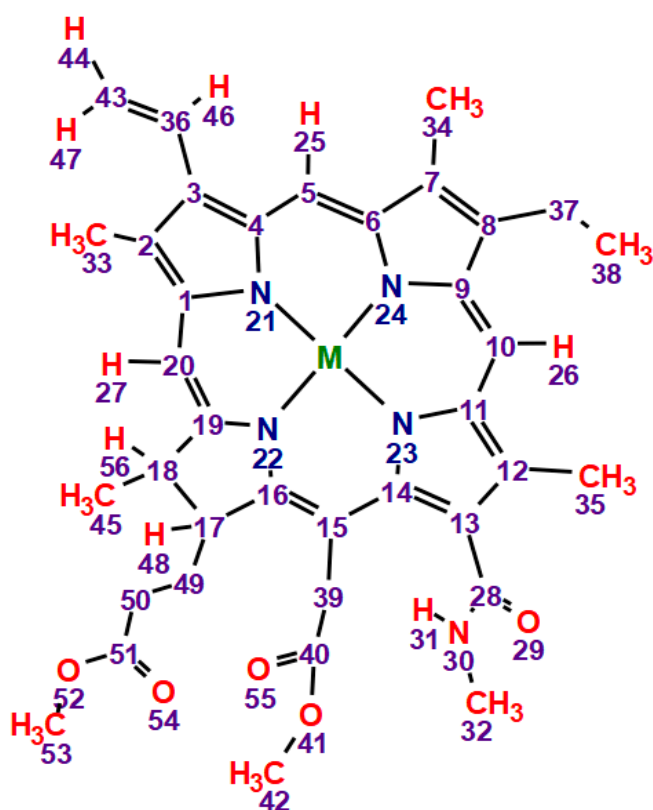


for

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Atom designations M-MADMECl for NMR spectra

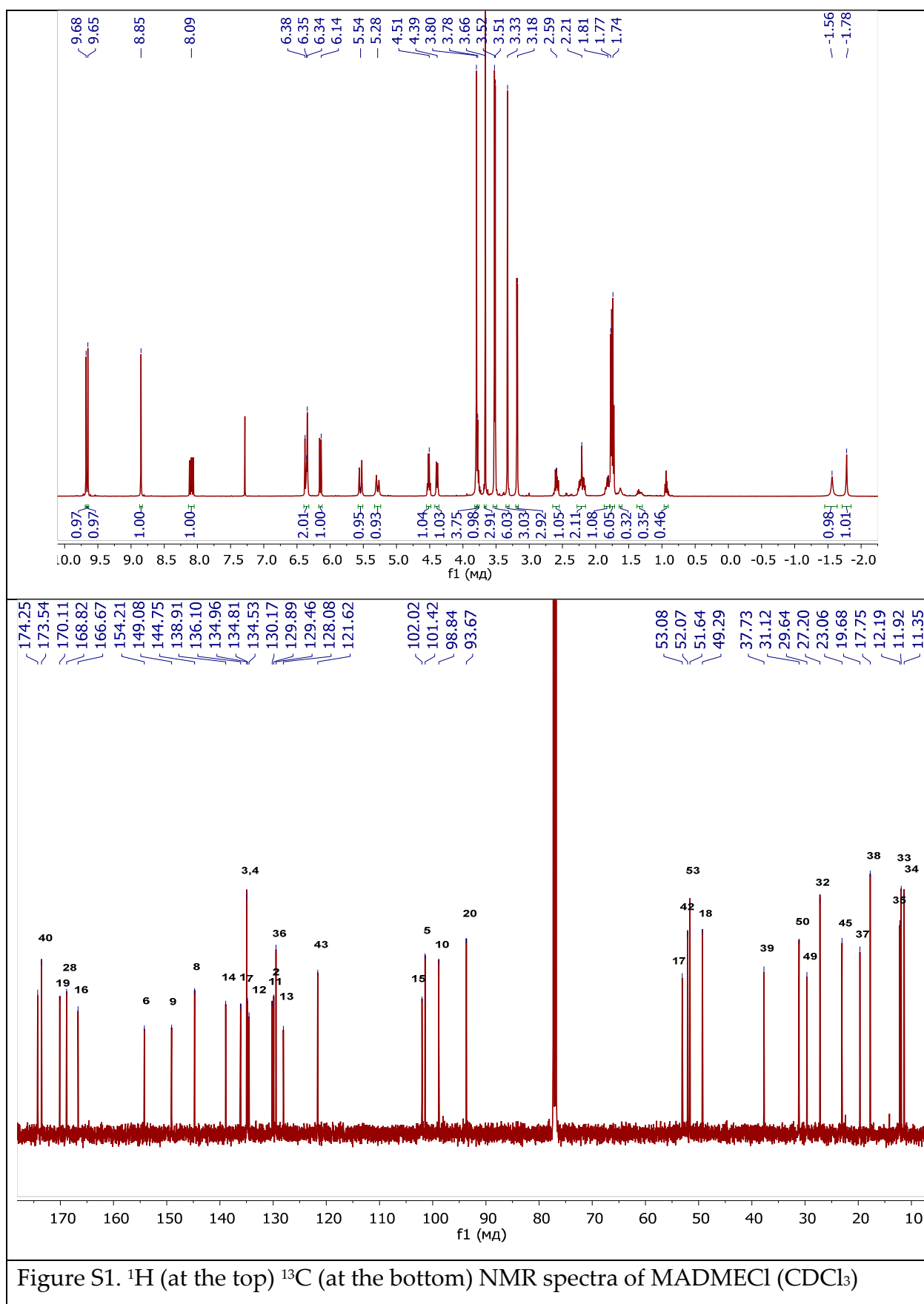


Figure S1. ¹H (at the top) ¹³C (at the bottom) NMR spectra of MADMECl (CDCl₃)

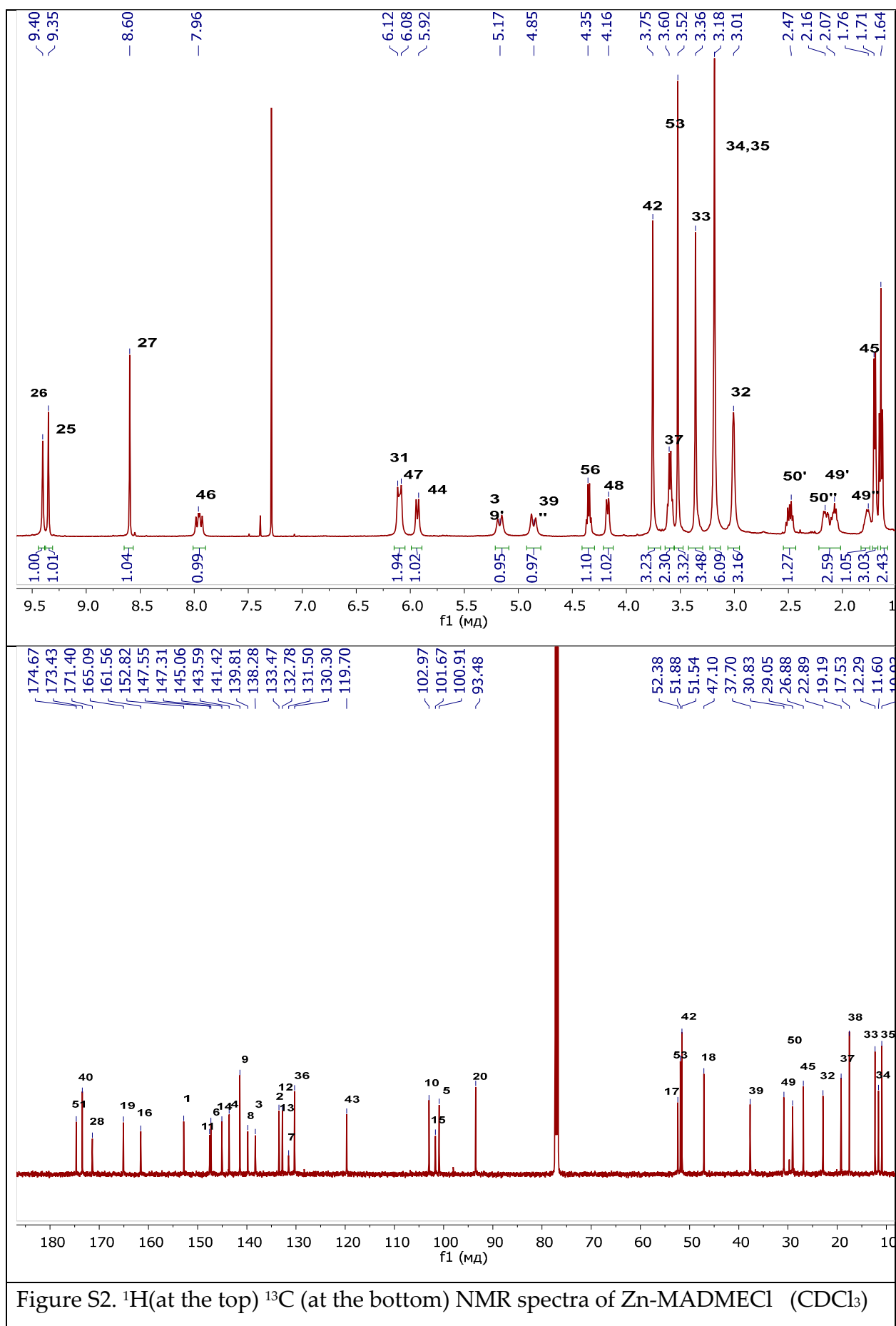


Figure S2. ¹H(at the top) ¹³C (at the bottom) NMR spectra of Zn-MADMECl (CDCl₃)

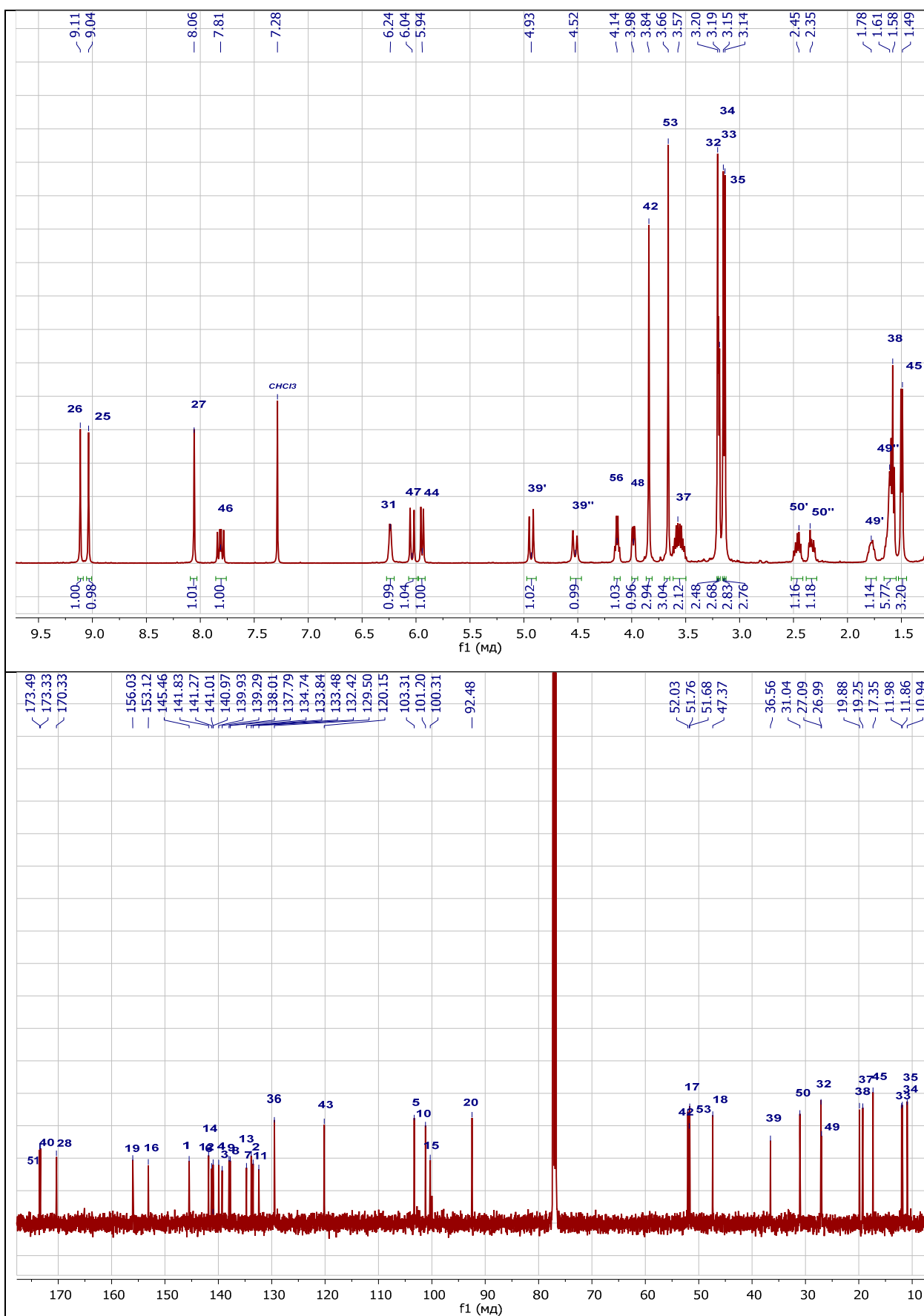


Figure S3. ¹H(at the top) ¹³C (at the bottom) NMR spectra of Ni-MADMECl (CDCl₃)

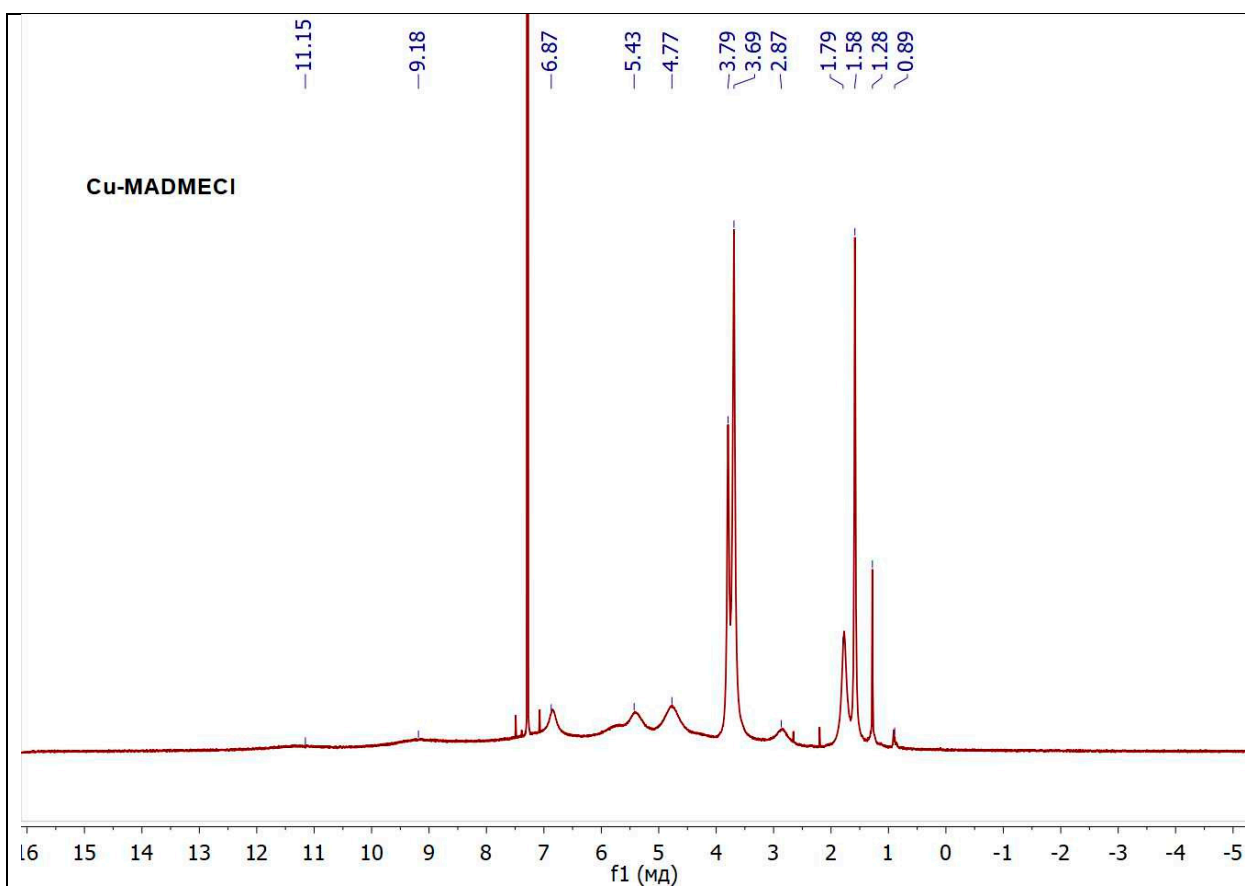


Figure S4. ^1H NMR spectra of Cu-MADMECl (CDCl_3)

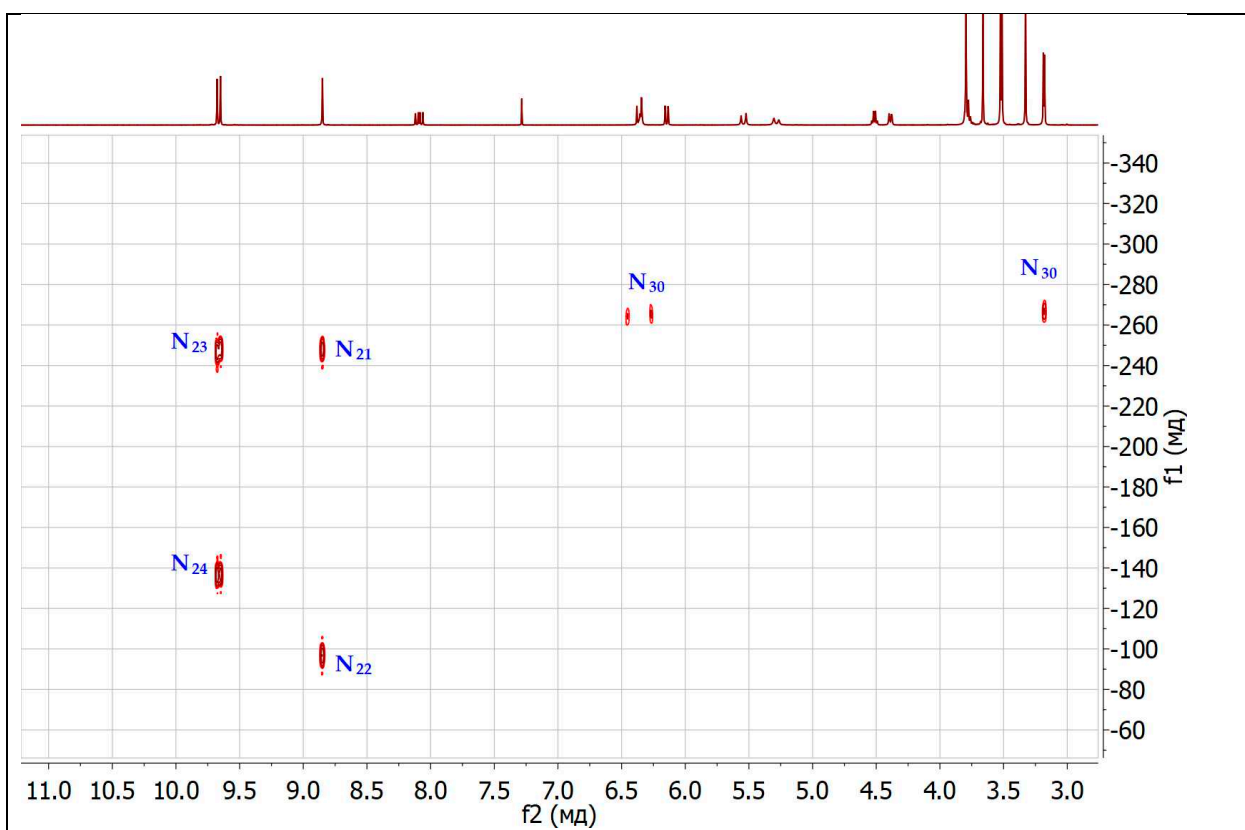


Figure S5. HMBC (^{15}N - ^1H) NMR spectra of MADMECl (CDCl_3)

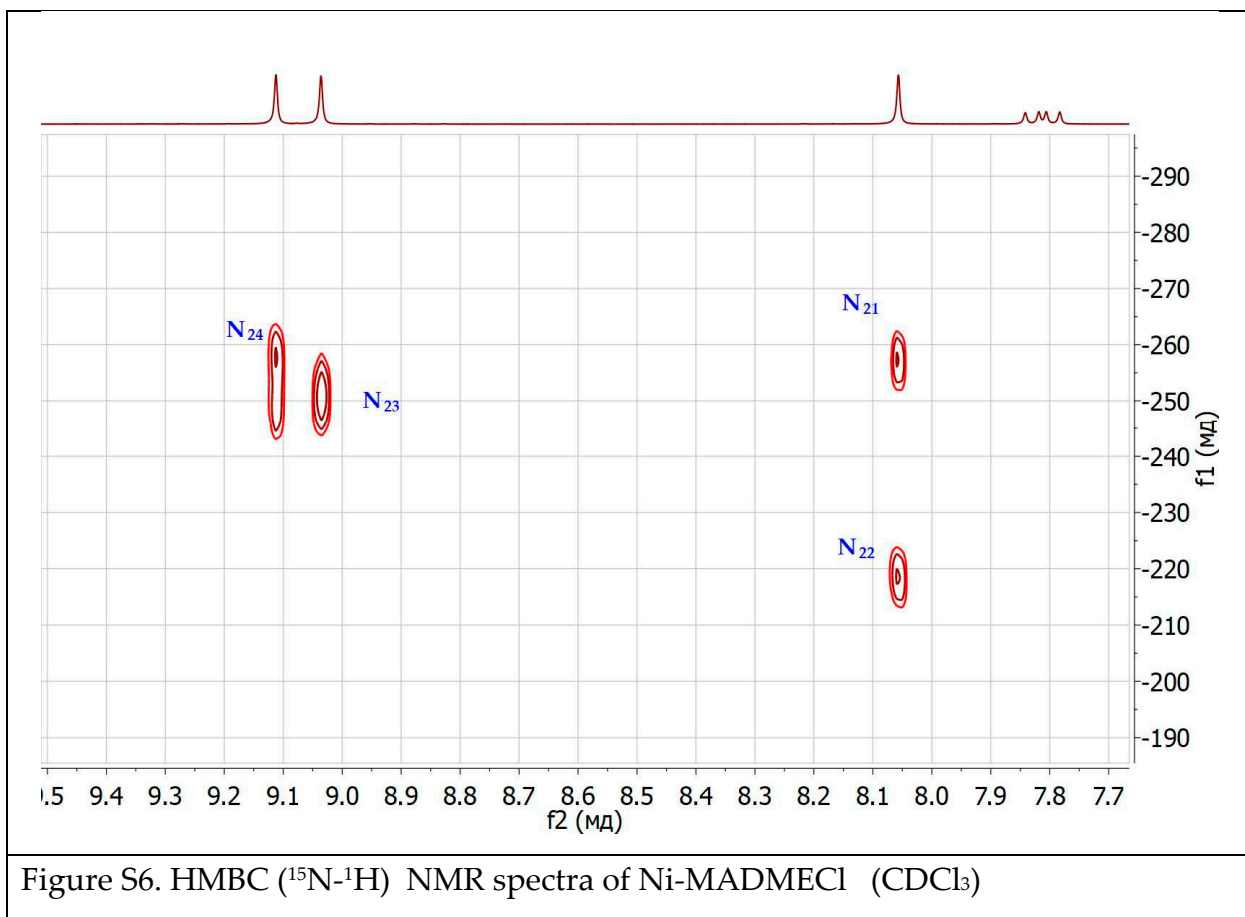


Figure S6. HMBC (^{15}N - ^1H) NMR spectra of Ni-MADMECl (CDCl_3)

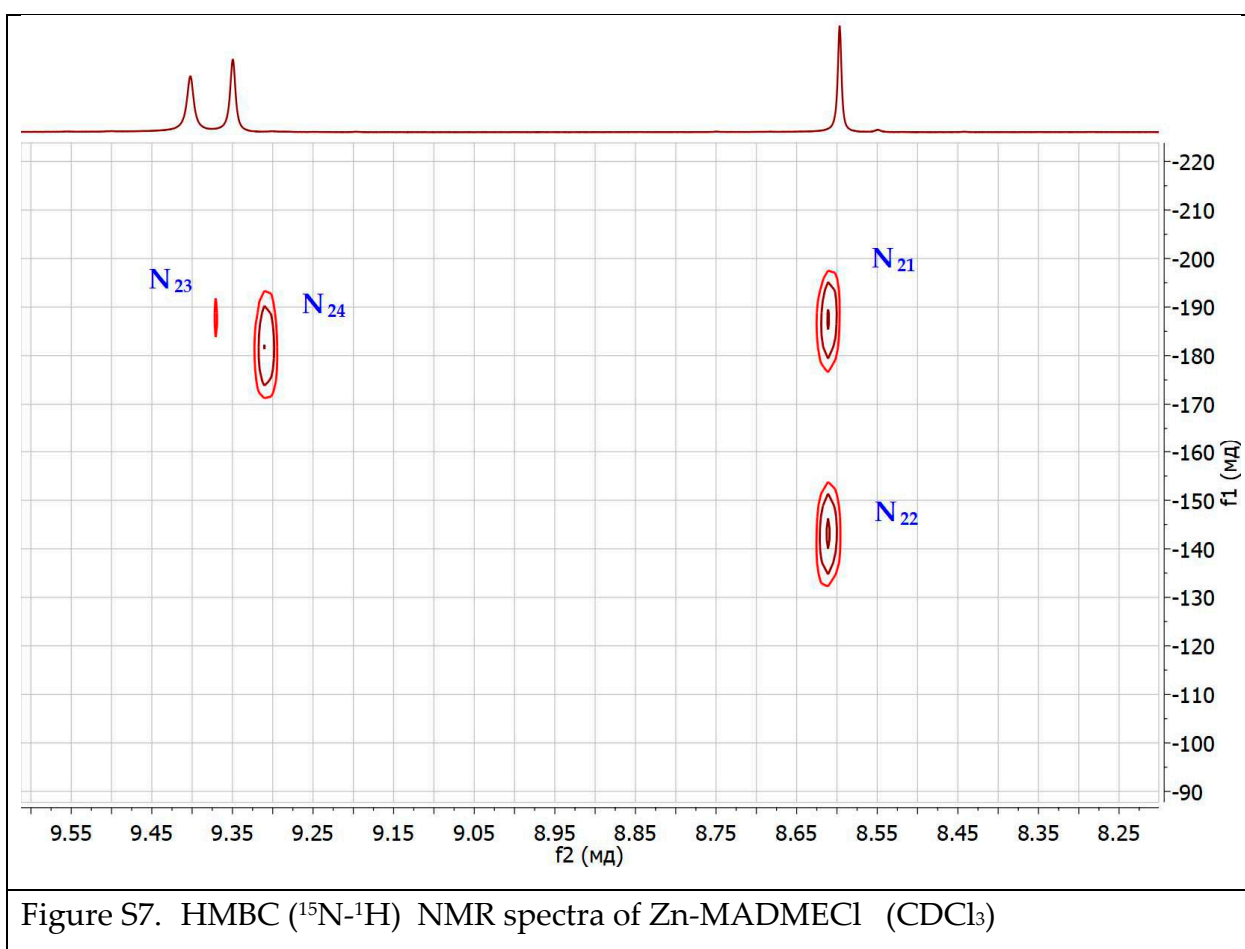


Figure S7. HMBC (^{15}N - ^1H) NMR spectra of Zn-MADMECl (CDCl_3)

Table S1. Experimental (CDCl₃) and calculated (DFT GIAO) chemical shifts of ¹³C

M=	H ₂		Zn		Ni	
No ¹³ C	CDCl ₃	GIAO	CDCl ₃	GIAO	CDCl ₃	GIAO
10	98.70	99.197	102.97	109.549	101.20	110.169
5	101.46	107.867	100.91	102.940	103.31	101.632
20	93.67	88.983	93.48	89.507	92.48	88.153
36	129.46	131.928	130.28	132.962	129.51	132.230
43	121.50	124.192	119.7	121.836	120.15	122.055
39	37.73	33.950	37.7	34.169	36.48	41.974
18	49.29	46.774	47.1	43.451	47.37	53.712
17	53.08	49.087	52.38	55.696	51.76	56.747
42	52.07	46.525	51.54	46.435	52.03	55.435
37	19.67	23.922	19.19	23.556	19.25	23.539
53	51.64	54.401	51.88	54.408	51.68	54.382
33	11.89	15.362	12.29	14.935	11.98	15.093
35	12.19	12.926	10.93	12.840	10.94	12.734
34	11.35	12.611	11.9	12.208	11.86	12.490
32	27.16	29.014	26.88	25.216	27.09	29.882
50	31.12	36.306	29.05	35.957	31.08	35.665
49	29.64	31.934	30.83	30.838	26.99	28.561
45	23.04	25.439	22.89	28.256	17.35	21.716
38	17.75	22.176	17.53	21.702	19.88	21.354
51	174.25	177.631	174.67	177.604	173.49	177.594
40	173.54	182.356	173.43	182.718	173.33	180.399
19	170.11	175.389	165.09	170.930	156.03	165.464
28	168.82	170.202	171.4	170.638	170.33	170.072
16	166.67	172.195	161.56	168.510	153.12	163.875
6	154.21	154.772	147.31	147.199	141.83	145.567
9	149.08	146.050	141.42	141.286	138.01	138.876
8	144.75	147.617	139.81	143.380	137.79	145.464
14	138.91	138.093	145.06	153.477	140.97	149.112
1	136.10	143.848	152.82	158.986	145.46	155.607
3	134.96	138.211	138.28	142.171	139.29	144.039
4	134.96	134.741	143.59	144.984	139.93	141.351
7	134.81	135.880	131.5	133.108	134.74	134.418
12	134.53	143.481	141.42	149.158	141.27	149.991
11	130.17	127.252	147.55	140.714	132.42	135.923
2	129.89	132.195	133.47	133.590	133.46	136.550
13	128.08	126.198	132.78	130.440	133.84	131.744
15	102.02	99.820	101.67	99.983	100.29	97.850
MAE	1.684		1.801		3.61	
R ²	0.9961		0.9957		0.996	

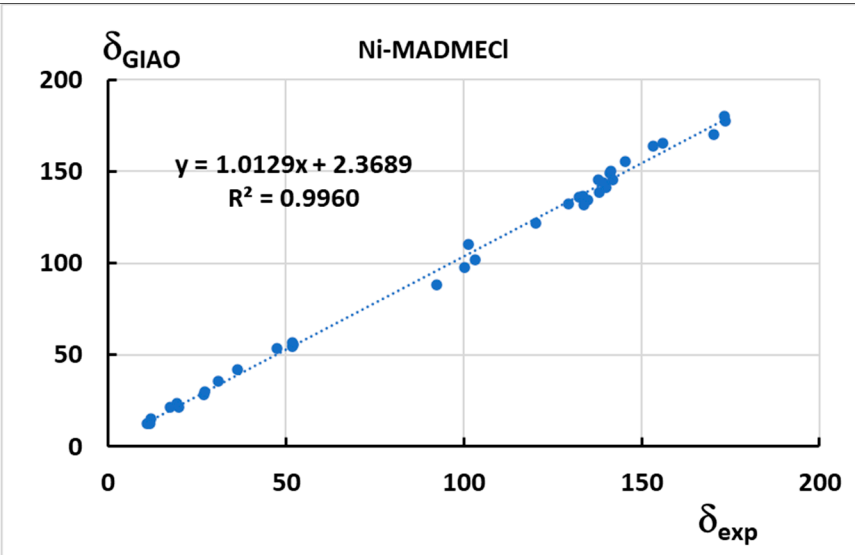
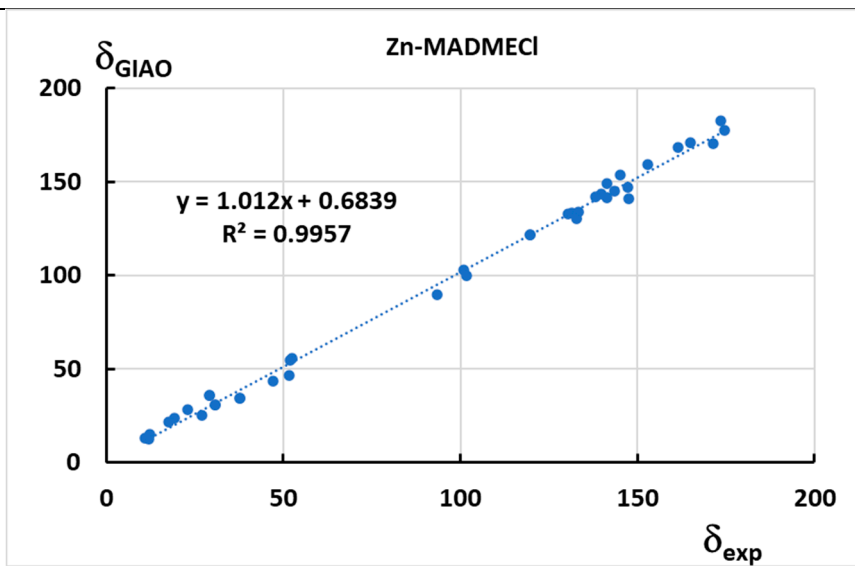
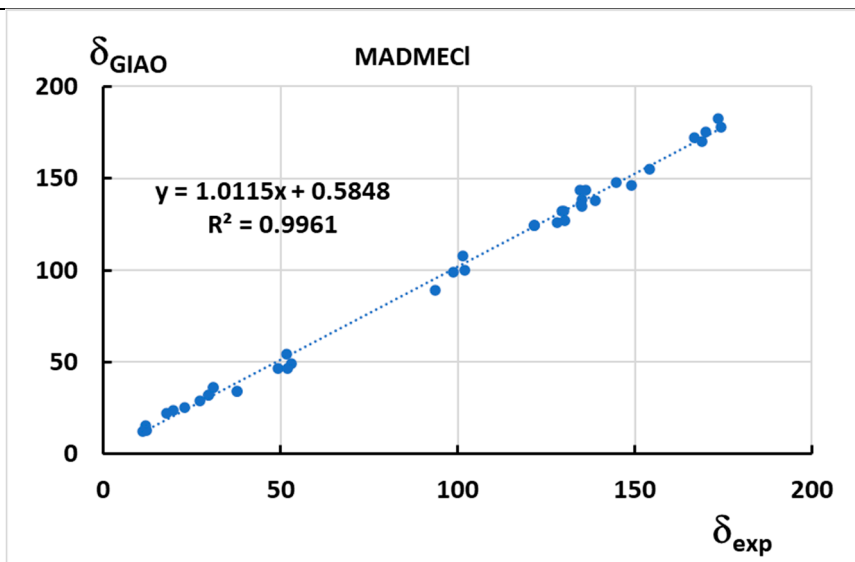


Figure S8. Correlations of calculated and experimental chemical shifts of ^{13}C

Table S2. Experimental (CDCl₃) and calculated (DFT GIAO) chemical shifts of ¹H

M=	NH2		Zn		Ni	
No ¹ H	CDCl3	GIAO	CDCl3	GIAO	CDCl3	GIAO
26	9.65	10.100	9.35	10.209	9.11	9.479
25	9.68	10.574	9.4	9.916	9.04	9.227
27	8.85	9.157	8.6	8.800	8.06	8.014
46	8.09	8.925	7.96	8.794	7.81	8.508
47	6.38	6.758	6.08	6.539	6.04	6.332
31	6.35	7.296	6.12	6.569	6.24	5.871
44	6.14	6.764	5.92	6.591	5.94	6.280
39'	5.54	5.229	5.17	5.022	4.93	4.642
39''	5.28	4.851	4.85	4.536	4.52	3.701
56	4.51	4.652	4.35	4.405	4.14	3.961
48	4.39	3.908	4.16	3.590	3.98	3.642
42	3.8	4.257	3.75	4.230	3.84	4.118
37	3.78	3.989	3.60	3.938	3.57	3.600
53	3.66	3.769	3.52	3.748	3.66	3.635
33	3.52	3.682	3.36	3.440	3.15	3.169
35	3.51	3.996	3.18	3.756	3.14	3.403
34	3.33	3.569	3.18	3.534	3.2	3.166
32	3.18	2.697	3.01	3.121	3.19	3.090
50'	2.59	3.161	2.47	3.083	2.45	2.818
50''	2.24	1.866	2.16	1.739	2.35	2.308
49'	2.21	3.020	2.07	2.888	1.78	1.546
49''	1.81	1.375	1.76	1.436	1.61	0.940
45	1.77	1.846	1.71	1.853	1.49	1.914
38	1.74	1.990	1.64	1.780	1.58	1.663
21	-1.56	-2.437				
23	-1.78	-2.639				
MAE		0.152		0.230		0.009
R ²		0.984		0.975		0.9806

Table S3. Experimental (CDCl₃) and calculated (DFT GIAO) chemical shifts of ¹⁵N

M=	NH2		Zn		Ni	
No ¹⁵ N	CDCl3	GIAO	CDCl3	GIAO	CDCl3	GIAO
24	-136.52	-149.195	-181.8	-194.282	-245.9	-239.09
21	-246.62	-273.603	-187.42	-211.27	-257.81	-257.76
22	-96.74	-127.499	-143.42	-175.76	-218.4	-222.36
23	-247.74	-268.111	-187.77	-203.35	-250.32	-244.74
30	-266.71	-289.51				

0.65% Cu-MADMECl at 72 °C	1.35% Cu-MADMECl at 71 °C	1.96% Cu-MADMECl at 70 °C
0.65% Cu-MADMECl at 25 °C	1.35% Cu-MADMECl at 25 °C	1.96% Cu-MADMECl at 25 °C
0,48% Zn-MADMECl at 70 °C	1,42% Zn-MADMECl at 68 °C	3,36% Zn-MADMECl at 71 °C
0,48% Zn-MADMECl at 25 °C	1,42% Zn-MADMECl at 25 °C	3,36% Zn-MADMECl at 25 °C
0,32% Ni-MADMECl at 71 °C	1,04% Ni-MADMECl at 71 °C	1,54% Ni-MADMECl at 70 °C
0,32% Ni-MADMECl at 25 °C	1,04% Ni-MADMECl at 25 °C	1,54% Ni-MADMECl at 25 °C
0,62% MADMECl at 69 °C	0,855% MADMECl at 70 °C	2,104% MADMECl at 68 °C
0,62% MADMECl at 25 °C	0,855% MADMECl at 25 °C	2,104% MADMECl at 25 °C

Fig S9 The "fingerprints" textures and the systems of Newton's rings of the mixture CB-2 with M-MADMECl

Cartesian coordinates of MADMECl optimized CAM-B3LYP/6-31g(d,p) level of theory:

N	-3.375768000000	0.658072000000	0.183966000000
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C	0.790639000000	2.046754000000	-0.017717000000
C	1.801365000000	1.047991000000	-0.124321000000
C	1.547761000000	-0.296314000000	-0.339460000000
C	-0.371880000000	3.975047000000	0.357676000000
C	2.650545000000	-1.353812000000	-0.363011000000
C	0.513139000000	-2.129897000000	-0.960215000000
C	-1.274644000000	2.877591000000	0.347907000000
C	-2.645070000000	2.955081000000	0.558474000000
C	-3.862686000000	-2.192188000000	-0.506082000000
C	-4.030479000000	-3.578380000000	-0.879008000000
C	-2.790689000000	-4.071803000000	-1.208991000000
C	-1.833991000000	-3.005952000000	-1.021232000000
C	-4.813766000000	-1.288371000000	-0.106278000000
C	-4.583718000000	0.062352000000	0.217509000000
C	-5.638187000000	0.992286000000	0.594878000000
C	-3.609539000000	1.958988000000	0.511537000000
C	-5.025288000000	2.193733000000	0.775944000000
C	-0.459109000000	-3.094160000000	-1.200315000000
N	0.328791000000	-0.868529000000	-0.550352000000
N	-0.530480000000	1.747740000000	0.105350000000
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H	6.863251000000	-5.150361000000	3.600134000000
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H	3.346116000000	2.447987000000	0.469543000000
H	3.751574000000	0.792100000000	0.774903000000
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O	5.320092000000	1.003019000000	-1.000083000000
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H	6.281136000000	2.009252000000	-2.548185000000
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H	2.217236000000	-3.454091000000	-0.819243000000
H	3.564104000000	-0.999142000000	-0.847234000000
H	3.553852000000	6.067233000000	-1.933269000000
H	-6.179427000000	-3.612814000000	-1.151353000000
H	-4.761895000000	-6.219411000000	-0.377016000000

Cartesian coordinates of Zn-MADMECl optimized CAM-B3LYP/6-31g(d,p) level of theory:

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C	0.829619000000	2.031362000000	-0.023000000000
C	1.868241000000	1.052598000000	-0.099379000000
C	1.648032000000	-0.287537000000	-0.319130000000
C	-0.244579000000	3.996251000000	0.354202000000

C	2.756482000000	-1.333950000000	-0.334515000000
C	0.660452000000	-2.151464000000	-1.019125000000
C	-1.159321000000	2.892138000000	0.357938000000
C	-2.507721000000	3.012822000000	0.619626000000
C	-3.626101000000	-2.138994000000	-0.539068000000
C	-3.857323000000	-3.513181000000	-0.952107000000
C	-2.640663000000	-4.021870000000	-1.313217000000
C	-1.676907000000	-2.961689000000	-1.095487000000
C	-4.590652000000	-1.274479000000	-0.089971000000
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C	-5.458364000000	0.958113000000	0.684869000000
C	-3.473841000000	2.009573000000	0.600084000000
C	-4.872058000000	2.184152000000	0.880792000000
C	-0.295315000000	-3.096759000000	-1.290846000000
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C	4.539982000000	-3.250464000000	2.549080000000
O	3.906063000000	-2.965974000000	3.535907000000
C	2.166458000000	4.351542000000	-0.185818000000
O	2.516870000000	5.237792000000	0.586944000000
N	2.773082000000	4.162650000000	-1.383931000000
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C	-5.517985000000	3.458152000000	1.336027000000

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C	-5.395835000000	3.688294000000	2.846948000000
H	-4.347055000000	3.727428000000	3.153031000000
H	-5.872775000000	4.627099000000	3.142348000000
H	-5.869892000000	2.875335000000	3.403301000000
O	5.599037000000	-4.078394000000	2.565134000000
C	5.937612000000	-4.605927000000	3.849388000000
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C	3.308267000000	1.461905000000	0.137043000000
H	3.380109000000	2.467099000000	0.555011000000
H	3.780064000000	0.820056000000	0.883313000000
C	4.179323000000	1.427783000000	-1.100579000000
O	3.810673000000	1.589720000000	-2.242839000000
O	5.461818000000	1.194568000000	-0.780729000000
C	6.381585000000	1.201660000000	-1.875392000000
H	7.352920000000	0.958344000000	-1.448610000000
H	6.092632000000	0.462556000000	-2.624496000000
H	6.409546000000	2.186291000000	-2.346249000000
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H	-6.010199000000	-3.497024000000	-1.221047000000
H	-4.645278000000	-6.138581000000	-0.475834000000
Zn	-1.404063000000	-0.068736000000	-0.194010000000

Cartesian coordinates of Cu-MADMECl optimized CAM-B3LYP/6-31g(d,p) level of theory:

N	-3.122408000000	0.824826000000	0.254650000000
N	-2.320643000000	-1.682388000000	-0.715125000000
C	1.123823000000	3.411446000000	0.035018000000
C	0.895462000000	1.984141000000	-0.022475000000
C	1.896111000000	0.968897000000	-0.023520000000
C	1.608190000000	-0.340358000000	-0.293506000000
C	-0.092935000000	4.006843000000	0.230577000000
C	2.650910000000	-1.445194000000	-0.329787000000
C	0.559042000000	-2.073758000000	-1.181886000000
C	-1.053929000000	2.947153000000	0.243130000000
C	-2.388276000000	3.127976000000	0.518023000000
C	-3.658454000000	-1.975299000000	-0.527398000000
C	-3.949729000000	-3.314671000000	-1.007205000000
C	-2.778740000000	-3.810798000000	-1.501887000000
C	-1.780341000000	-2.785227000000	-1.279988000000
C	-4.573567000000	-1.125446000000	0.022998000000
C	-4.326619000000	0.203783000000	0.382487000000
C	-5.336866000000	1.117137000000	0.830222000000
C	-3.355431000000	2.136216000000	0.575264000000

C	-4.728053000000	2.340437000000	0.939213000000
C	-0.420430000000	-2.957903000000	-1.541849000000
N	0.375954000000	-0.850346000000	-0.625609000000
N	-0.432424000000	1.725298000000	0.048553000000
C	2.026914000000	-2.385297000000	-1.367031000000
H	-5.585008000000	-1.490169000000	0.155939000000
H	-2.707584000000	4.142416000000	0.728674000000
H	-0.105920000000	-3.894936000000	-1.984770000000
C	2.808025000000	-2.097148000000	1.054360000000
H	2.976541000000	-1.333001000000	1.818170000000
H	1.870979000000	-2.588634000000	1.335189000000
C	3.952363000000	-3.101804000000	1.106021000000
H	4.904706000000	-2.627691000000	0.839522000000
H	3.819658000000	-3.916904000000	0.387505000000
C	4.119482000000	-3.716564000000	2.473854000000
O	3.498396000000	-3.409783000000	3.462145000000
C	2.366839000000	4.198848000000	-0.198491000000
O	2.749205000000	5.087135000000	0.555115000000
N	3.021933000000	3.923367000000	-1.355485000000
H	2.697331000000	3.176567000000	-1.950020000000
C	4.230287000000	4.639275000000	-1.703088000000
H	4.586871000000	4.275690000000	-2.667171000000
C	-2.521970000000	-5.119641000000	-2.173751000000
H	-1.816818000000	-5.008802000000	-3.001834000000
H	-2.100616000000	-5.860581000000	-1.484722000000
H	-3.449599000000	-5.534299000000	-2.573296000000
C	-6.765763000000	0.760955000000	1.094266000000
H	-7.248808000000	0.335066000000	0.208700000000
H	-6.857221000000	0.024627000000	1.899405000000
H	-7.342663000000	1.639285000000	1.389805000000
C	2.493149000000	-2.076926000000	-2.793850000000
H	1.918648000000	-2.648694000000	-3.526877000000
H	2.380041000000	-1.012556000000	-3.015684000000
H	3.550572000000	-2.329420000000	-2.913544000000
C	-0.392374000000	5.464500000000	0.365687000000
H	0.532567000000	6.035983000000	0.432719000000
H	-0.979417000000	5.832862000000	-0.481822000000
H	-0.971497000000	5.661609000000	1.272929000000
C	-5.275187000000	-3.928401000000	-0.976769000000
C	-5.327071000000	3.639323000000	1.388045000000
H	-4.917498000000	4.463064000000	0.793289000000
H	-6.401786000000	3.632722000000	1.181350000000
C	-5.099899000000	3.925771000000	2.877024000000
H	-4.032446000000	3.964913000000	3.109749000000
H	-5.547764000000	4.880400000000	3.167173000000
H	-5.541777000000	3.140033000000	3.495463000000
O	5.071819000000	-4.665555000000	2.465804000000
C	5.311818000000	-5.294819000000	3.726209000000
H	5.627574000000	-4.559976000000	4.469193000000
H	4.408051000000	-5.789384000000	4.087150000000
H	6.101379000000	-6.023375000000	3.549941000000
C	3.320719000000	1.319994000000	0.344510000000

H	3.383656000000	2.276085000000	0.866529000000
H	3.717824000000	0.596560000000	1.063065000000
C	4.305436000000	1.356310000000	-0.805736000000
O	4.064564000000	1.137715000000	-1.971733000000
O	5.538117000000	1.641950000000	-0.358657000000
C	6.568399000000	1.654789000000	-1.349189000000
H	7.494602000000	1.847859000000	-0.810832000000
H	6.616515000000	0.694408000000	-1.865609000000
H	6.385909000000	2.440142000000	-2.084550000000
H	5.007732000000	4.487225000000	-0.947908000000
C	-5.530432000000	-5.226600000000	-0.812779000000
H	-6.548467000000	-5.600363000000	-0.817817000000
H	2.218056000000	-3.438706000000	-1.142004000000
H	3.617935000000	-1.078106000000	-0.677224000000
H	4.039274000000	5.713116000000	-1.770753000000
H	-6.117708000000	-3.250691000000	-1.097489000000
H	-4.742833000000	-5.952858000000	-0.645812000000
Cu	-1.384831000000	0.006686000000	-0.246977000000

Cartesian coordinates of Ni-MADMECl optimized CAM-B3LYP/6-31g(d,p) level of theory:

N	3.032311000000	-0.810666000000	0.208845000000
N	2.218804000000	1.585854000000	-0.739417000000
C	-1.071912000000	-3.450477000000	0.006398000000
C	-0.850235000000	-2.024917000000	0.007854000000
C	-1.842792000000	-1.011625000000	0.112183000000
C	-1.555740000000	0.263063000000	-0.270906000000
C	0.158657000000	-4.048992000000	-0.023801000000
C	-2.575777000000	1.378756000000	-0.372026000000
C	-0.558823000000	1.835496000000	-1.455113000000
C	1.111783000000	-2.986794000000	-0.046872000000
C	2.456006000000	-3.166712000000	0.155495000000
C	3.477040000000	2.003320000000	-0.343062000000
C	3.755646000000	3.330822000000	-0.855891000000
C	2.675874000000	3.684545000000	-1.610262000000
C	1.722670000000	2.605254000000	-1.479861000000
C	4.360650000000	1.227068000000	0.342458000000
C	4.163557000000	-0.136372000000	0.560717000000
C	5.196484000000	-1.031166000000	0.989725000000
C	3.352270000000	-2.136412000000	0.363782000000
C	4.695962000000	-2.295808000000	0.834865000000
C	0.401647000000	2.691172000000	-1.910675000000
N	-0.335290000000	0.702495000000	-0.741508000000
N	0.476221000000	-1.754782000000	-0.066641000000
C	-2.034522000000	2.113302000000	-1.607327000000
H	5.309246000000	1.655337000000	0.640590000000
H	2.819206000000	-4.184084000000	0.239687000000
H	0.092428000000	3.559970000000	-2.477502000000
C	-2.585126000000	2.240693000000	0.900144000000
H	-2.728835000000	1.607686000000	1.780207000000
H	-1.605715000000	2.711827000000	1.033004000000

C	-3.674044000000	3.306995000000	0.886621000000
H	-4.659857000000	2.854998000000	0.719510000000
H	-3.540727000000	4.030778000000	0.077182000000
C	-3.748836000000	4.070332000000	2.186319000000
O	-3.182318000000	3.772225000000	3.209481000000
C	-2.336654000000	-4.234859000000	-0.072533000000
O	-2.591269000000	-5.164481000000	0.685054000000
N	-3.165933000000	-3.910986000000	-1.096533000000
H	-2.937860000000	-3.139553000000	-1.704209000000
C	-4.403096000000	-4.633436000000	-1.297605000000
H	-4.929292000000	-4.193616000000	-2.145174000000
C	2.460619000000	4.912675000000	-2.432023000000
H	1.920051000000	4.682611000000	-3.353993000000
H	1.880589000000	5.671943000000	-1.894851000000
H	3.416927000000	5.363826000000	-2.704279000000
C	6.553089000000	-0.616635000000	1.464899000000
H	7.095412000000	-0.047661000000	0.702365000000
H	6.494140000000	0.012564000000	2.358871000000
H	7.162811000000	-1.486012000000	1.717918000000
C	-2.595684000000	1.555098000000	-2.918953000000
H	-2.079904000000	1.988615000000	-3.779490000000
H	-2.487542000000	0.468651000000	-2.957164000000
H	-3.661667000000	1.782489000000	-3.005816000000
C	0.474104000000	-5.509303000000	-0.038321000000
H	-0.436463000000	-6.094981000000	0.081422000000
H	0.969610000000	-5.802488000000	-0.969368000000
H	1.145136000000	-5.772848000000	0.784930000000
C	5.000072000000	4.058503000000	-0.621177000000
C	5.359336000000	-3.603482000000	1.147007000000
H	5.052905000000	-4.359198000000	0.415737000000
H	6.441804000000	-3.496960000000	1.024428000000
C	5.057941000000	-4.111503000000	2.561851000000
H	3.983495000000	-4.251556000000	2.706967000000
H	5.555527000000	-5.066748000000	2.751837000000
H	5.399220000000	-3.394308000000	3.313048000000
O	-4.554713000000	5.140741000000	2.074676000000
C	-4.711051000000	5.909454000000	3.269181000000
H	-5.138980000000	5.298920000000	4.066644000000
H	-3.747531000000	6.296828000000	3.605503000000
H	-5.382705000000	6.726711000000	3.011783000000
C	-3.207768000000	-1.326617000000	0.678929000000
H	-3.203897000000	-2.269717000000	1.229163000000
H	-3.484376000000	-0.576253000000	1.427178000000
C	-4.356803000000	-1.379177000000	-0.306713000000
O	-4.299956000000	-1.187877000000	-1.501290000000
O	-5.505159000000	-1.643570000000	0.332802000000
C	-6.678922000000	-1.670895000000	-0.482592000000
H	-7.510482000000	-1.831807000000	0.201100000000
H	-6.796972000000	-0.726693000000	-1.017093000000
H	-6.623197000000	-2.482583000000	-1.209725000000
H	-5.036468000000	-4.577667000000	-0.407173000000
C	5.124486000000	5.383346000000	-0.538793000000

H	6.092605000000	5.843689000000	-0.374926000000
H	-2.217854000000	3.190631000000	-1.563269000000
H	-3.577609000000	0.993234000000	-0.563484000000
H	-4.211656000000	-5.690364000000	-1.501352000000
H	5.894298000000	3.450977000000	-0.500625000000
H	4.271282000000	6.048827000000	-0.607276000000
Ni	1.352385000000	-0.070857000000	-0.329102000000