily set to zero.

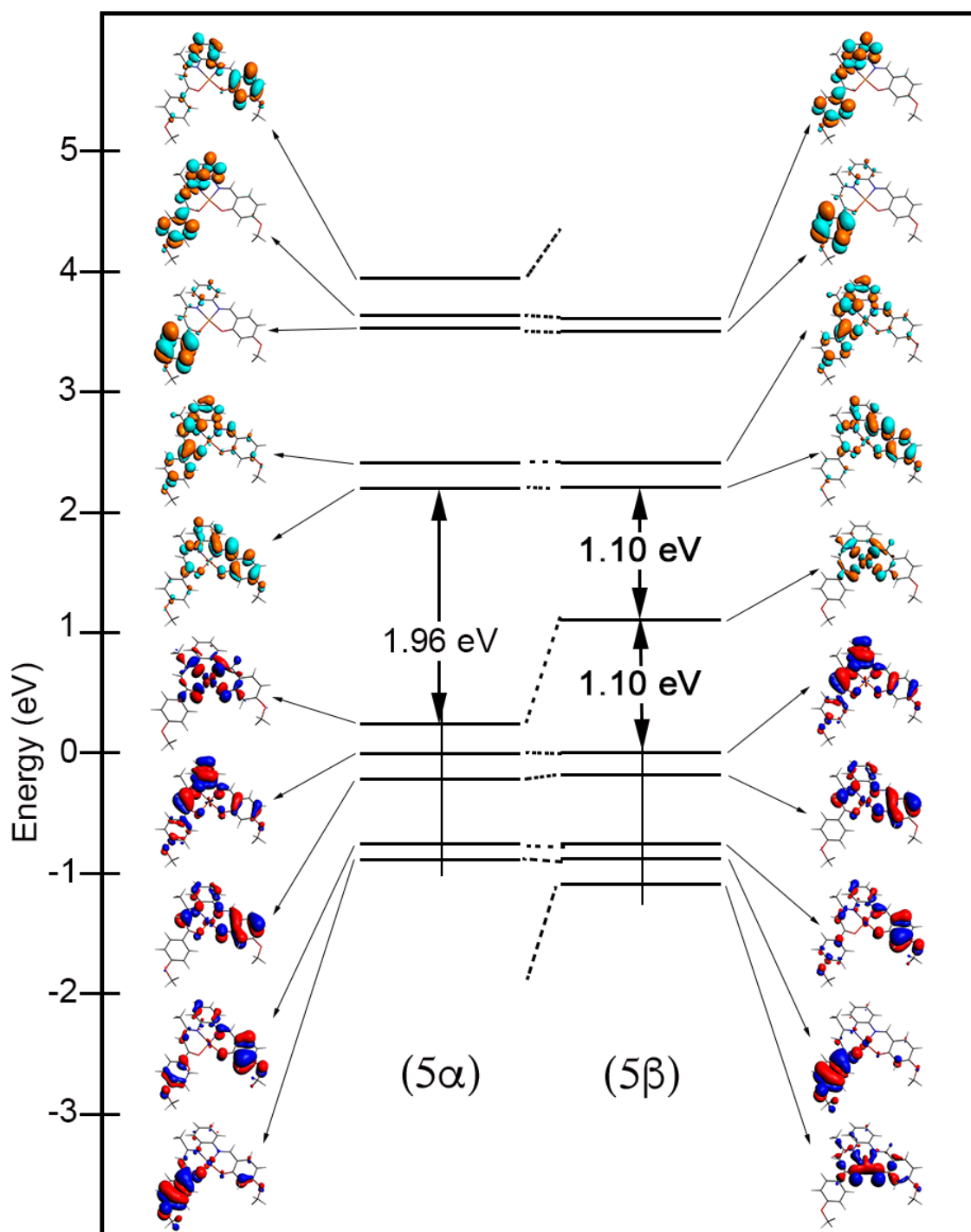


Fig. S18 MO diagram of compound **5**. The HOMO energy has been arbitrarily set to zero.

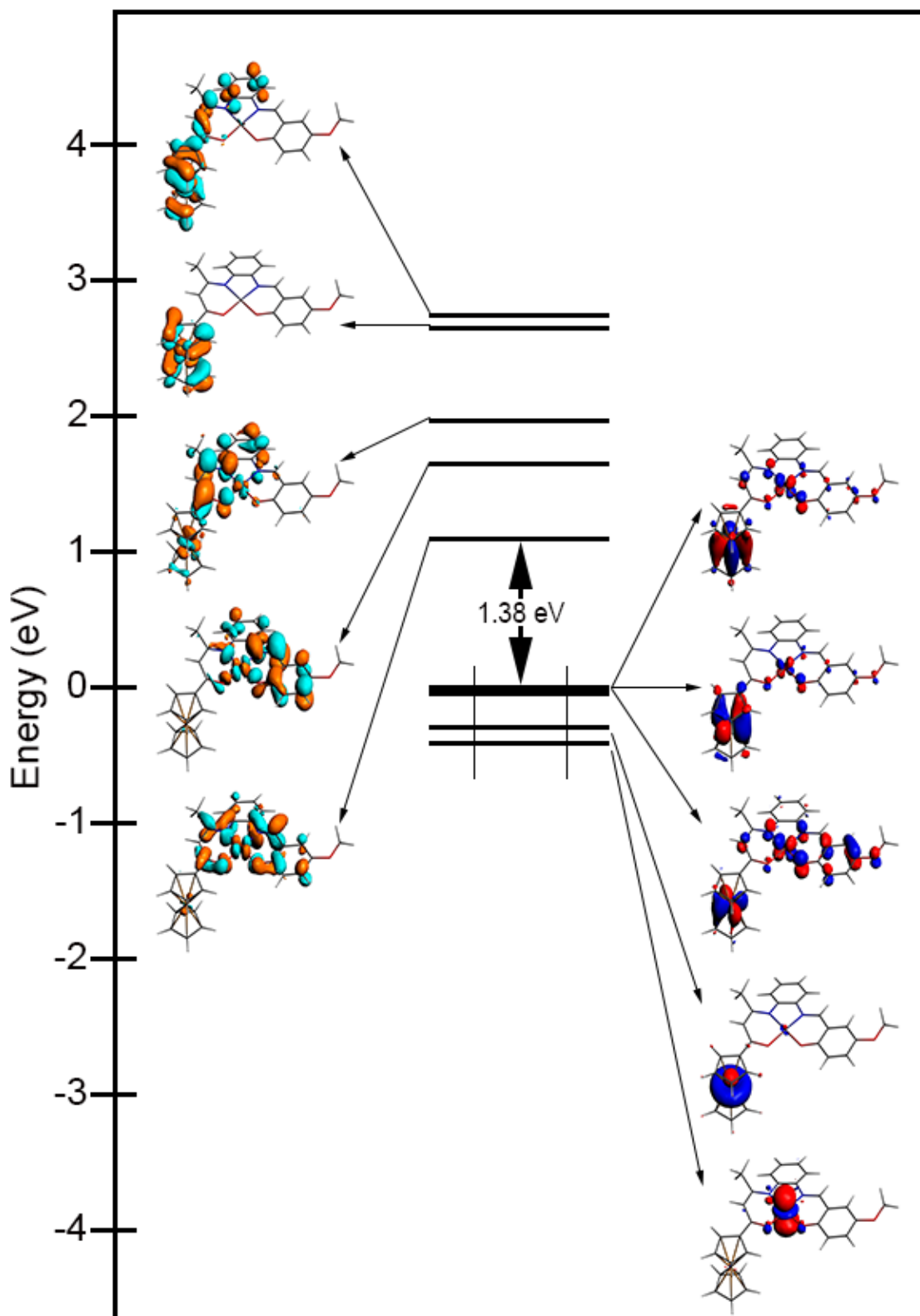


Fig. S91 MO diagram of compound **6**. The HOMO energy has been arbitrarily set to zero.

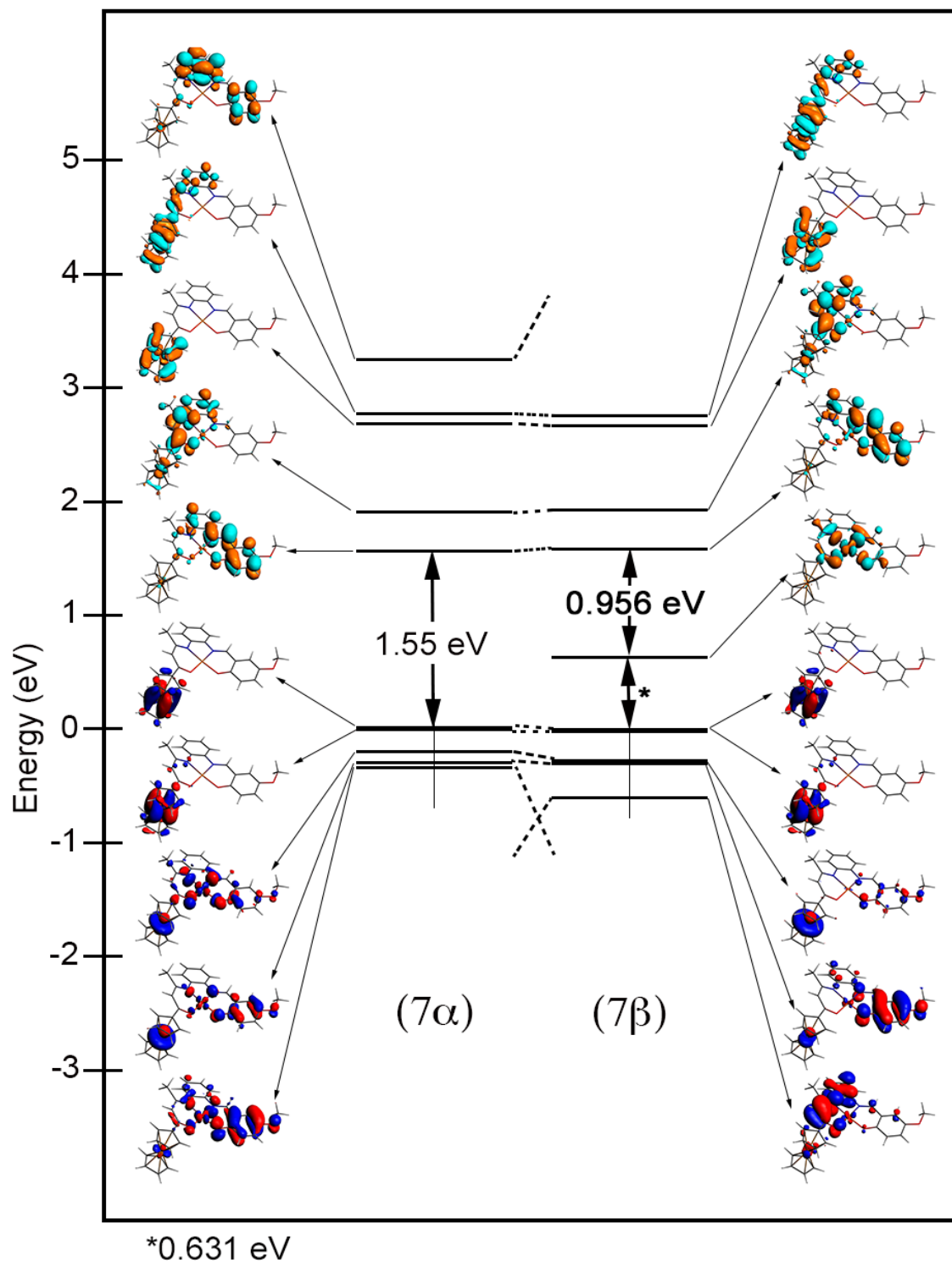


Fig. S20 MO diagram of compound **7**. The HOMO energy has been arbitrarily set to zero.

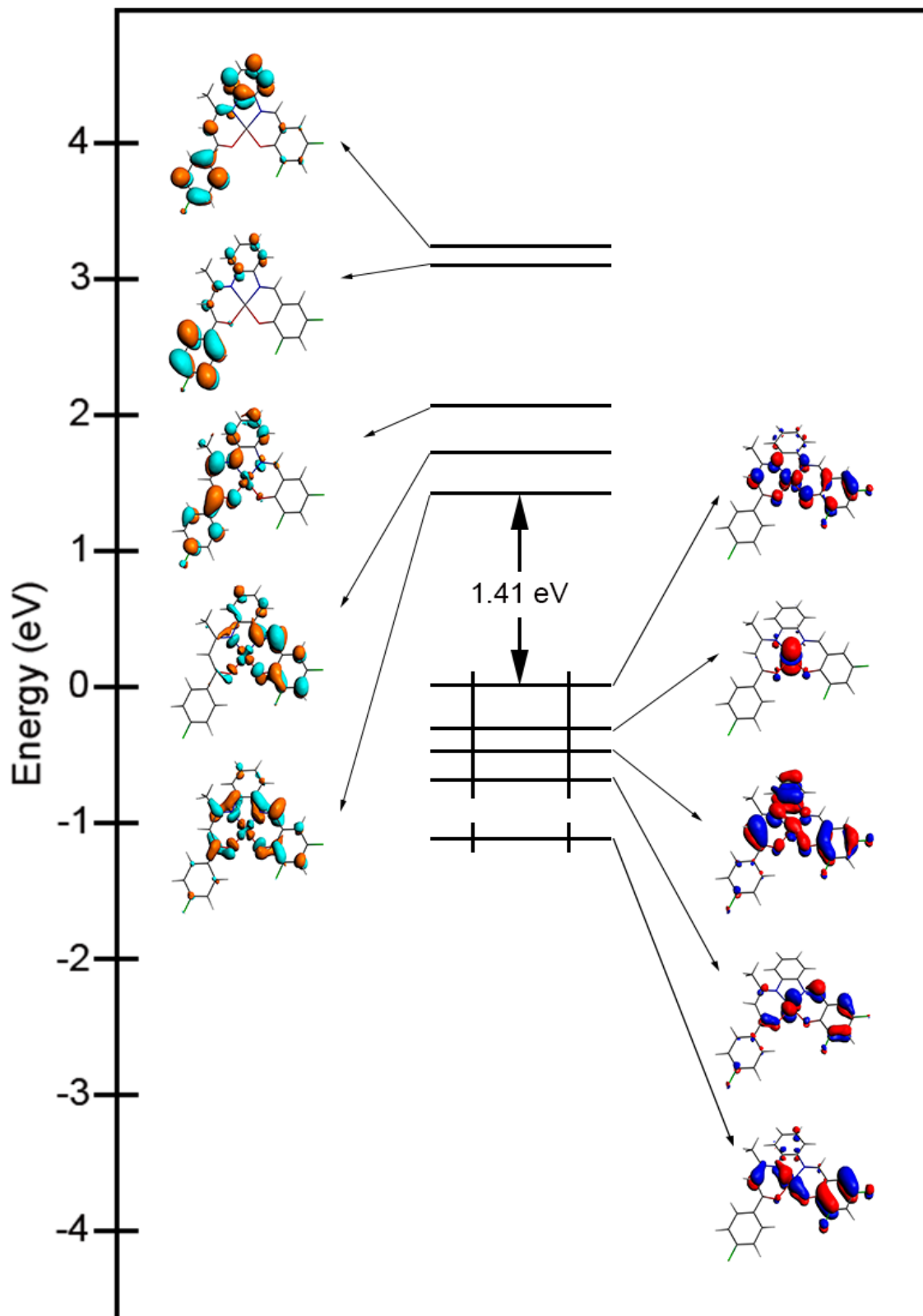


Fig. S21 MO diagram of compound **8**. The HOMO energy has been arbitrarily set to zero.

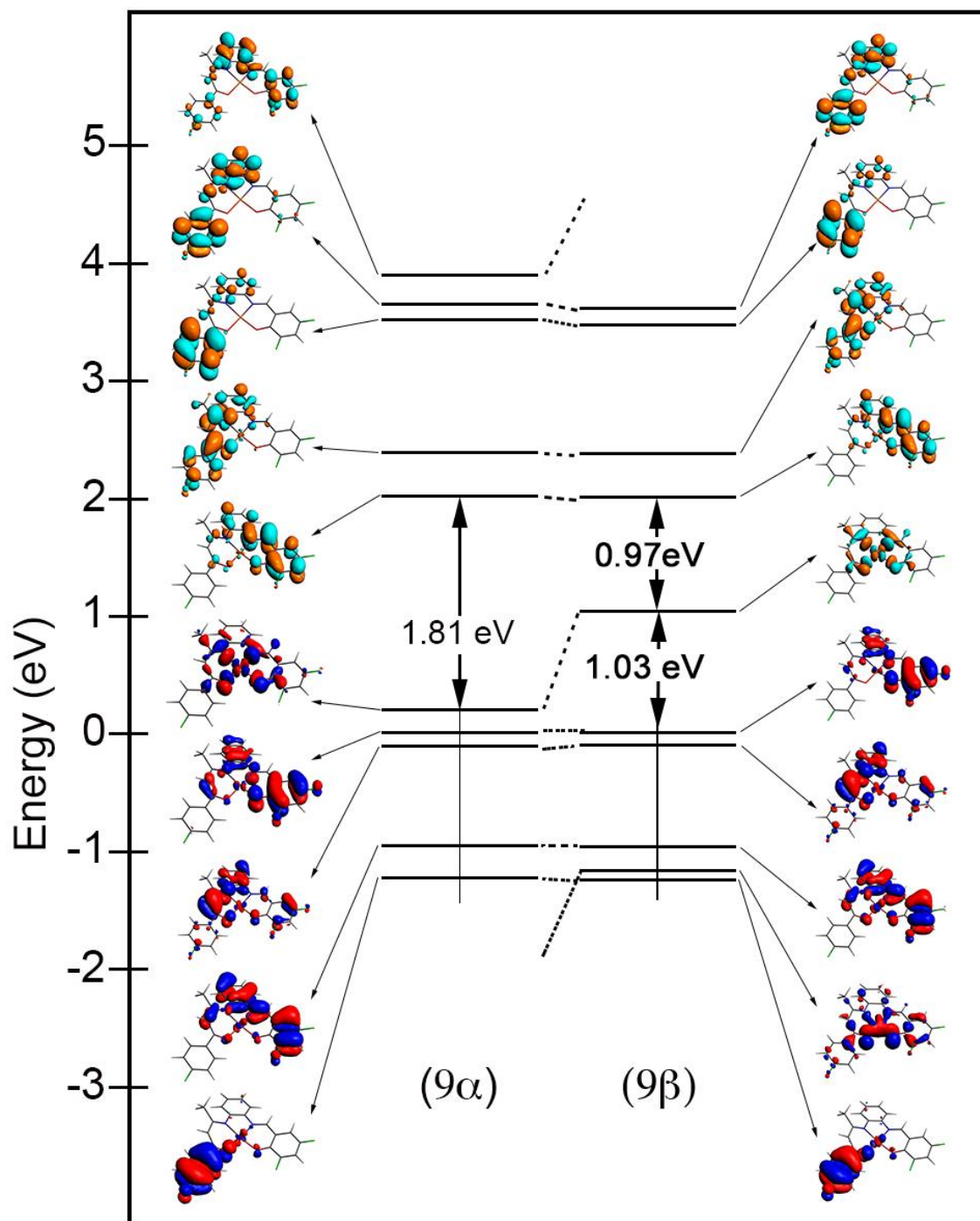


Fig. S22 MO diagram of compound **9**. The HOMO energy has been arbitrarily set to zero.

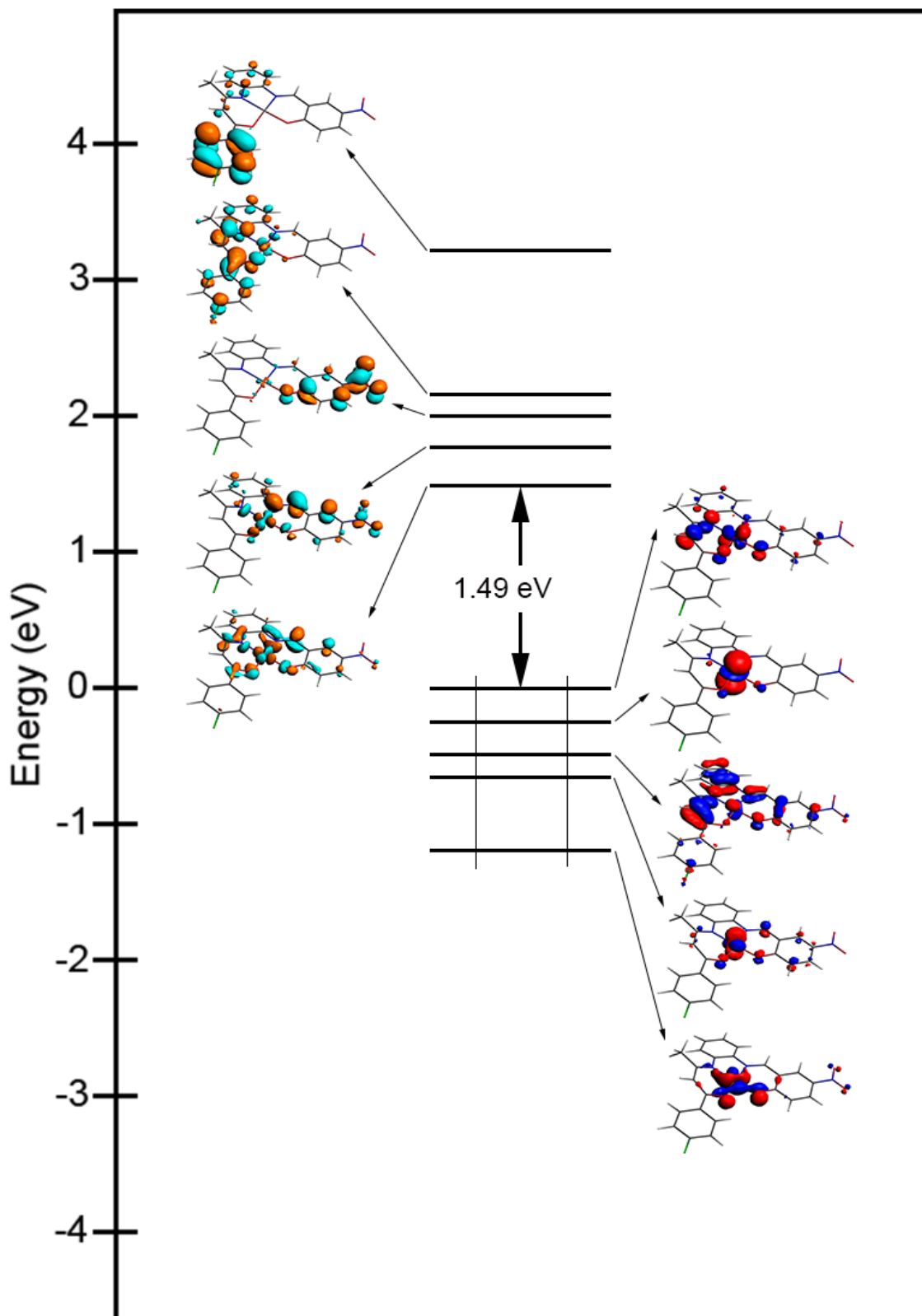


Fig. S23 MO diagram of compound **10**. The HOMO energy has been arbitrarily set to zero.

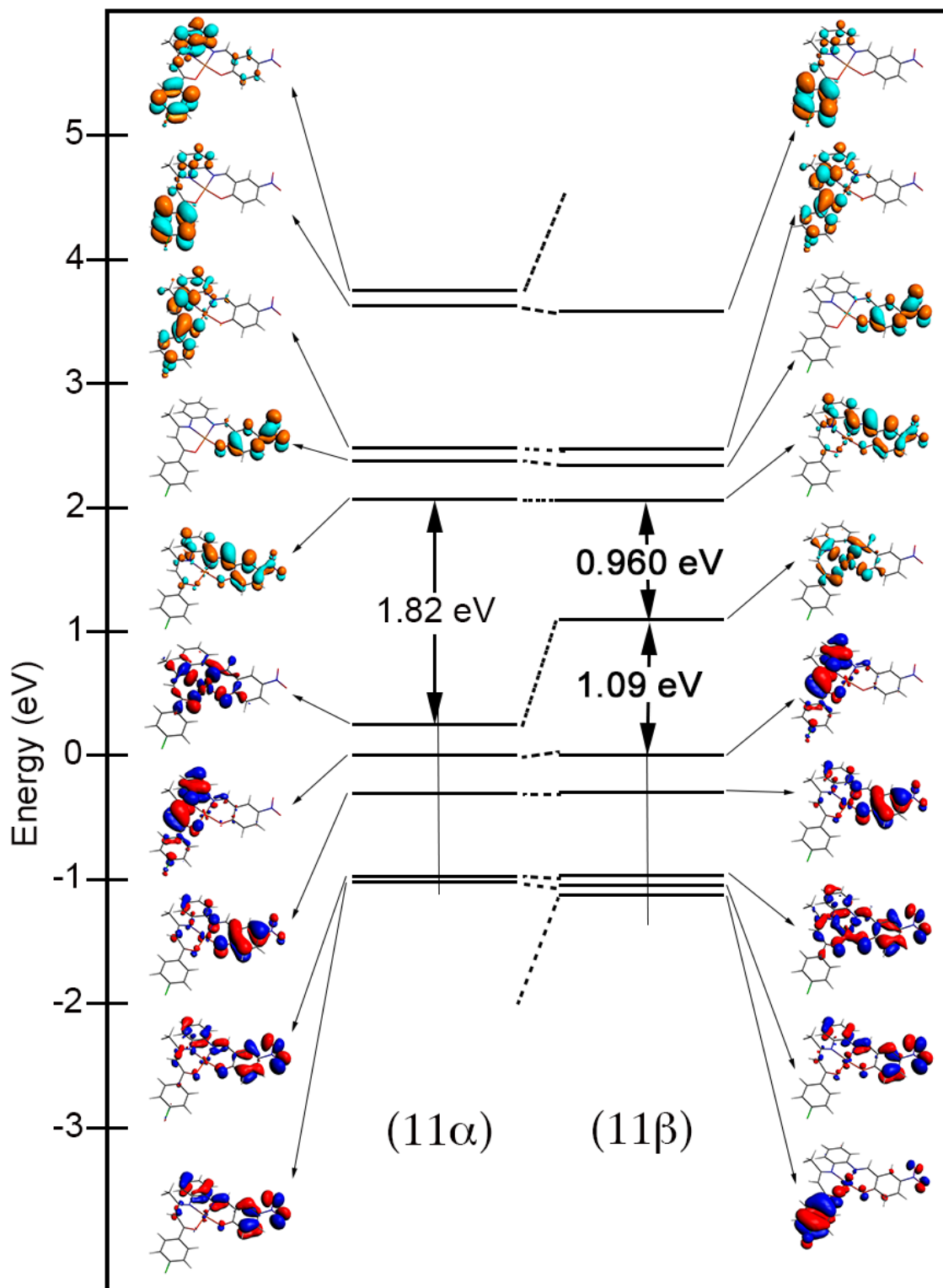


Fig. S24 MO diagram of compound **11**. The HOMO energy has been arbitrarily set to zero.

Table S1. Selected bond distances (Å) and angles (°) for compounds **4**·H₂O and **5**·CH₂Cl₂ with their theoretically computed values into brackets

	4·H ₂ O	5·CH ₂ Cl ₂
Bond distances		
O(1)-C(8)	1.286(5) [1.286]	1.288(4) [1.285]
O(2)-C(20)	1.306(5) [1.297]	1.299(4) [1.295]
O(3)-C(1)	1.418(6) [1.429]	1.410(5) [1.429]
O(3)-C(2)	1.370(5) [1.367]	1.367(4) [1.367]
O(4)-C(22)	1.368(6) [1.365]	1.367(4) [1.365]
O(4)-C(25)	1.416(7) [1.430]	1.414(5) [1.430]
N(1)-C(10)	1.330(6) [1.345]	1.320(5) [1.339]
N(1)-C(12)	1.415(6) [1.405]	1.410(5) [1.397]
N(2)-C(17)	1.417(6) [1.409]	1.408(4) [1.403]
N(2)-C(18)	1.299(6) [1.319]	1.297(4) [1.314]
C(8)-C(9)	1.380(6) [1.405]	1.386(5) [1.410]
C(9)-C(10)	1.392(6) [1.401]	1.398(5) [1.406]
C(12)-C(17)	1.386(7) [1.417]	1.408(5) [1.428]
C(18)-C(19)	1.419(6) [1.408]	1.411(5) [1.414]
C(19)-C(20)	1.413(6) [1.441]	1.422(5) [1.450]
Angles		
M(1)-O(1)-C(8)	125.5(3) [126]	123.5(2) [124]
M(1)-O(2)-C(20)	127.6(3) [127]	126.6(2) [126]
M(1)-N(1)-C(10)	122.6(3) [123]	121.6(2) [121]
M(1)-N(1)-C(12)	112.0(3) [112]	111.8(2) [111]
M(1)-N(2)-C(17)	112.9(3) [113]	112.9(2) [112]
M(1)-N(2)-C(18)	125.1(3) [125]	124.8(2) [124]
O(1)-C(8)-C(9)	123.6(4) [124]	124.6(3) [125]
C(8)-C(9)-C(10)	125.8(4) [126]	127.9(3) [128]
C(9)-C(10)-N(1)	122.2(4) [123]	121.4(3) [123]
O(2)-C(20)-C(19)	123.4(4) [124]	124.2(3) [125]
N(2)-C(18)-C(19)	125.9(4) [126]	126.3(3) [127]
C(18)-C(19)-C(20)	121.9(4) [122]	123.5(3) [124]

M = Ni, **4**; Cu, **5**.

Table S2. Selected bond distances (Å) and angles (°) for compound **7**·CH₃OH with its theoretically computed values into brackets

Bond distances			
O(1)-C(11)	1.284(3) [1.283]	O(2)-C(23)	1.316(3) [1.295]
N(1)-C(13)	1.333(3) [1.328]	N(1)-C(15)	1.415(3) [1.408]
N(2)-C(20)	1.419(3) [1.289]	N(2)-C(21)	1.291(3) [1.421]
O(3)-C(27)	1.384(3) [1.400]	O(3)-C(28)	1.413(4) [1.320]
C(10)-C(11)	1.476(3) [1.540]	C(11)-C(12)	1.388(3) [1.370]
C(12)-C(13)	1.404(3) [1.408]	C(15)-C(20)	1.411(3) [1.408]
C(21)-C(22)	1.426(3) [1.421]	C(22)-C(23)	1.414(3) [1.423]
Fe(1)-C(Cp) avg	2.037(3)	Fe(1)-C(Cp') avg	2.039(2)
Angles			
Cu(1)-O(1)-C(11)	124.78(15) [125]	Cu(1)-O(2)-C(23)	126.53(15) [126]
Cu(1)-N(1)-C(13)	121.55(16) [122]	Cu(1)-N(1)-C(15)	111.43(14) [112]
Cu(1)-N(2)-C(20)	112.55(14) [125]	Cu(1)-N(2)-C(21)	125.24(16) [125]
O(1)-C(11)-C(12)	124.6(2) [125]	O(2)-C(23)-C(22)	124.2(2) [126]
N(1)-C(13)-C(12)	122.1(2) [121]	N(2)-C(21)-C(22)	126.2(2) [126]
C(11)-C(12)-C(13)	127.7(2) [128]	C(21)-C(22)-C(23)	123.3(2) [122]

Abbreviations: Cp = C₅H₅, Cp' = C₅H₄

Table S3. Selected bond distances (Å) and angles (°) for compounds **9**·2CH₃OH and **11** with their theoretically computed values into brackets

	9·2CH ₃ OH	11
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Bond distances		
O(1)-C(7)	1.2861(19) [1.283]	1.284(3) [1.285]
O(2)-C(19)	1.3074(19) [1.292]	1.295(3) [1.289]
N(1)-C(9)	1.325(2) [1.339]	1.331(4) [1.339]
N(1)-C(11)	1.4157(19) [1.396]	1.413(4) [1.397]
N(2)-C(16)	1.419(2) [1.405]	1.416(4) [1.407]
N(2)-C(17)	1.293(2) [1.310]	1.290(4) [1.306]
C(7)-C(8)	1.386(2) [1.409]	1.400(4) [1.408]
C(8)-C(9)	1.416(2) [1.406]	1.414(4) [1.406]
C(11)-C(16)	1.406(2) [1.427]	1.405(4) [1.426]
C(17)-C(18)	1.432(2) [1.423]	1.433(4) [1.427]
C(18)-C(19)	1.419(2) [1.444]	1.437(4) [1.453]
F(1)-C(1)	1.354(2) [1.360]	1.363(4) [1.359]
F(2)-C(20)	1.351(2) [1.352]	-
F(3)-C(22)	1.367(2) [1.364]	-
N(3)-C(22)	-	1.467(4) [1.459]
N(3)-O(3)	-	1.220(5) [1.242]
N(3)-O(4)	-	1.214(4) [1.241]
Angles		
Cu(1)-O(1)-C(7)	124.15(10) [124]	124.53(19) [124]
Cu(1)-O(2)-C(19)	126.08(10) [126]	126.84(18) [127]
Cu(1)-N(1)-C(9)	122.52(10) [121]	122.8(2) [121]
Cu(1)-N(1)-C(11)	111.21(10) [111]	110.68(17) [111]
Cu(1)-N(2)-C(16)	111.87(10) [112]	111.0(2) [112]
Cu(1)-N(2)-C(17)	126.01(11) [125]	125.5(2) [124]
O(1)-C(7)-C(8)	124.68(14) [125]	125.1(3) [125]
C(7)-C(8)-C(9)	127.26(15) [128]	127.1(3) [128]
C(8)-C(9)-N(1)	121.76(14) [123]	122.0(3) [123]
O(2)-C(19)-C(18)	125.51(14) [126]	124.0(3) [125]
N(2)-C(17)-C(18)	125.21(14) [127]	125.7(3) [126]
C(17)-C(18)-C(19)	122.74(14) [123]	123.0(3) [124]

Table S4. Hydrogen Bonding interaction parameters for compounds **4**·H₂O, **5**·CH₂Cl₂, **7**·CH₃OH and **9**·2CH₃OH

Compd	D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
4 ·H ₂ O	O(5)-H(5B)···O(2)	0.80	2.15	2.880(6)	152.4
	O(5)-H(5A)···O(3)	0.80	2.11	2.943(8)	165.4
5 ·CH ₂ Cl ₂	C(26)-H(26A)···O(2)	0.97	2.32	3.289(5)	174.8
	C(26)-H(26A)···O(3) ^{#1}	0.97	2.61	3.401(6)	139.0
7 ·CH ₃ OH	O(4)-H(4A)···O(2) ^{#2}	0.82	1.97	2.789(3)	172.6
9 ·2CH ₃ OH	O(3)-H(3)···O(2)	0.82	2.04	2.8424(18)	168.0
	O(4)-H(4A)···O(3)	0.82	1.93	2.745(3)	176.1

Symmetry transformations: #1 2-X,2-Y,2-Z; #2 1-X,-Y,-Z.

Table S5. Computed bond distances (Å) and angles (°) of the [Ni(N₂O₂)] coordination core for compounds **6**, **8** and **10**

	6	8	10
Bond distances			
Ni(1)-O(1)	1.877	1.874	1.873
Ni(1)-O(2)	1.875	1.878	1.882
Ni(1)-N(1)	1.905	1.898	1.897
Ni(1)-N(2)	1.869	1.870	1.871
Angles			
O(1)-Ni(1)-N(2)	178	177	178
O(2)-Ni(1)-N(1)	178	177	177
O(1)-Ni(1)-O(2)	83	83	84
O(1)-Ni(1)-N(1)	96	96	96
O(2)-Ni(1)-N(2)	95	95	95
N(1)-Ni(1)-N(2)	86	86	86

Table S6. Computed bond distances (Å) and angles (°) for compound **6**

Bond distances			
O(1)-C(11)	1.286	O(2)-C(23)	1.299
N(1)-C(13)	1.348	N(1)-C(15)	1.404
N(2)-C(20)	1.409	N(2)-C(21)	1.320
O(3)-C(27)	1.377	O(3)-C(28)	1.423
C(10)-C(11)	1.471	C(11)-C(12)	1.408
C(12)-C(13)	1.398	C(15)-C(20)	1.418
C(21)-C(22)	1.411	C(22)-C(23)	1.435
Fe(1)-Cp _{CNT} avg	1.688	Fe(1)-Cp' _{CNT} avg	1.679
Angles			
Ni(1)-O(1)-C(11)	125	Ni(1)-O(2)-C(23)	127
Ni(1)-N(1)-C(13)	112	Ni(1)-N(1)-C(15)	112
Ni(1)-N(2)-C(20)	113	Ni(1)-N(2)-C(21)	125
O(1)-C(11)-C(12)	124	O(2)-C(23)-C(22)	124
N(1)-C(13)-C(12)	122	N(2)-C(21)-C(22)	126
C(11)-C(12)-C(13)	126	C(21)-C(22)-C(23)	121

Abbreviations: Cp = C₅H₅, Cp' = C₅H₄

Table S7. Computed bond distances (Å) and angles (°) for compounds **8** and **10**

	8	10
Bond distances		

O(1)-C(7)	1.284	1.286
O(2)-C(19)	1.294	1.291
N(1)-C(9)	1.345	1.345
N(1)-C(11)	1.404	1.405
N(2)-C(16)	1.411	1.414
N(2)-C(17)	1.316	1.312
C(7)-C(8)	1.404	1.404
C(8)-C(9)	1.401	1.401
C(11)-C(16)	1.416	1.415
C(17)-C(18)	1.415	1.420
C(18)-C(19)	1.436	1.444
F(1)-C(1)	1.359	1.359
F(2)-C(20)	1.352	-
F(3)-C(22)	1.364	-
N(3)-C(22)	-	1.459
N(3)-O(3)	-	1.242
N(3)-O(4)	-	1.241
Angles		
Ni(1)-O(1)-C(7)	126	125
Ni(1)-O(2)-C(19)	126	127
Ni(1)-N(1)-C(9)	123	123
Ni(1)-N(1)-C(11)	111	111
Ni(1)-N(2)-C(16)	113	113
Ni(1)-N(2)-C(17)	125	125
O(1)-C(7)-C(8)	124	124
C(7)-C(8)-C(9)	126	126
C(8)-C(9)-N(1)	122	122
O(2)-C(19)-C(18)	125	124
N(2)-C(17)-C(18)	126	126
C(17)-C(18)-C(19)	121	122

Table S8. Computed geometry optimization parameters of compound **4**

ATOMS	X	Y	Z	CHARGE		
				Nucl	+Core	At.Mass
	(Angstrom)					

1	Ni	-0.0805	0.0927	-0.0807	28.00	10.00	57.9353
2	N	-0.2163	1.9856	-0.0064	7.00	5.00	14.0031
3	O	0.0834	-1.7736	-0.2484	8.00	6.00	15.9949
4	H	1.3205	4.5583	-1.4715	1.00	1.00	1.0078
5	O	1.7948	0.0413	-0.0690	8.00	6.00	15.9949
6	H	-0.4308	4.4156	-1.1782	1.00	1.00	1.0078
7	N	-1.9504	0.0941	-0.0394	7.00	5.00	14.0031
8	C	2.5710	1.0437	-0.2853	6.00	4.00	12.0000
9	C	-2.4869	1.3620	0.2590	6.00	4.00	12.0000
10	C	-3.2323	-3.3146	-0.6566	6.00	4.00	12.0000
11	H	-4.2870	-3.0385	-0.6889	1.00	1.00	1.0078
12	C	-2.8709	-4.6276	-0.8094	6.00	4.00	12.0000
13	C	-2.7126	-0.9625	-0.2473	6.00	4.00	12.0000
14	H	-3.7959	-0.8140	-0.2532	1.00	1.00	1.0078
15	C	-1.5198	2.3964	0.3176	6.00	4.00	12.0000
16	C	-0.8729	-2.6346	-0.4096	6.00	4.00	12.0000
17	C	5.0242	1.7114	-0.2576	6.00	4.00	12.0000
18	H	4.7547	2.7598	-0.1454	1.00	1.00	1.0078
19	C	-1.9280	3.6659	0.7680	6.00	4.00	12.0000
20	H	-1.1986	4.4509	0.9296	1.00	1.00	1.0078
21	C	-3.8301	1.6297	0.5495	6.00	4.00	12.0000
22	H	-4.5714	0.8341	0.5165	1.00	1.00	1.0078
23	C	-2.2702	-2.2836	-0.4502	6.00	4.00	12.0000
24	C	4.0197	0.7259	-0.3242	6.00	4.00	12.0000
25	C	-0.5201	-4.0057	-0.5541	6.00	4.00	12.0000
26	C	0.7891	2.7978	-0.3793	6.00	4.00	12.0000
27	H	0.6628	4.9143	0.1291	1.00	1.00	1.0078
28	C	4.4197	-0.6153	-0.4234	6.00	4.00	12.0000
29	H	3.6487	-1.3816	-0.4655	1.00	1.00	1.0078
30	C	-4.2237	2.9092	0.9340	6.00	4.00	12.0000
31	H	-5.2679	3.1049	1.1726	1.00	1.00	1.0078
32	C	-1.4920	-4.9717	-0.7527	6.00	4.00	12.0000
33	H	0.1199	-7.8061	-0.9903	1.00	1.00	1.0078
34	C	-3.2666	3.9196	1.0612	6.00	4.00	12.0000
35	H	-3.5574	4.9081	1.4140	1.00	1.00	1.0078
36	C	2.1106	2.3521	-0.5097	6.00	4.00	12.0000
37	H	2.8374	3.0936	-0.8272	1.00	1.00	1.0078
38	C	5.7653	-0.9719	-0.4740	6.00	4.00	12.0000
39	H	6.0378	-2.0215	-0.5595	1.00	1.00	1.0078
40	C	6.3671	1.3719	-0.3035	6.00	4.00	12.0000
41	H	7.1441	2.1326	-0.2447	1.00	1.00	1.0078
42	C	6.7494	0.0252	-0.4172	6.00	4.00	12.0000

43	C	0.5611	4.2536	-0.7432	6.00	4.00	12.0000
44	H	-3.6036	-5.4158	-0.9665	1.00	1.00	1.0078
45	H	8.1924	-2.1621	0.2985	1.00	1.00	1.0078
46	O	8.0955	-0.2101	-0.4600	8.00	6.00	15.9949
47	C	8.5281	-1.5676	-0.5645	6.00	4.00	12.0000
48	H	8.1643	-2.0330	-1.4930	1.00	1.00	1.0078
49	H	9.6213	-1.5317	-0.5793	1.00	1.00	1.0078
50	O	-1.2311	-6.3024	-0.9090	8.00	6.00	15.9949
51	C	0.1346	-6.7210	-0.8520	6.00	4.00	12.0000
52	H	0.7265	-6.2541	-1.6533	1.00	1.00	1.0078
53	H	0.5839	-6.4782	0.1226	1.00	1.00	1.0078
54	H	0.5387	-4.2469	-0.5110	1.00	1.00	1.0078

Table S9. Computed geometry optimization parameters of compound **5**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Cu	0.0000	0.0000	0.0000	29.00	11.00	62.9296
2	N	-0.1620	1.9511	0.0000	7.00	5.00	14.0031
3	O	0.0913	-1.9050	-0.1822	8.00	6.00	15.9949
4	H	1.2017	4.3232	-1.6436	1.00	1.00	1.0078
5	O	1.9013	0.0000	0.0000	8.00	6.00	15.9949
6	H	-0.3079	4.2245	-1.2335	1.00	1.00	1.0078
7	N	-1.9372	0.0444	-0.0408	7.00	5.00	14.0031
8	C	2.6330	1.0328	-0.2118	6.00	4.00	12.0000
9	C	-2.4592	1.3426	0.2066	6.00	4.00	12.0000
10	C	-3.2849	-3.2908	-0.5825	6.00	4.00	12.0000
11	H	-4.1773	-3.0338	-0.6441	1.00	1.00	1.0078
12	C	-2.9602	-4.5922	-0.6260	6.00	4.00	12.0000
13	C	-2.7025	-0.9620	-0.2913	6.00	4.00	12.0000
14	H	-3.6112	-0.7899	-0.3792	1.00	1.00	1.0078
15	C	-1.4873	2.3612	0.2418	6.00	4.00	12.0000
16	C	-0.9149	-2.6965	-0.3774	6.00	4.00	12.0000
17	C	5.0578	1.7757	-0.2355	6.00	4.00	12.0000
18	H	4.7874	2.6658	-0.2324	1.00	1.00	1.0078
19	C	-1.8910	3.6384	0.6138	6.00	4.00	12.0000
20	H	-1.2601	4.3184	0.6910	1.00	1.00	1.0078
21	C	-3.7800	1.6419	0.4859	6.00	4.00	12.0000
22	H	-4.4168	0.9638	0.4648	1.00	1.00	1.0078
23	C	-2.2832	-2.3110	-0.4455	6.00	4.00	12.0000
24	C	4.0991	0.7676	-0.2127	6.00	4.00	12.0000
25	C	-0.6829	-4.0922	-0.5038	6.00	4.00	12.0000
26	C	0.8229	2.7390	-0.4155	6.00	4.00	12.0000
27	H	0.7497	4.7668	-0.2103	1.00	1.00	1.0078
28	C	4.5383	-0.5356	-0.1549	6.00	4.00	12.0000
29	H	3.9155	-1.2231	-0.1011	1.00	1.00	1.0078
30	C	-4.1657	2.9215	0.7929	6.00	4.00	12.0000
31	H	-5.0603	3.1181	0.9483	1.00	1.00	1.0078
32	C	-1.6569	-5.0267	-0.6127	6.00	4.00	12.0000
33	H	0.2731	-7.3855	-1.1727	1.00	1.00	1.0078
34	C	-3.2198	3.9073	0.8691	6.00	4.00	12.0000
35	H	-3.4765	4.7717	1.0962	1.00	1.00	1.0078
36	C	2.1564	2.2914	-0.4673	6.00	4.00	12.0000
37	H	2.7915	2.9293	-0.7046	1.00	1.00	1.0078
38	C	5.8827	-0.8416	-0.1753	6.00	4.00	12.0000
39	H	6.1730	-1.7265	-0.1487	1.00	1.00	1.0078
40	C	6.4000	1.4761	-0.2625	6.00	4.00	12.0000
41	H	7.0381	2.1511	-0.2993	1.00	1.00	1.0078
42	C	6.7669	0.1783	-0.2339	6.00	4.00	12.0000
43	C	0.5960	4.1405	-0.9214	6.00	4.00	12.0000

44	H	-3.7678	-5.3077	-0.6730	1.00	1.00	1.0078
45	H	8.4044	-2.0639	-0.5145	1.00	1.00	1.0078
46	O	8.1284	-0.1366	-0.3182	8.00	6.00	15.9949
47	C	8.2794	-1.1829	-1.1087	6.00	4.00	12.0000
48	H	7.4132	-1.2901	-1.7277	1.00	1.00	1.0078
49	H	9.1429	-1.0427	-1.7248	1.00	1.00	1.0078
50	O	-1.3451	-6.3882	-0.7082	8.00	6.00	15.9949
51	C	-0.2916	-6.5339	-1.4901	6.00	4.00	12.0000
52	H	-0.6143	-6.6763	-2.5003	1.00	1.00	1.0078
53	H	0.3202	-5.6581	-1.4312	1.00	1.00	1.0078
54	H	0.3258	-4.4778	-0.5184	1.00	1.00	1.0078

Table S10. Computed geometry optimization parameters of compound **6**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Ni	0.0000	0.0000	0.0000	28.00	10.00	57.9353
2	N	-0.1620	1.9511	0.0000	7.00	5.00	14.0031
3	O	0.0913	-1.9050	-0.1822	8.00	6.00	15.9949
4	H	1.2017	4.3232	-1.6436	1.00	1.00	1.0078
5	O	1.9013	0.0000	0.0000	8.00	6.00	15.9949
6	H	-0.3079	4.2245	-1.2335	1.00	1.00	1.0078
7	N	-1.9372	0.0444	-0.0408	7.00	5.00	14.0031
8	C	2.6330	1.0328	-0.2118	6.00	4.00	12.0000
9	C	-2.4592	1.3426	0.2066	6.00	4.00	12.0000
10	C	-3.2849	-3.2908	-0.5825	6.00	4.00	12.0000
11	H	-4.1773	-3.0338	-0.6441	1.00	1.00	1.0078
12	C	-2.9602	-4.5922	-0.6260	6.00	4.00	12.0000
13	C	-2.7025	-0.9620	-0.2913	6.00	4.00	12.0000
14	H	-3.6112	-0.7899	-0.3792	1.00	1.00	1.0078
15	C	-1.4873	2.3612	0.2418	6.00	4.00	12.0000
16	C	-0.9149	-2.6965	-0.3774	6.00	4.00	12.0000
17	H	3.2810	-1.0753	-0.0127	1.00	1.00	1.0078
18	O	-4.0070	-5.5198	-0.6869	8.00	6.00	15.9949
19	C	-1.8910	3.6384	0.6138	6.00	4.00	12.0000
20	H	-1.2601	4.3184	0.6910	1.00	1.00	1.0078
21	C	-3.7800	1.6419	0.4859	6.00	4.00	12.0000
22	H	-4.4168	0.9638	0.4648	1.00	1.00	1.0078
23	C	-2.2832	-2.3110	-0.4455	6.00	4.00	12.0000
24	H	0.3258	-4.4778	-0.5184	1.00	1.00	1.0078
25	C	-0.6829	-4.0922	-0.5038	6.00	4.00	12.0000
26	C	0.8229	2.7390	-0.4155	6.00	4.00	12.0000
27	H	0.7497	4.7668	-0.2103	1.00	1.00	1.0078
28	C	0.5960	4.1405	-0.9214	6.00	4.00	12.0000
29	H	-5.3810	-4.2977	-0.0179	1.00	1.00	1.0078
30	C	-4.1657	2.9215	0.7929	6.00	4.00	12.0000
31	H	-5.0603	3.1181	0.9483	1.00	1.00	1.0078
32	C	-1.6569	-5.0267	-0.6127	6.00	4.00	12.0000
33	C	-5.1414	-4.8750	-0.8863	6.00	4.00	12.0000
34	C	-3.2198	3.9073	0.8691	6.00	4.00	12.0000
35	H	-3.4765	4.7717	1.0962	1.00	1.00	1.0078
36	C	2.1564	2.2914	-0.4673	6.00	4.00	12.0000
37	H	2.7915	2.9293	-0.7046	1.00	1.00	1.0078
38	H	-5.0385	-4.2245	-1.7297	1.00	1.00	1.0078
39	H	-5.9244	-5.5800	-1.0731	1.00	1.00	1.0078
40	Fe	5.1474	0.2896	1.6091	26.00	8.00	55.9349
41	C	6.3714	0.2824	3.2451	6.00	4.00	12.0000
42	C	6.3576	0.2779	-0.0270	6.00	4.00	12.0000
43	C	5.5325	-0.8722	3.2451	6.00	4.00	12.0000

44	C	5.5325	1.4370	3.2451	6.00	4.00	12.0000
45	C	5.5187	1.4326	-0.0270	6.00	4.00	12.0000
46	C	5.5187	-0.8767	-0.0270	6.00	4.00	12.0000
47	C	4.1751	-0.4312	3.2451	6.00	4.00	12.0000
48	C	4.1751	0.9960	3.2451	6.00	4.00	12.0000
49	C	4.1614	0.9915	-0.0270	6.00	4.00	12.0000
50	C	4.1614	-0.4357	-0.0270	6.00	4.00	12.0000
51	H	7.4595	0.2824	3.2309	1.00	1.00	1.0078
52	H	7.4458	0.2779	-0.0127	1.00	1.00	1.0078
53	H	5.8687	-1.9071	3.2309	1.00	1.00	1.0078
54	H	5.8687	2.4720	3.2309	1.00	1.00	1.0078
55	H	5.8550	2.4675	-0.0127	1.00	1.00	1.0078
56	H	5.8550	-1.9116	-0.0127	1.00	1.00	1.0078
57	H	3.2948	-1.0708	3.2309	1.00	1.00	1.0078
58	H	3.2948	1.6356	3.2309	1.00	1.00	1.0078
59	H	-1.4050	-6.0744	-0.6857	1.00	1.00	1.0078

Table S11. Computed geometry optimization parameters of compound **7**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Cu	-0.0848	-0.0551	0.1005	29.00	11.00	62.9296
2	N	-0.1728	1.9416	0.0369	7.00	5.00	14.0031
3	O	-0.0875	-2.0111	0.0624	8.00	6.00	15.9949
4	H	1.5579	4.3226	-1.5404	1.00	1.00	1.0078
5	O	1.8609	-0.1210	0.2751	8.00	6.00	15.9949
6	H	-0.2149	4.2483	-1.3651	1.00	1.00	1.0078
7	N	-2.0446	0.0705	-0.0324	7.00	5.00	14.0031
8	C	2.6282	0.8684	-0.0133	6.00	4.00	12.0000
9	C	-2.4998	1.3844	0.1550	6.00	4.00	12.0000
10	C	-3.4927	-3.2438	-0.7197	6.00	4.00	12.0000
11	H	-4.4966	-2.8568	-0.8887	1.00	1.00	1.0078
12	C	-3.2337	-4.5947	-0.7874	6.00	4.00	12.0000
13	C	-2.8312	-0.9406	-0.3209	6.00	4.00	12.0000
14	H	-3.8920	-0.7326	-0.5093	1.00	1.00	1.0078
15	C	-1.4838	2.3867	0.2204	6.00	4.00	12.0000
16	C	-1.1098	-2.7698	-0.1881	6.00	4.00	12.0000
17	H	4.0063	-1.6760	0.0899	1.00	1.00	1.0078
18	O	-4.1582	-5.5764	-1.0687	8.00	6.00	15.9949
19	C	-1.8780	3.6978	0.5580	6.00	4.00	12.0000
20	H	-1.1261	4.4633	0.7133	1.00	1.00	1.0078
21	C	-3.8440	1.7321	0.3499	6.00	4.00	12.0000
22	H	-4.6110	0.9604	0.3267	1.00	1.00	1.0078
23	C	-2.4572	-2.3045	-0.4140	6.00	4.00	12.0000
24	H	0.1140	-4.5400	-0.0758	1.00	1.00	1.0078
25	C	-0.8985	-4.1836	-0.2560	6.00	4.00	12.0000
26	C	0.8849	2.6762	-0.3381	6.00	4.00	12.0000
27	H	0.7957	4.8310	-0.0289	1.00	1.00	1.0078
28	C	0.7394	4.1003	-0.8476	6.00	4.00	12.0000
29	H	-5.9176	-4.6348	-0.4341	1.00	1.00	1.0078
30	C	-4.2096	3.0468	0.6227	6.00	4.00	12.0000
31	H	-5.2572	3.2979	0.7812	1.00	1.00	1.0078
32	C	-1.9158	-5.0591	-0.5469	6.00	4.00	12.0000
33	C	-5.4929	-5.1475	-1.3126	6.00	4.00	12.0000
34	C	-3.2187	4.0258	0.7420	6.00	4.00	12.0000
35	H	-3.4875	5.0482	1.0045	1.00	1.00	1.0078
36	C	2.1953	2.1717	-0.3420	6.00	4.00	12.0000
37	H	2.9667	2.8607	-0.6757	1.00	1.00	1.0078
38	H	-5.5464	-4.4746	-2.1839	1.00	1.00	1.0078
39	H	-6.0706	-6.0539	-1.5178	1.00	1.00	1.0078
40	Fe	5.3327	0.3475	1.5837	26.00	8.00	55.9349
41	C	6.5608	0.8583	3.1822	6.00	4.00	12.0000
42	C	6.3911	0.6930	-0.1717	6.00	4.00	12.0000
43	C	6.1805	-0.5215	3.2702	6.00	4.00	12.0000

44	C	5.3650	1.6489	3.2100	6.00	4.00	12.0000
45	C	5.1896	1.4680	-0.1488	6.00	4.00	12.0000
46	C	6.0310	-0.6915	-0.0764	6.00	4.00	12.0000
47	C	4.7500	-0.5829	3.3518	6.00	4.00	12.0000
48	C	4.2487	0.7580	3.3169	6.00	4.00	12.0000
49	C	4.0707	0.5592	-0.0555	6.00	4.00	12.0000
50	C	4.6078	-0.7777	0.0071	6.00	4.00	12.0000
51	H	7.5751	1.2368	3.0993	1.00	1.00	1.0078
52	H	7.4006	1.0875	-0.2335	1.00	1.00	1.0078
53	H	6.8569	-1.3709	3.2645	1.00	1.00	1.0078
54	H	5.3135	2.7319	3.1514	1.00	1.00	1.0078
55	H	5.1361	2.5510	-0.1906	1.00	1.00	1.0078
56	H	6.7222	-1.5284	-0.0559	1.00	1.00	1.0078
57	H	4.1488	-1.4846	3.4118	1.00	1.00	1.0078
58	H	3.2014	1.0447	3.3330	1.00	1.00	1.0078
59	H	-1.7316	-6.1322	-0.5996	1.00	1.00	1.0078

Table S12. Computed geometry optimization parameters of compound **8**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Ni	0.0000	0.0000	0.0000	28.00	10.00	57.9353
2	N	-0.1620	1.9511	0.0000	7.00	5.00	14.0031
3	O	0.0913	-1.9050	-0.1822	8.00	6.00	15.9949
4	H	1.2017	4.3232	-1.6436	1.00	1.00	1.0078
5	O	1.9013	0.0000	0.0000	8.00	6.00	15.9949
6	H	-0.3079	4.2245	-1.2335	1.00	1.00	1.0078
7	N	-1.9372	0.0444	-0.0408	7.00	5.00	14.0031
8	C	2.6330	1.0328	-0.2118	6.00	4.00	12.0000
9	C	-2.4592	1.3426	0.2066	6.00	4.00	12.0000
10	C	-3.2849	-3.2908	-0.5825	6.00	4.00	12.0000
11	H	-4.1773	-3.0338	-0.6441	1.00	1.00	1.0078
12	C	-2.9602	-4.5922	-0.6260	6.00	4.00	12.0000
13	C	-2.7025	-0.9620	-0.2913	6.00	4.00	12.0000
14	H	-3.6112	-0.7899	-0.3792	1.00	1.00	1.0078
15	C	-1.4873	2.3612	0.2418	6.00	4.00	12.0000
16	C	-0.9149	-2.6965	-0.3774	6.00	4.00	12.0000
17	C	5.0578	1.7757	-0.2355	6.00	4.00	12.0000
18	H	4.7874	2.6658	-0.2324	1.00	1.00	1.0078
19	C	-1.8910	3.6384	0.6138	6.00	4.00	12.0000
20	H	-1.2601	4.3184	0.6910	1.00	1.00	1.0078
21	C	-3.7800	1.6419	0.4859	6.00	4.00	12.0000
22	H	-4.4168	0.9638	0.4648	1.00	1.00	1.0078
23	C	-2.2832	-2.3110	-0.4455	6.00	4.00	12.0000
24	C	4.0991	0.7676	-0.2127	6.00	4.00	12.0000
25	C	-0.6829	-4.0922	-0.5038	6.00	4.00	12.0000
26	C	0.8229	2.7390	-0.4155	6.00	4.00	12.0000
27	H	0.7497	4.7668	-0.2103	1.00	1.00	1.0078
28	C	4.5383	-0.5356	-0.1549	6.00	4.00	12.0000
29	H	3.9155	-1.2231	-0.1011	1.00	1.00	1.0078
30	C	-4.1657	2.9215	0.7929	6.00	4.00	12.0000
31	H	-5.0603	3.1181	0.9483	1.00	1.00	1.0078
32	C	-1.6569	-5.0267	-0.6127	6.00	4.00	12.0000
33	F	0.6246	-4.5921	-0.5228	9.00	7.00	18.9984
34	C	-3.2198	3.9073	0.8691	6.00	4.00	12.0000
35	H	-3.4765	4.7717	1.0962	1.00	1.00	1.0078
36	C	2.1564	2.2914	-0.4673	6.00	4.00	12.0000
37	H	2.7915	2.9293	-0.7046	1.00	1.00	1.0078
38	C	5.8827	-0.8416	-0.1753	6.00	4.00	12.0000
39	H	6.1730	-1.7265	-0.1487	1.00	1.00	1.0078
40	C	6.4000	1.4761	-0.2625	6.00	4.00	12.0000
41	H	7.0381	2.1511	-0.2993	1.00	1.00	1.0078
42	C	6.7669	0.1783	-0.2339	6.00	4.00	12.0000
43	C	0.5960	4.1405	-0.9214	6.00	4.00	12.0000

44	F	-4.0594	-5.5661	-0.6900	9.00	7.00	18.9984
45	H	-1.4493	-5.9331	-0.6763	1.00	1.00	1.0078
46	F	8.1284	-0.1366	-0.3182	9.00	7.00	18.9984

Table S13. Computed geometry optimization parameters of compound **9**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Cu	0.0000	0.0000	0.0000	29.00	11.00	62.9296
2	N	-0.1620	1.9511	0.0000	7.00	5.00	14.0031
3	O	0.0913	-1.9050	-0.1822	8.00	6.00	15.9949
4	H	1.2017	4.3232	-1.6436	1.00	1.00	1.0078
5	O	1.9013	0.0000	0.0000	8.00	6.00	15.9949
6	H	-0.3079	4.2245	-1.2335	1.00	1.00	1.0078
7	N	-1.9372	0.0444	-0.0408	7.00	5.00	14.0031
8	C	2.6330	1.0328	-0.2118	6.00	4.00	12.0000
9	C	-2.4592	1.3426	0.2066	6.00	4.00	12.0000
10	C	-3.2849	-3.2908	-0.5825	6.00	4.00	12.0000
11	H	-4.1773	-3.0338	-0.6441	1.00	1.00	1.0078
12	C	-2.9602	-4.5922	-0.6260	6.00	4.00	12.0000
13	C	-2.7025	-0.9620	-0.2913	6.00	4.00	12.0000
14	H	-3.6112	-0.7899	-0.3792	1.00	1.00	1.0078
15	C	-1.4873	2.3612	0.2418	6.00	4.00	12.0000
16	C	-0.9149	-2.6965	-0.3774	6.00	4.00	12.0000
17	C	5.0578	1.7757	-0.2355	6.00	4.00	12.0000
18	H	4.7874	2.6658	-0.2324	1.00	1.00	1.0078
19	C	-1.8910	3.6384	0.6138	6.00	4.00	12.0000
20	H	-1.2601	4.3184	0.6910	1.00	1.00	1.0078
21	C	-3.7800	1.6419	0.4859	6.00	4.00	12.0000
22	H	-4.4168	0.9638	0.4648	1.00	1.00	1.0078
23	C	-2.2832	-2.3110	-0.4455	6.00	4.00	12.0000
24	C	4.0991	0.7676	-0.2127	6.00	4.00	12.0000
25	C	-0.6829	-4.0922	-0.5038	6.00	4.00	12.0000
26	C	0.8229	2.7390	-0.4155	6.00	4.00	12.0000
27	H	0.7497	4.7668	-0.2103	1.00	1.00	1.0078
28	C	4.5383	-0.5356	-0.1549	6.00	4.00	12.0000
29	H	3.9155	-1.2231	-0.1011	1.00	1.00	1.0078
30	C	-4.1657	2.9215	0.7929	6.00	4.00	12.0000
31	H	-5.0603	3.1181	0.9483	1.00	1.00	1.0078
32	C	-1.6569	-5.0267	-0.6127	6.00	4.00	12.0000
33	F	0.6246	-4.5921	-0.5228	9.00	7.00	18.9984
34	C	-3.2198	3.9073	0.8691	6.00	4.00	12.0000
35	H	-3.4765	4.7717	1.0962	1.00	1.00	1.0078
36	C	2.1564	2.2914	-0.4673	6.00	4.00	12.0000
37	H	2.7915	2.9293	-0.7046	1.00	1.00	1.0078
38	C	5.8827	-0.8416	-0.1753	6.00	4.00	12.0000
39	H	6.1730	-1.7265	-0.1487	1.00	1.00	1.0078
40	C	6.4000	1.4761	-0.2625	6.00	4.00	12.0000
41	H	7.0381	2.1511	-0.2993	1.00	1.00	1.0078
42	C	6.7669	0.1783	-0.2339	6.00	4.00	12.0000
43	C	0.5960	4.1405	-0.9214	6.00	4.00	12.0000

44	F	-4.0594	-5.5661	-0.6900	9.00	7.00	18.9984
45	H	-1.4493	-5.9331	-0.6763	1.00	1.00	1.0078
46	F	8.1284	-0.1366	-0.3182	9.00	7.00	18.9984

Table S14. Computed geometry optimization parameters of compound **10**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Ni	-0.0718	0.0949	-0.0380	28.00	10.00	57.9353
2	N	-0.1942	1.9874	-0.0589	7.00	5.00	14.0031
3	O	0.0813	-1.7790	-0.1172	8.00	6.00	15.9949
4	H	1.3520	4.4664	-1.6625	1.00	1.00	1.0078
5	O	1.8002	0.0334	-0.0074	8.00	6.00	15.9949
6	H	-0.3978	4.3546	-1.3517	1.00	1.00	1.0078
7	N	-1.9431	0.1089	-0.0101	7.00	5.00	14.0031
8	C	2.5832	1.0201	-0.2648	6.00	4.00	12.0000
9	C	-2.4711	1.3975	0.2341	6.00	4.00	12.0000
10	C	-3.2386	-3.2928	-0.5021	6.00	4.00	12.0000
11	H	-4.2968	-3.0443	-0.5582	1.00	1.00	1.0078
12	C	-2.8586	-4.6161	-0.5998	6.00	4.00	12.0000
13	C	-2.7115	-0.9409	-0.1795	6.00	4.00	12.0000
14	H	-3.7935	-0.7890	-0.1972	1.00	1.00	1.0078
15	C	-1.4951	2.4220	0.2452	6.00	4.00	12.0000
16	C	-0.8724	-2.6378	-0.2569	6.00	4.00	12.0000
17	C	5.0314	1.6798	-0.1942	6.00	4.00	12.0000
18	H	4.7588	2.7306	-0.1192	1.00	1.00	1.0078
19	C	-1.8919	3.7142	0.6369	6.00	4.00	12.0000
20	H	-1.1570	4.5008	0.7614	1.00	1.00	1.0078
21	C	-3.8110	1.6833	0.5165	6.00	4.00	12.0000
22	H	-4.5577	0.8925	0.5234	1.00	1.00	1.0078
23	C	-2.2703	-2.2823	-0.3270	6.00	4.00	12.0000
24	C	4.0334	0.6919	-0.2594	6.00	4.00	12.0000
25	C	-0.5348	-4.0247	-0.3477	6.00	4.00	12.0000
26	C	0.8153	2.7743	-0.4716	6.00	4.00	12.0000
27	H	0.7090	4.9143	-0.0797	1.00	1.00	1.0078
28	C	4.4224	-0.6590	-0.3075	6.00	4.00	12.0000
29	H	3.6478	-1.4216	-0.3475	1.00	1.00	1.0078
30	C	-4.1939	2.9816	0.8422	6.00	4.00	12.0000
31	H	-5.2351	3.1966	1.0750	1.00	1.00	1.0078
32	C	-1.4976	-4.9888	-0.5197	6.00	4.00	12.0000
33	H	0.5196	-4.2865	-0.2836	1.00	1.00	1.0078
34	C	-3.2278	3.9888	0.9198	6.00	4.00	12.0000
35	H	-3.5109	4.9943	1.2272	1.00	1.00	1.0078
36	C	2.1352	2.3151	-0.5689	6.00	4.00	12.0000
37	H	2.8688	3.0333	-0.9214	1.00	1.00	1.0078
38	C	5.7667	-1.0182	-0.3087	6.00	4.00	12.0000
39	H	6.0819	-2.0590	-0.3530	1.00	1.00	1.0078
40	C	6.3810	1.3367	-0.1914	6.00	4.00	12.0000
41	H	7.1635	2.0906	-0.1335	1.00	1.00	1.0078
42	C	6.7222	-0.0097	-0.2529	6.00	4.00	12.0000
43	C	0.5951	4.2084	-0.9141	6.00	4.00	12.0000

44	O	-5.0662	-5.2832	-0.8399	8.00	6.00	15.9949
45	H	-1.2401	-6.0423	-0.5967	1.00	1.00	1.0078
46	F	8.0374	-0.3506	-0.2526	9.00	7.00	18.9984
47	N	-3.8794	-5.6432	-0.7787	7.00	5.00	14.0031
48	O	-3.5012	-6.8224	-0.8585	8.00	6.00	15.9949

Table S15. Computed geometry optimization parameters of compound **11**

ATOMS	X	Y	Z	CHARGE	
	(Angstrom)			Nucl + Core	At.Mass

1	Cu	0.0000	0.0000	0.0000	29.00	11.00	62.9296
2	N	-0.1620	1.9511	0.0000	7.00	5.00	14.0031
3	O	0.0913	-1.9050	-0.1822	8.00	6.00	15.9949
4	H	1.2017	4.3232	-1.6436	1.00	1.00	1.0078
5	O	1.9013	0.0000	0.0000	8.00	6.00	15.9949
6	H	-0.3079	4.2245	-1.2335	1.00	1.00	1.0078
7	N	-1.9372	0.0444	-0.0408	7.00	5.00	14.0031
8	C	2.6330	1.0328	-0.2118	6.00	4.00	12.0000
9	C	-2.4592	1.3426	0.2066	6.00	4.00	12.0000
10	C	-3.2849	-3.2908	-0.5825	6.00	4.00	12.0000
11	H	-4.1773	-3.0338	-0.6441	1.00	1.00	1.0078
12	C	-2.9602	-4.5922	-0.6260	6.00	4.00	12.0000
13	C	-2.7025	-0.9620	-0.2913	6.00	4.00	12.0000
14	H	-3.6112	-0.7899	-0.3792	1.00	1.00	1.0078
15	C	-1.4873	2.3612	0.2418	6.00	4.00	12.0000
16	C	-0.9149	-2.6965	-0.3774	6.00	4.00	12.0000
17	C	5.0578	1.7757	-0.2355	6.00	4.00	12.0000
18	H	4.7874	2.6658	-0.2324	1.00	1.00	1.0078
19	C	-1.8910	3.6384	0.6138	6.00	4.00	12.0000
20	H	-1.2601	4.3184	0.6910	1.00	1.00	1.0078
21	C	-3.7800	1.6419	0.4859	6.00	4.00	12.0000
22	H	-4.4168	0.9638	0.4648	1.00	1.00	1.0078
23	C	-2.2832	-2.3110	-0.4455	6.00	4.00	12.0000
24	C	4.0991	0.7676	-0.2127	6.00	4.00	12.0000
25	C	-0.6829	-4.0922	-0.5038	6.00	4.00	12.0000
26	C	0.8229	2.7390	-0.4155	6.00	4.00	12.0000
27	H	0.7497	4.7668	-0.2103	1.00	1.00	1.0078
28	C	4.5383	-0.5356	-0.1549	6.00	4.00	12.0000
29	H	3.9155	-1.2231	-0.1011	1.00	1.00	1.0078
30	C	-4.1657	2.9215	0.7929	6.00	4.00	12.0000
31	H	-5.0603	3.1181	0.9483	1.00	1.00	1.0078
32	C	-1.6569	-5.0267	-0.6127	6.00	4.00	12.0000
33	H	0.3258	-4.4778	-0.5184	1.00	1.00	1.0078
34	C	-3.2198	3.9073	0.8691	6.00	4.00	12.0000
35	H	-3.4765	4.7717	1.0962	1.00	1.00	1.0078
36	C	2.1564	2.2914	-0.4673	6.00	4.00	12.0000
37	H	2.7915	2.9293	-0.7046	1.00	1.00	1.0078
38	C	5.8827	-0.8416	-0.1753	6.00	4.00	12.0000
39	H	6.1730	-1.7265	-0.1487	1.00	1.00	1.0078
40	C	6.4000	1.4761	-0.2625	6.00	4.00	12.0000
41	H	7.0381	2.1511	-0.2993	1.00	1.00	1.0078
42	C	6.7669	0.1783	-0.2339	6.00	4.00	12.0000
43	C	0.5960	4.1405	-0.9214	6.00	4.00	12.0000

44	O	-5.0329	-5.3416	-0.6469	8.00	6.00	15.9949
45	H	-1.4493	-5.9331	-0.6763	1.00	1.00	1.0078
46	F	8.1284	-0.1366	-0.3182	9.00	7.00	18.9984
47	N	-4.0594	-5.5661	-0.6900	7.00	5.00	14.0031
48	O	-3.9493	-6.5557	-0.7833	8.00	6.00	15.9949
