

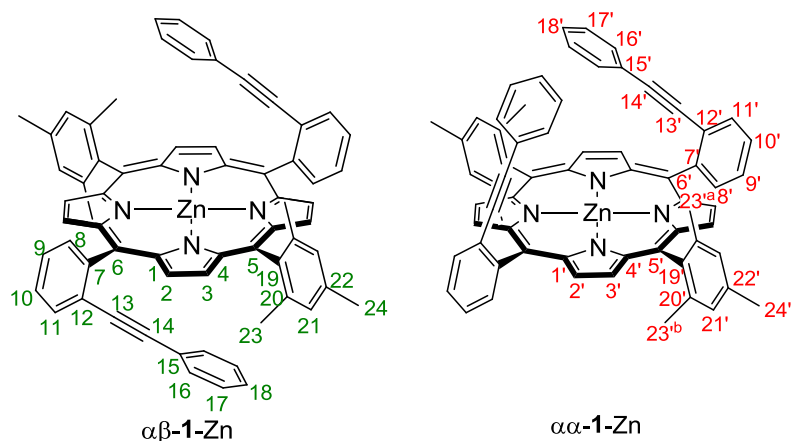
$\alpha\alpha$ - and $\alpha\beta$ -Zinc-meso-A₂B₂-Tetraarylporphyrins with large optical response to volatile amines

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and Katja Heinze*^a**

Supplementary Information

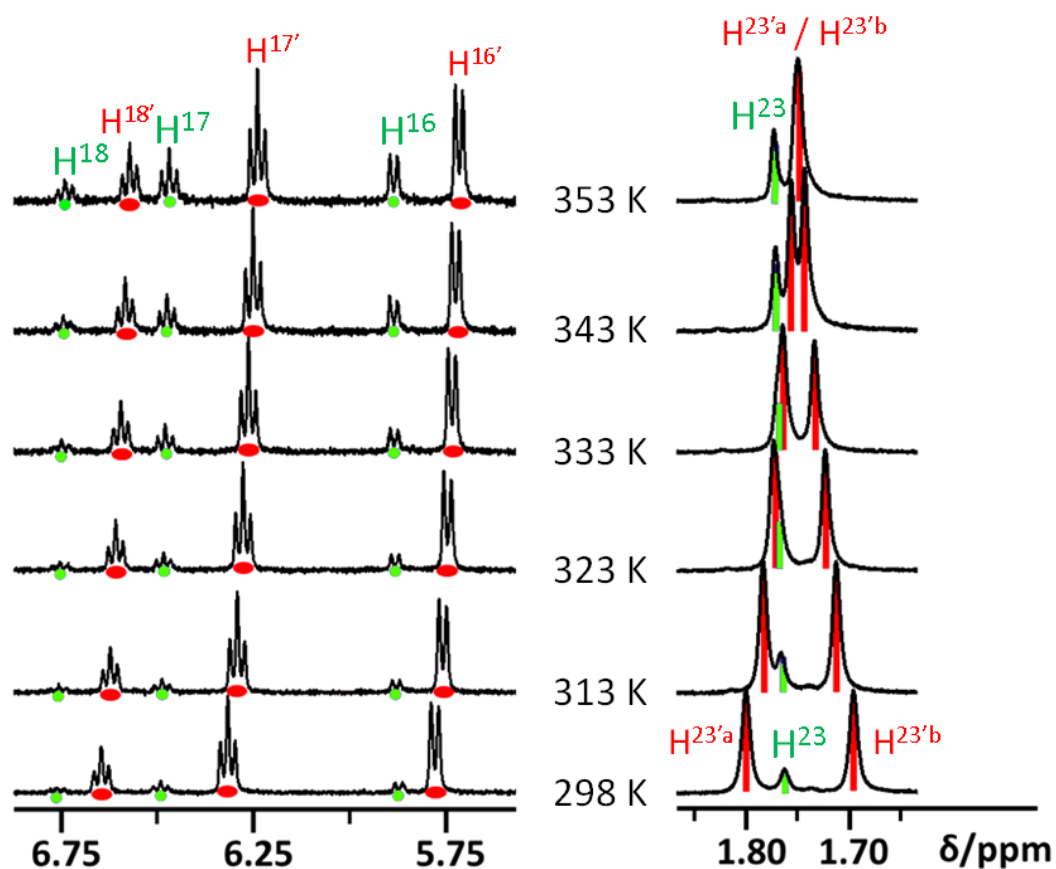
- **Figure S1** Atom numbering as used for NMR assignments
- NOESY (CD₂Cl₂, 298 K, 400 MHz) of $\alpha\alpha$ -**1**-2H and $\alpha\beta$ -**1**-2H
- Temperature dependent NMR ($T = 278 - 353$ K) of $\alpha\alpha$ - and $\alpha\beta$ -**1**-Zn in DMSO-d₆
- ¹³C{¹H}-NMR (CD₂Cl₂, 298 K, 100 MHz) of $\alpha\alpha$ -**1**-Zn
- HMBC (CD₂Cl₂, 298 K) of $\alpha\alpha$ -**1**-Zn
- HMBC (CD₂Cl₂, 298 K) of $\alpha\alpha$ -**1**-Zn (aromatic region)
- HSQC (CD₂Cl₂, 298 K) of $\alpha\alpha$ -**1**-Zn
- HSQC (CD₂Cl₂, 298 K) of $\alpha\alpha$ -**1**-Zn (aromatic region)
- NOESY (CD₂Cl₂, 298 K, 400 MHz) of $\alpha\alpha$ -**1**-Zn
- ¹³C{¹H}-NMR (CD₂Cl₂, 298 K, 100 MHz) of $\alpha\beta$ -**1**-Zn
- HMBC (CD₂Cl₂, 298 K) of $\alpha\beta$ -**1**-Zn
- HMBC (CD₂Cl₂, 298 K) of $\alpha\beta$ -**1**-Zn (aromatic region)
- HSQC (CD₂Cl₂, 298 K) of $\alpha\beta$ -**1**-Zn
- HSQC (CD₂Cl₂, 298 K) of $\alpha\beta$ -**1**-Zn (aromatic region)
- Normalized (to Soret band) absorption spectra of $\alpha\beta$ -**1**-Zn
- Cartesian Coordinates of DFT optimised of $\alpha\alpha$ -**1**-Zn, $\alpha\alpha$ -**1**-Zn(NEt₃)-dist, $\alpha\alpha$ -**1**-Zn(NEt₃)-prox, $\alpha\beta$ -**1**-Zn and $\alpha\beta$ -**1**-Zn(NEt₃)

Figure S1. Atom numbering as used for NMR assignments



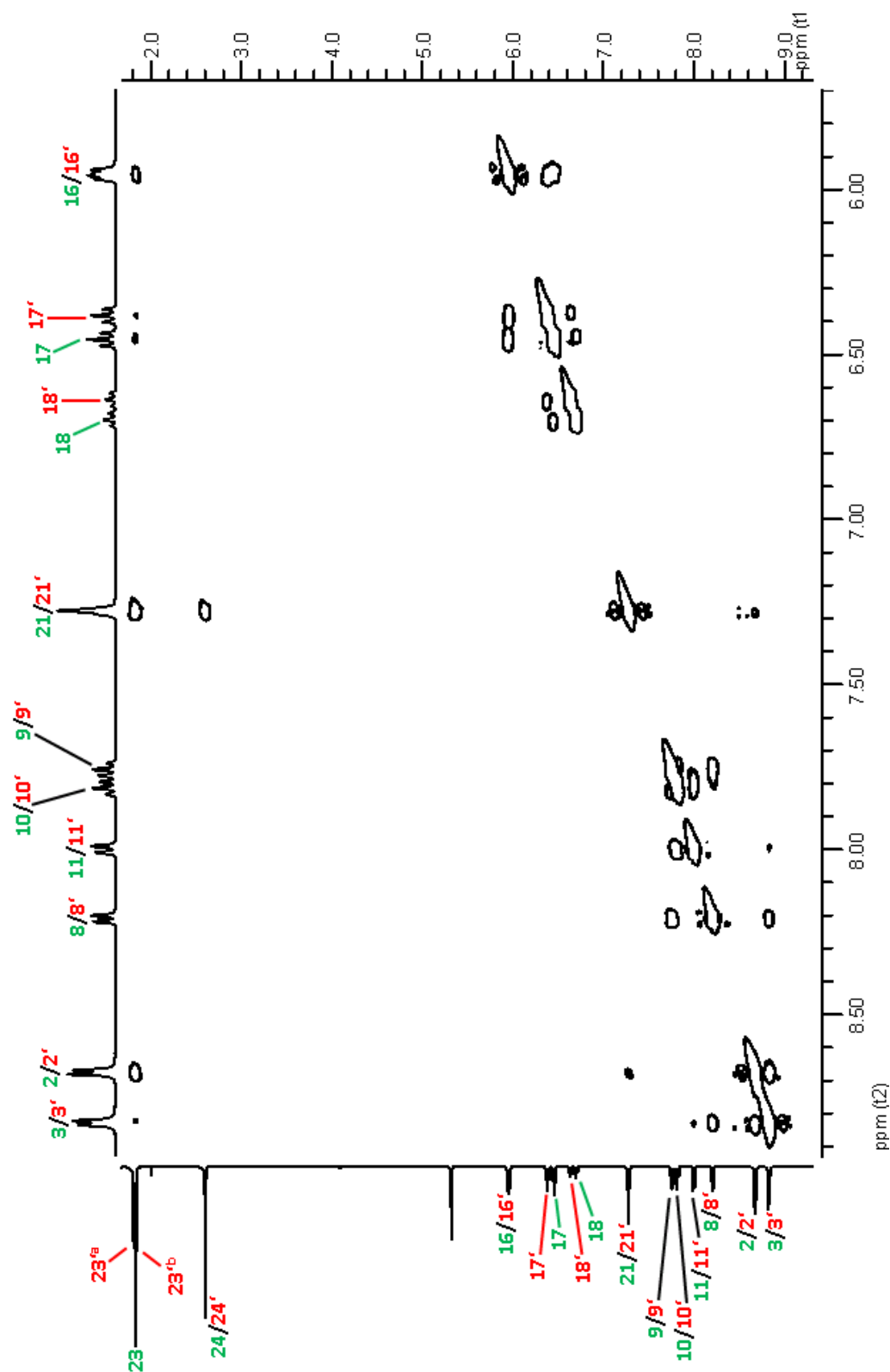
Temperature dependent NMR ($T = 278 - 353$ K) of $\alpha\alpha$ - and $\alpha\beta$ -1-Zn in DMSO- d_6

Partial NMR spectra of $\alpha\alpha$ -1-Zn (red) and $\alpha\beta$ -1-Zn (green) mixture in DMSO- d_6 at different temperatures. Increasing signal intensity for $\alpha\beta$ -1-Zn is due to increasing solubility at higher temperatures.



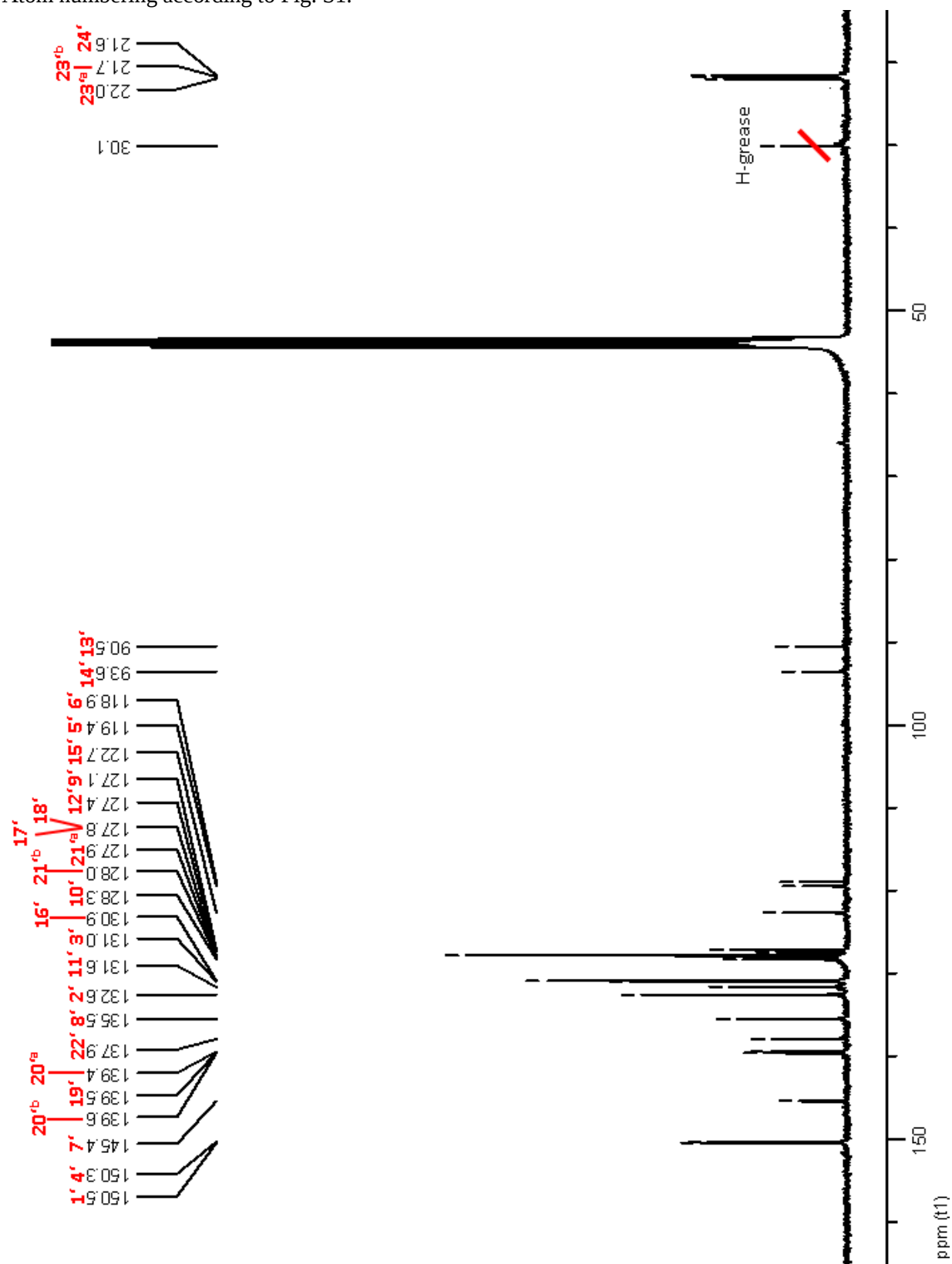
NOESY (CD₂Cl₂, 298 K, 400 MHz) of αα-1-2H and αβ-1-2H

Proton numbering according to Fig. S1.



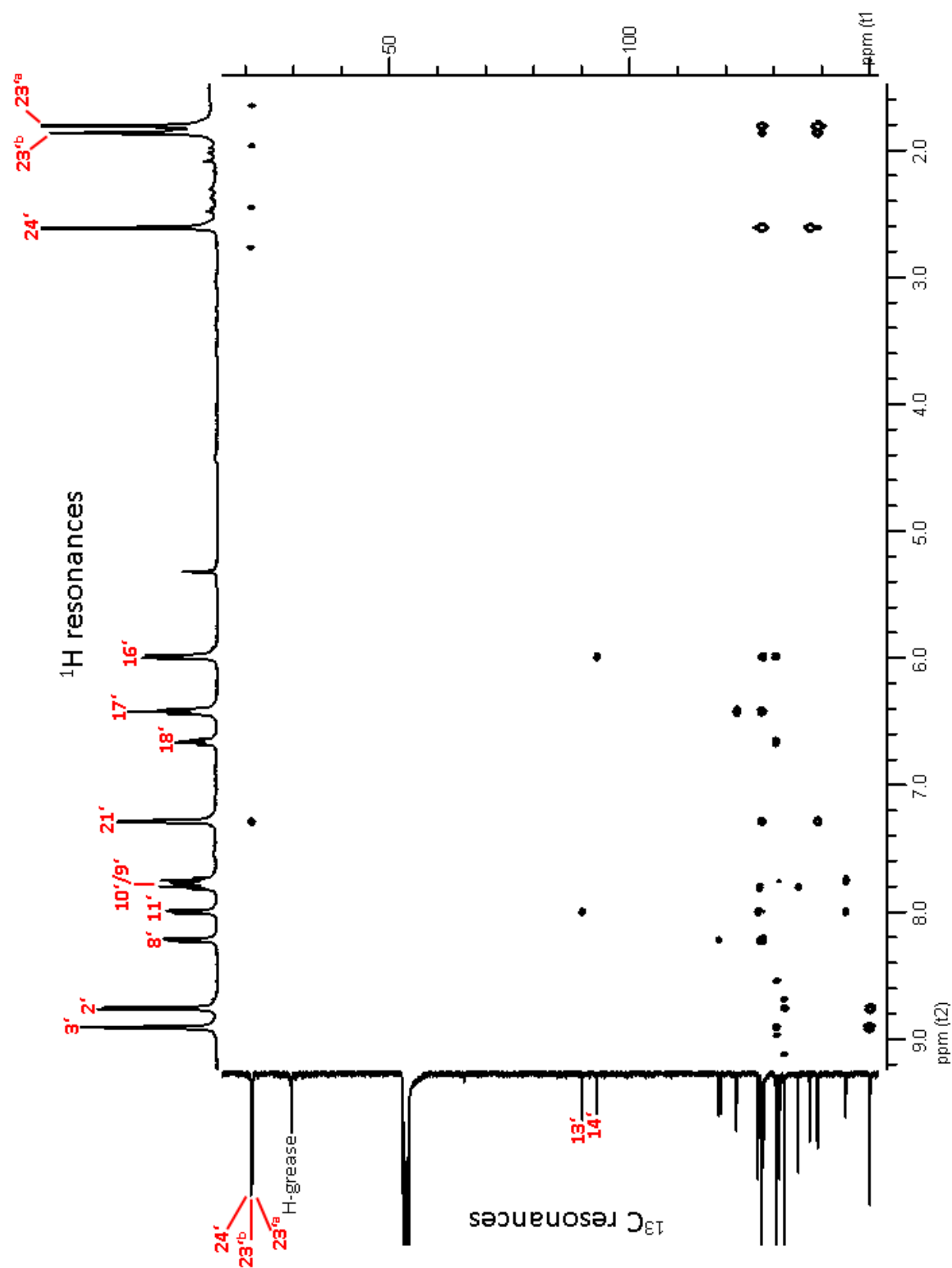
$^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 298 K, 100 MHz) of $\alpha\alpha$ -1-Zn

Atom numbering according to Fig. S1.



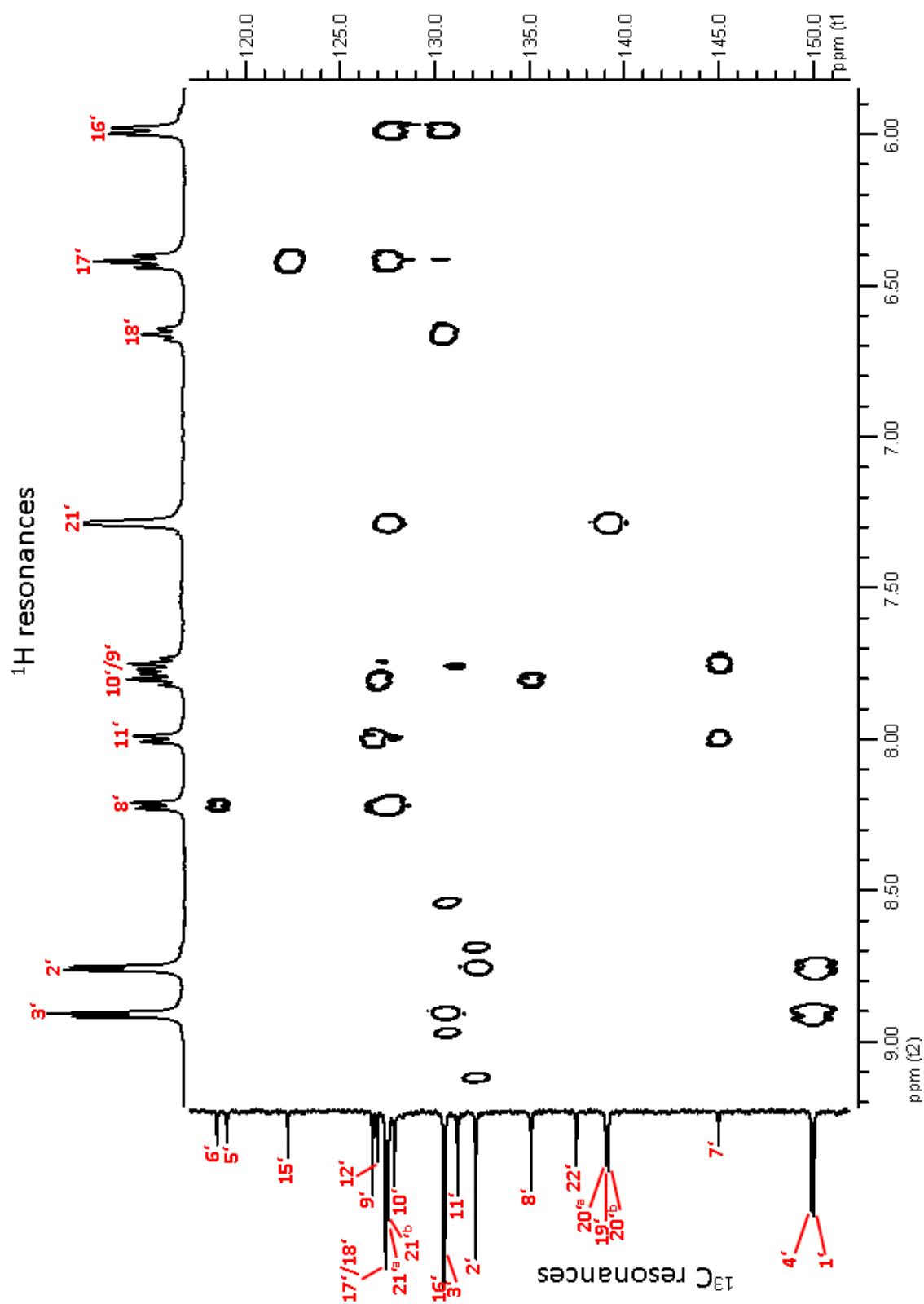
HMBC (CD₂Cl₂, 298 K) of αα-1-Zn

Atom numbering according to Fig. S1.



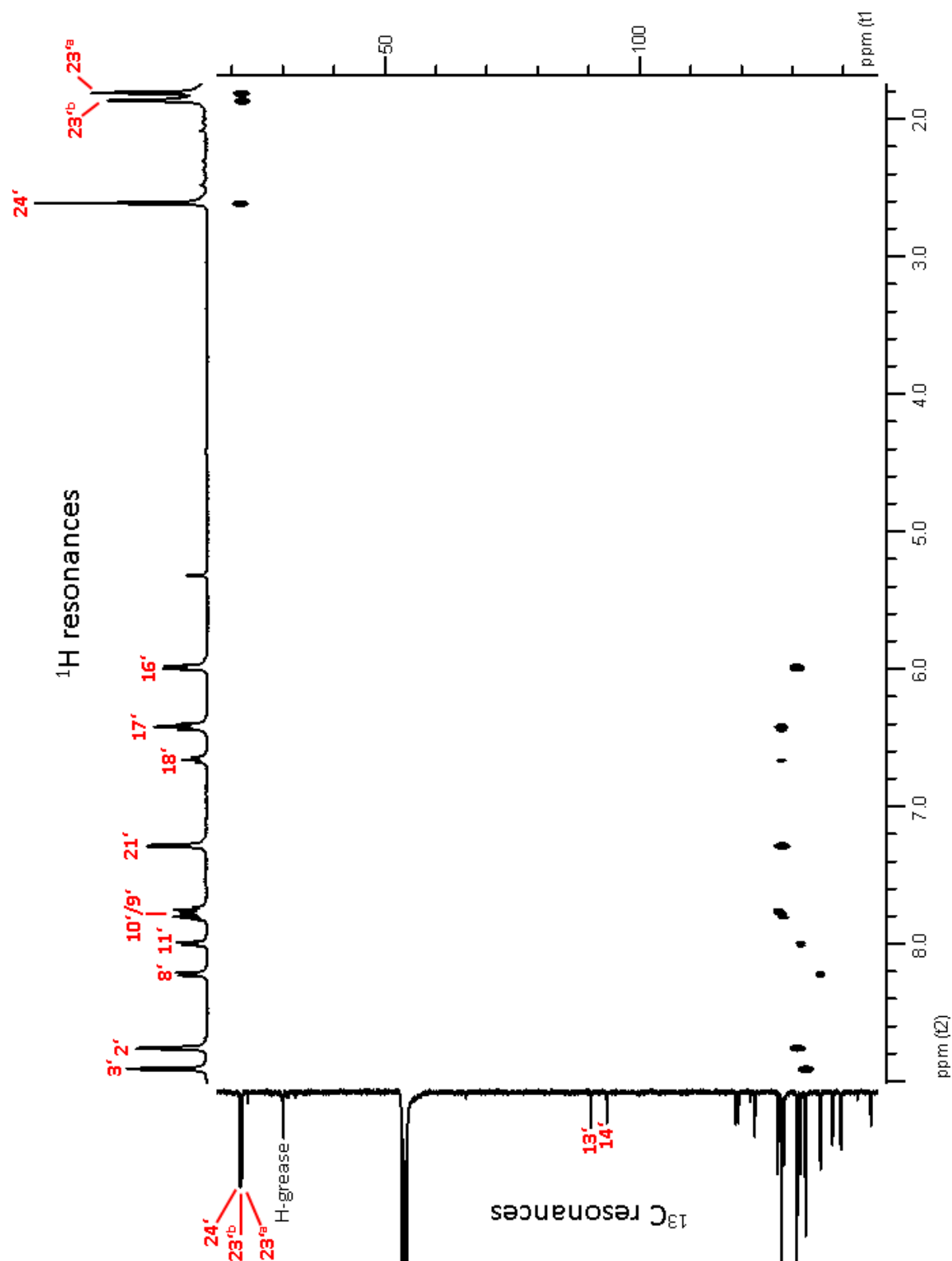
HMBC (CD₂Cl₂, 298 K) of $\alpha\alpha$ -1-Zn (aromatic region)

Atom numbering according to Fig. S1.



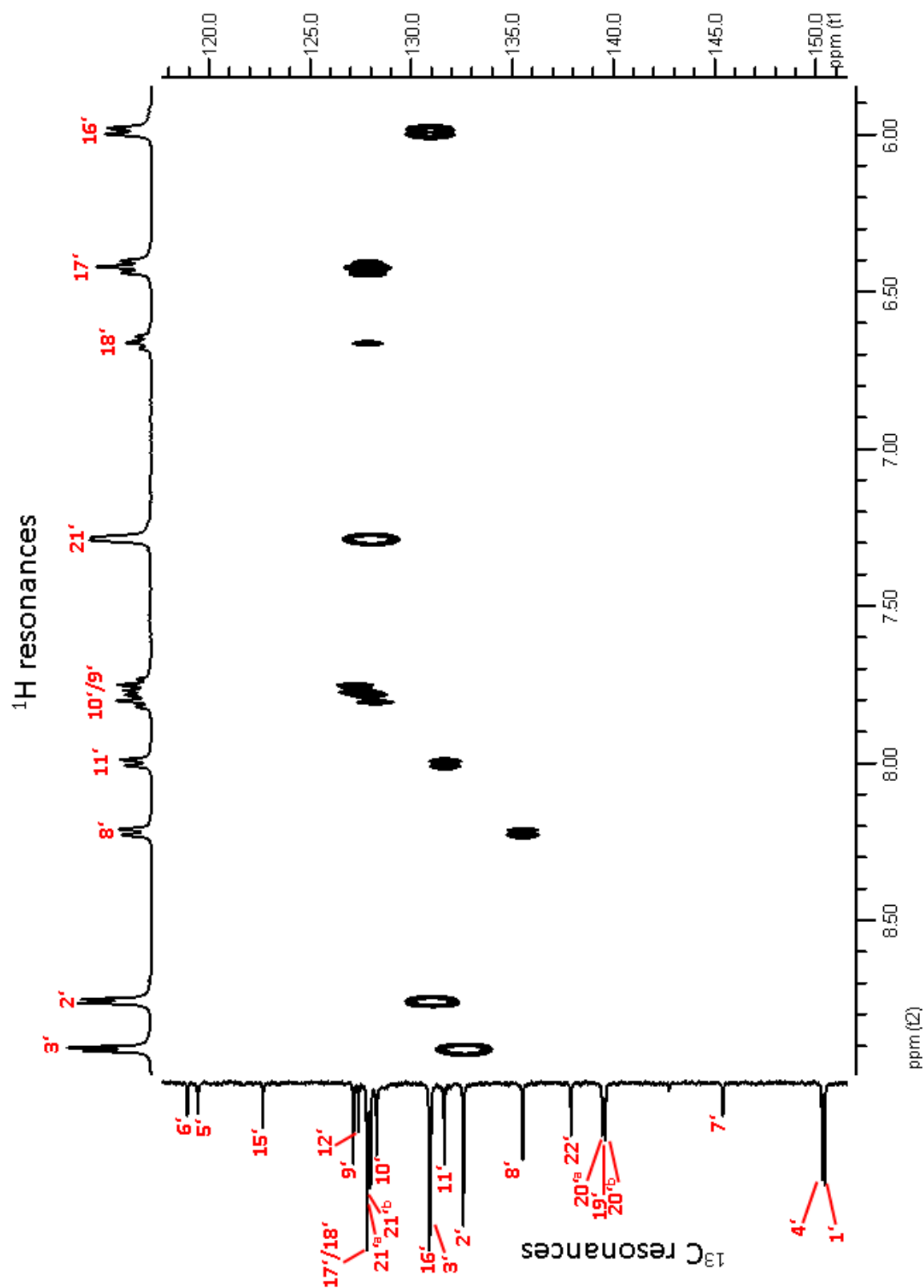
HSQC (CD_2Cl_2 , 298 K) of $\alpha\alpha$ -1-Zn

Atom numbering according to Fig. S1



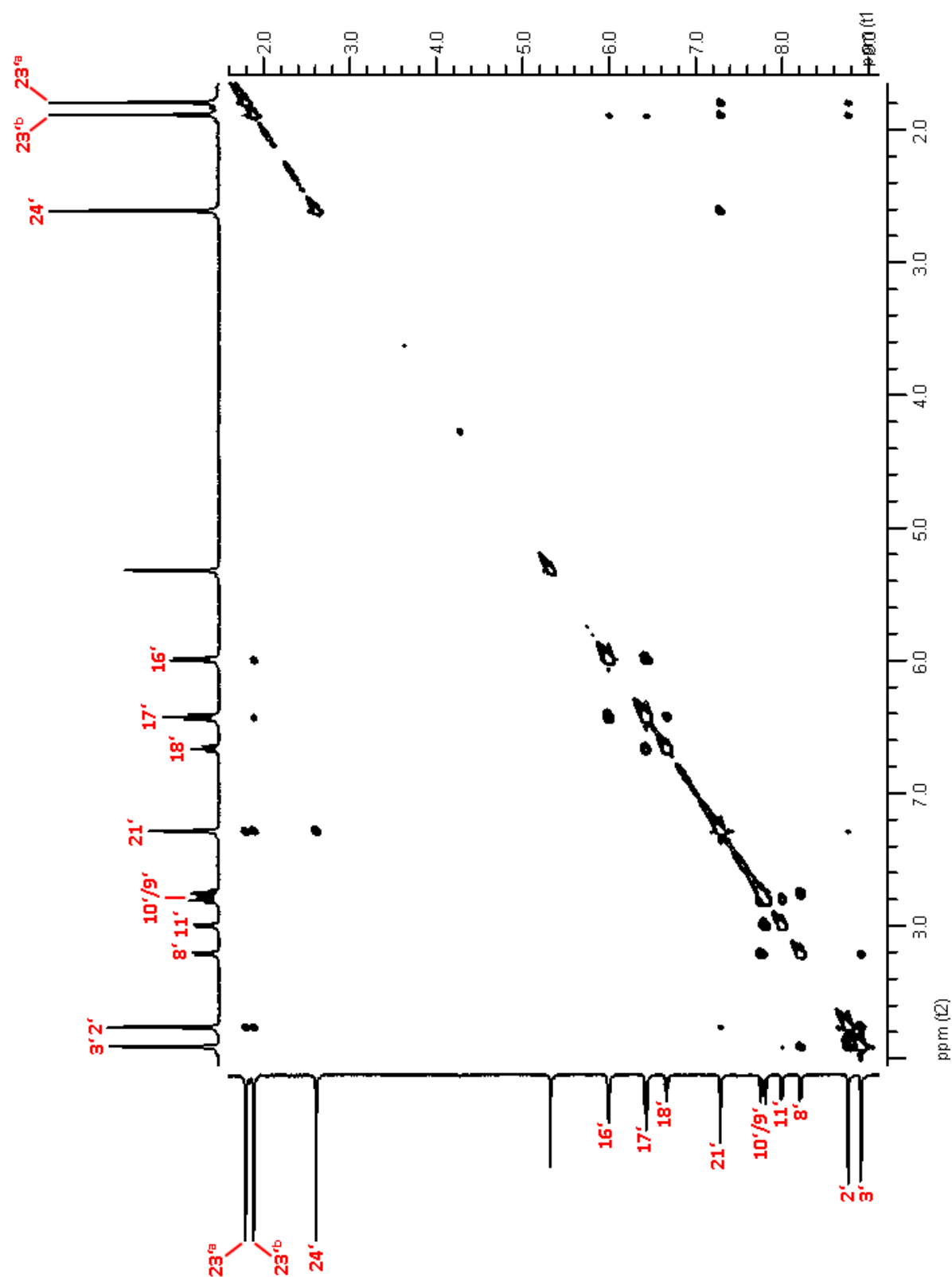
HSQC (CD₂Cl₂, 298 K) of αα-1-Zn (aromatic region)

Atom numbering according to Fig. S1



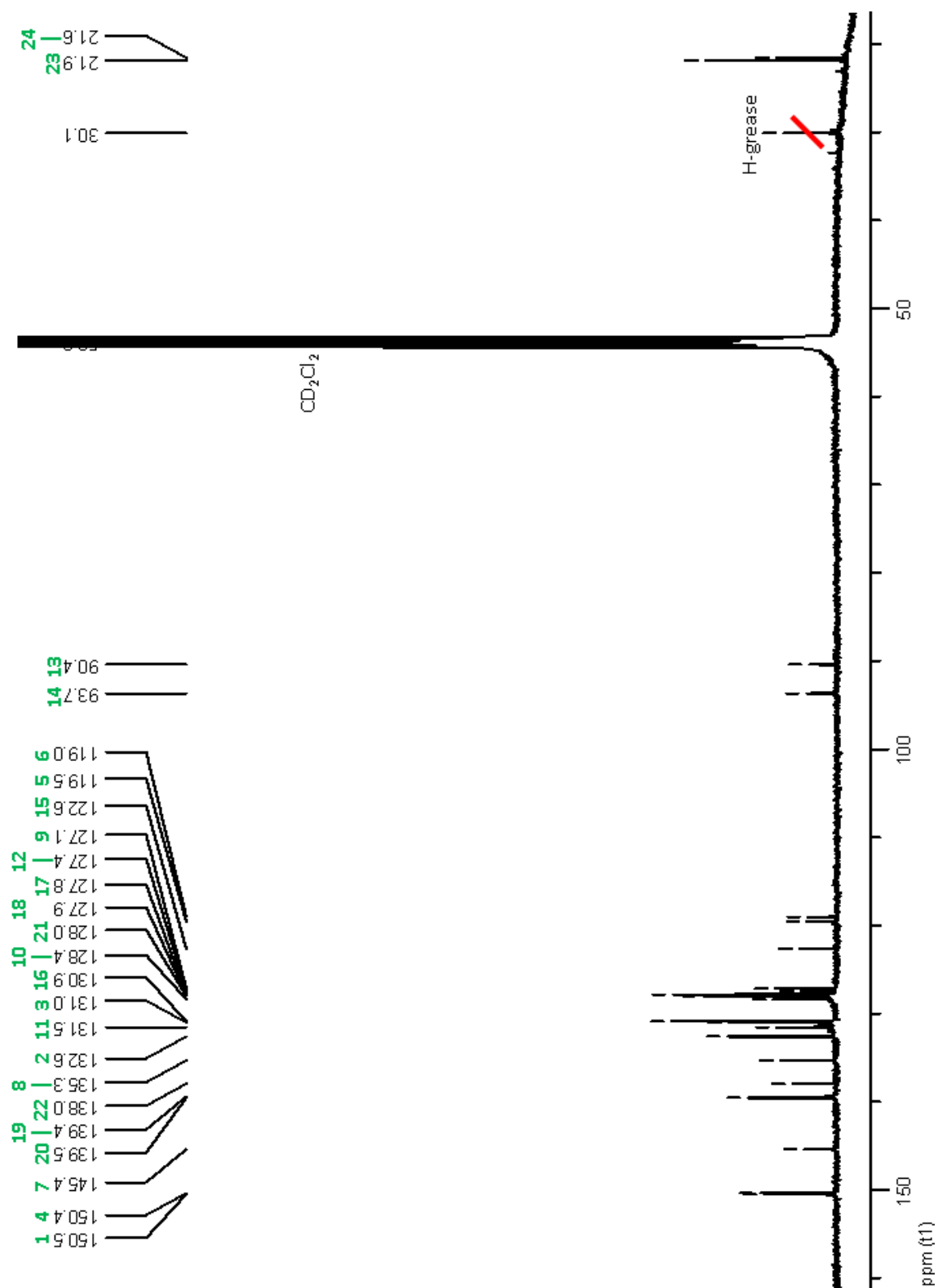
NOESY (CD₂Cl₂, 298 K, 400 MHz) of αα-1-Zn

Proton numbering according to Fig. S1.



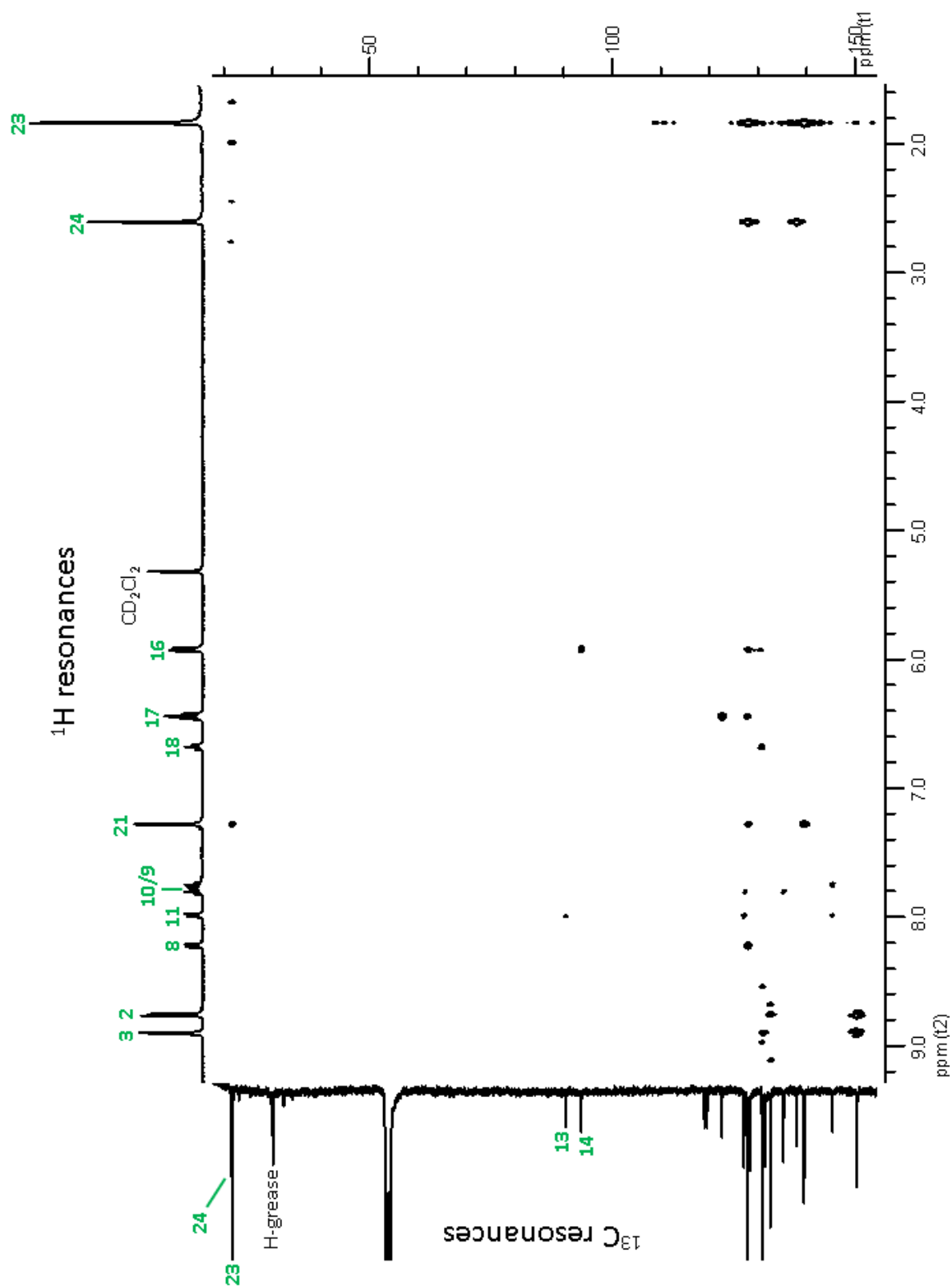
$^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 298 K, 100 MHz) of $\alpha\beta$ -1-Zn

Atom numbering according to Fig. S1.



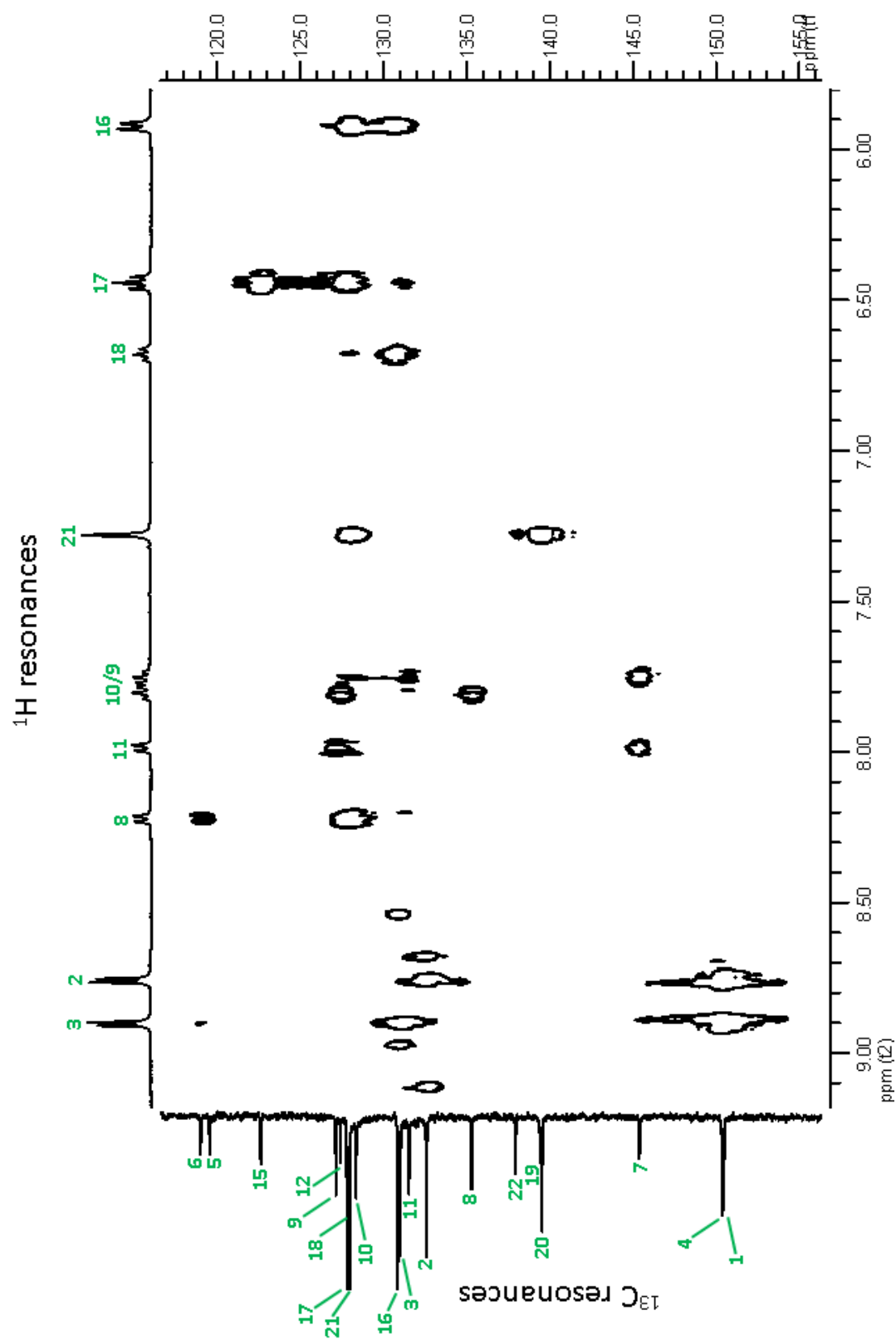
HMBC (CD_2Cl_2 , 298 K) of $\alpha\beta$ -1-Zn

Atom numbering according to Fig. S1.



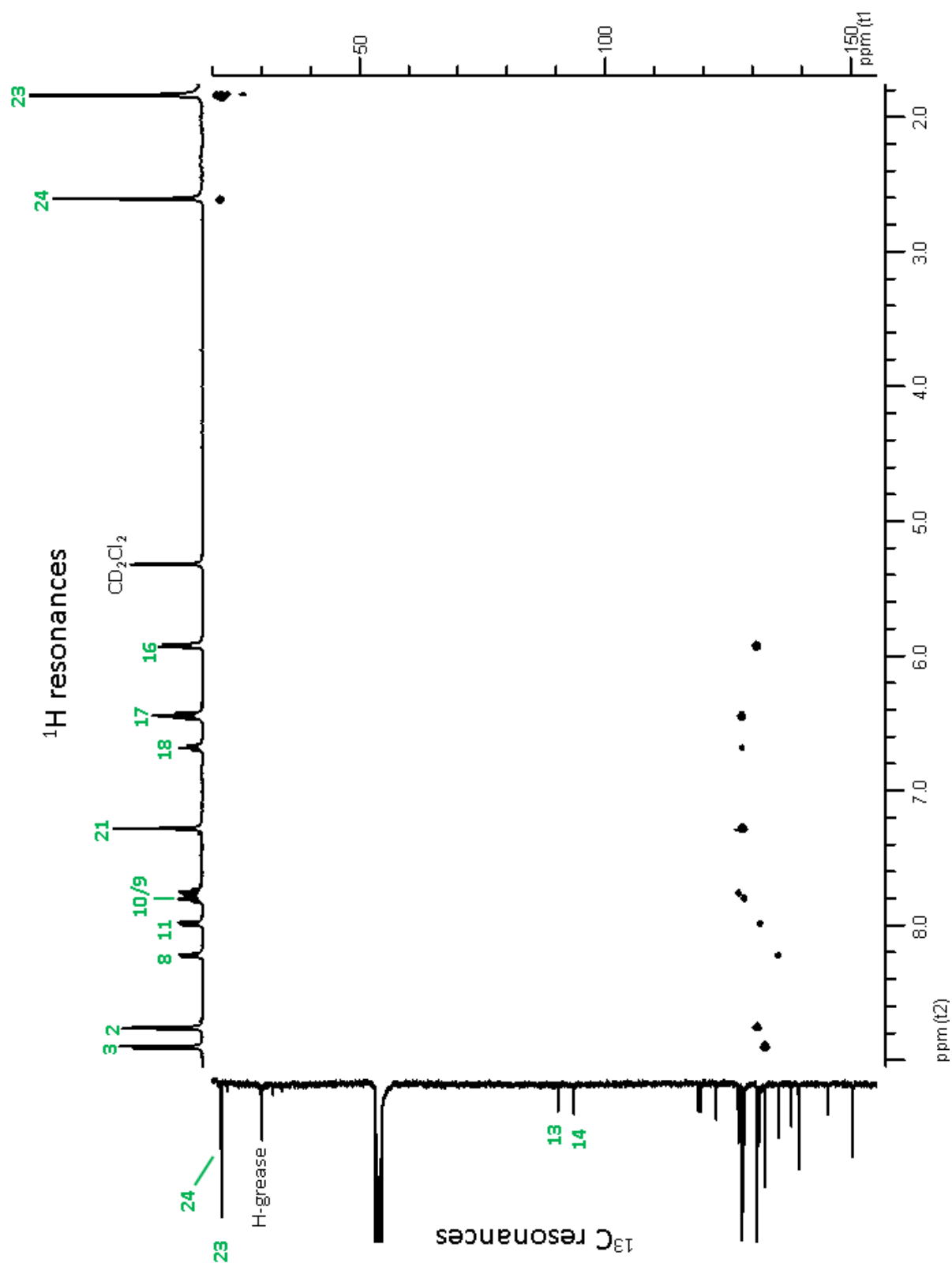
HMBC (CD₂Cl₂, 298 K) of αβ-1-Zn (aromatic region)

Atom numbering according to Fig. S1.



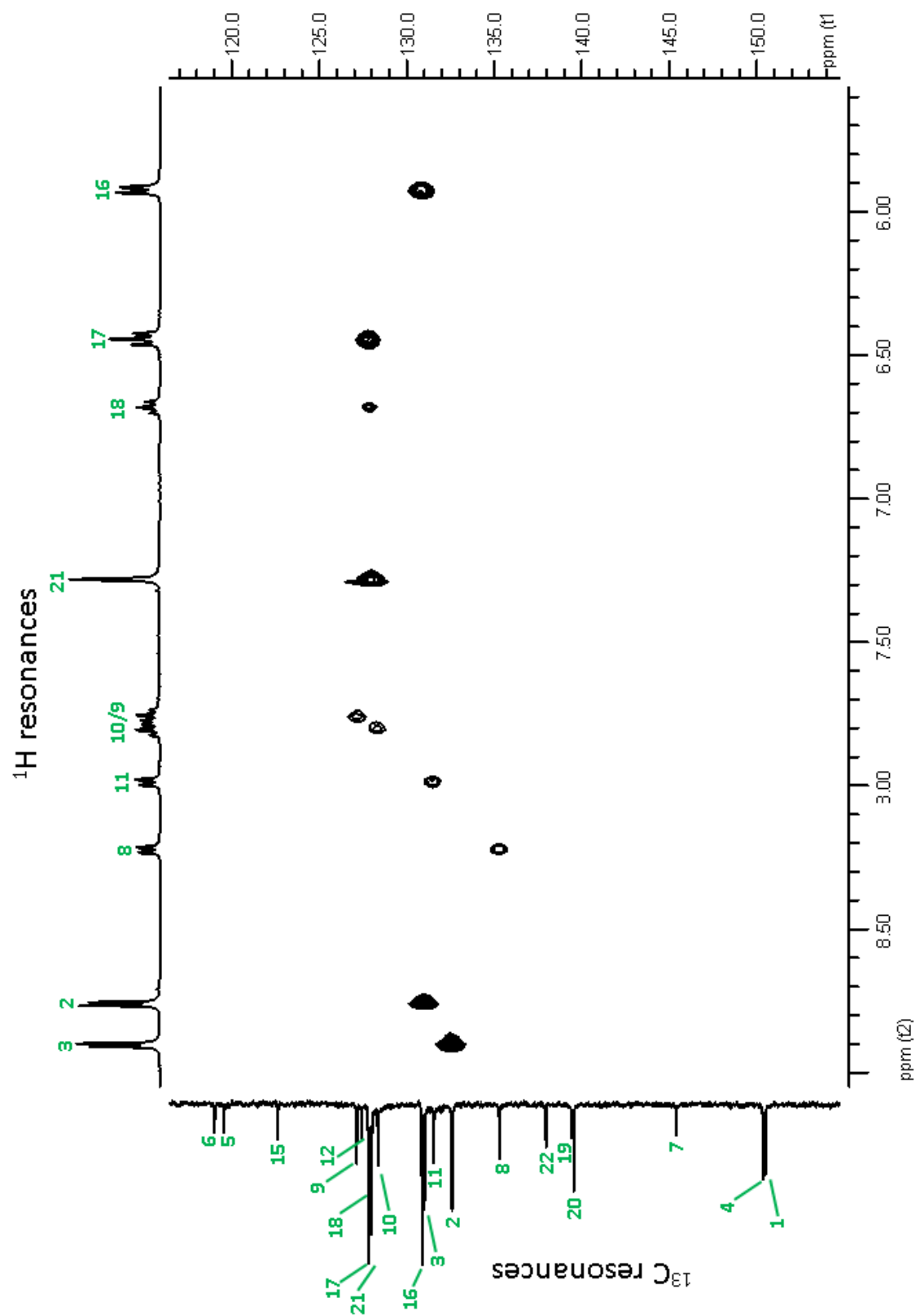
HSQC (CD_2Cl_2 , 298 K) of $\alpha\beta$ -1-Zn

Atom numbering according to Fig. S1



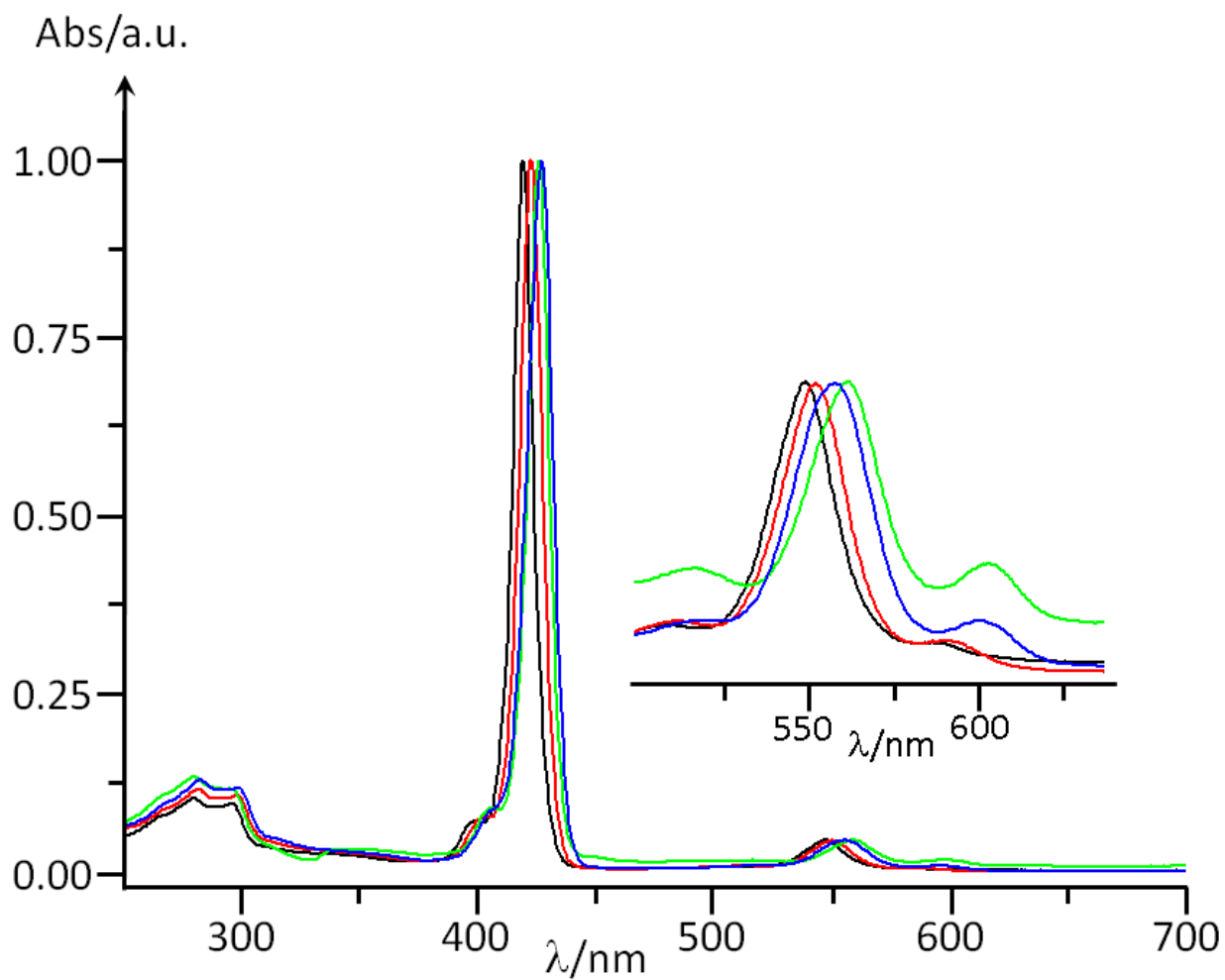
HSQC (CD_2Cl_2 , 298 K) of $\alpha\beta$ -1-Zn (aromatic region)

Atom numbering according to Fig. S1

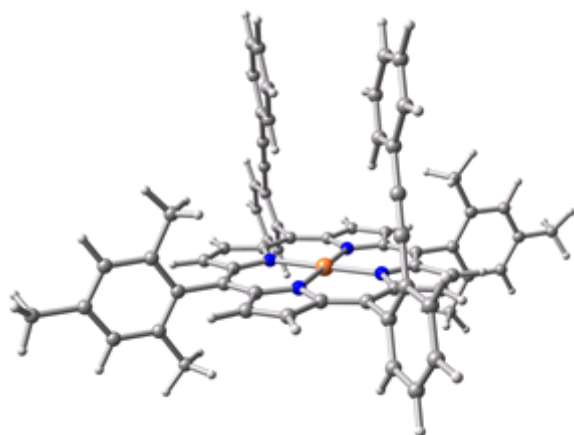


Normalized (to Soret band) absorption spectra of $\alpha\beta$ -1-Zn

in *n*-hexane (—), dichloromethane (—), acetonitrile (—) and chloroform (—). Inset shows magnification of Q-band region.



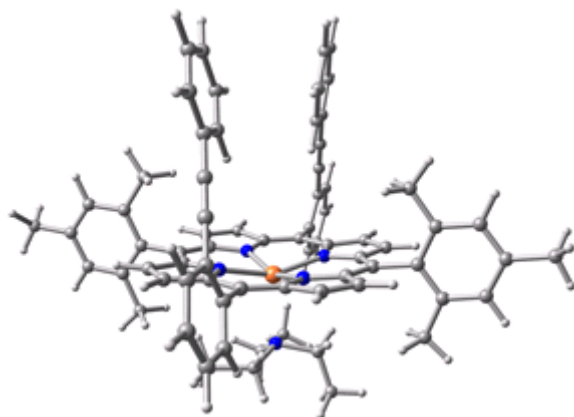
Cartesian Coordinates of DFT optimized $\alpha\alpha$ -1-Zn(NEt₃)



N	1.51615	1.18053	0.75796
N	0.94473	-1.68389	0.72952
N	-0.9448	1.68594	-0.72945
C	1.6115	2.5697	0.66543
C	2.83208	3.01006	1.32922
C	3.46258	1.88801	1.81462
C	2.63937	0.73954	1.45663
H	3.15548	4.03826	1.40666
H	4.39405	1.83705	2.35986
C	2.94464	-0.60367	1.77223
C	0.6842	3.42945	0.03327
C	2.4693	-3.10417	1.76107
C	1.45752	-3.88894	1.25838
C	0.50027	-3.00129	0.61021
C	2.14934	-1.7208	1.43083
H	3.3489	-3.42544	2.30024
H	1.36221	-4.96394	1.31405
C	-0.68356	-3.42753	-0.03438
C	-2.14968	1.7229	-1.43029
C	-2.46964	3.10628	-1.76049
C	-1.45746	3.89097	-1.25852
C	-0.50008	3.00327	-0.61059
H	-3.34944	3.42762	-2.2993
H	-1.36198	4.96595	-1.31465
C	-2.83103	-3.0082	-1.33103
C	-3.46197	-1.88607	-1.81566
C	-2.63941	-0.73748	-1.45658
C	-1.61094	-2.56771	-0.66639
H	-3.15377	-4.03653	-1.4097
H	-4.39322	-1.83518	-2.36128
C	-2.94502	0.60578	-1.77161
C	4.21105	-0.86454	2.54428
C	4.22159	-0.85744	3.97052
C	5.43862	-1.10939	4.65757
C	6.6239	-1.3633	3.95232
C	6.61345	-1.3693	2.54361
C	0.97782	4.90901	0.04901
C	0.48807	5.72062	1.10798
C	0.76957	7.101	1.10395
C	2.00102	6.88097	-0.96367
C	1.74053	5.49386	-0.99459
H	0.3899	7.71801	1.91724
C	-4.21173	0.86672	-2.54314
C	-5.4536	1.07877	-1.87446
C	-6.6236	1.32057	-2.64211
C	-6.57105	1.35333	-4.04315
C	-5.34415	1.14487	-4.70336
C	-4.17951	0.90456	-3.95083
C	-0.9767	-4.90717	-0.05145
C	-1.74495	-5.49259	0.98962

C	-2.00991	-6.87717	0.95489
C	-1.53013	-7.69947	-0.08433
C	-0.77392	-7.09799	-1.10994
C	-0.48745	-5.71701	-1.11017
H	-2.60214	-7.31971	1.75438
H	-0.3989	-7.713	-1.92648
C	5.41203	-1.12063	1.85427
H	2.58465	7.32439	-1.76859
H	5.3989	-1.12446	0.7674
H	5.43623	-1.10153	5.74416
H	7.52776	-1.56535	1.98917
H	-3.23061	0.74287	-4.45571
H	-5.2946	1.16847	-5.78908
H	-7.56473	1.48117	-2.12325
N	-1.51618	-1.17845	-0.75791
C	1.52684	7.70219	0.07704
H	-7.47573	1.53941	-4.61667
H	7.54754	-1.55465	4.49296
C	-0.33315	5.12273	2.23801
H	-1.2497	4.64937	1.86246
H	0.22793	4.34594	2.77411
H	-0.62202	5.89285	2.9619
C	2.27752	4.65414	-2.1415
H	2.96186	3.87409	-1.78281
H	1.46774	4.14308	-2.67846
H	2.82193	5.27612	-2.86073
C	-2.28715	-4.65147	2.13305
H	-1.47948	-4.14	2.67283
H	-2.96975	-3.87163	1.77066
H	-2.83459	-5.27265	2.8507
C	0.33289	-5.11924	-2.2409
H	-0.22777	-4.3414	-2.77592
H	1.25045	-4.64733	-1.86597
H	0.62021	-5.88919	-2.96557
C	-1.80106	-9.19359	-0.08622
H	-1.02713	-9.73639	0.47602
H	-2.76643	-9.42679	0.37931
H	-1.80914	-9.59854	-1.10529
C	1.82596	9.19081	0.10251
H	0.90968	9.78044	0.23917
H	2.50228	9.44632	0.93053
H	2.30192	9.51957	-0.82836
C	-5.53863	1.05389	-0.44438
C	3.02743	-0.59882	4.7189
C	2.01015	-0.37738	5.36817
C	-5.62096	1.0354	0.77968
C	-5.6888	1.00876	2.21104
C	-4.51963	0.76939	2.98015
C	-6.92029	1.22035	2.88402
C	-4.58463	0.74322	4.38217
H	-3.57477	0.6071	2.46853
C	-6.97816	1.19273	4.28663
H	-7.81854	1.40407	2.30053
C	-5.81226	0.95437	5.04181
H	-3.68203	0.55919	4.95984
H	-7.92759	1.35629	4.79095
H	-5.8596	0.9337	6.12793
C	0.80719	-0.1155	6.10194
C	0.80932	-0.10661	7.52116
C	-0.40967	0.14019	5.41665
C	-0.37352	0.15088	8.23251
H	1.73785	-0.30164	8.05113
C	-1.5886	0.39697	6.13413
H	-0.41532	0.13447	4.33001
C	-1.57682	0.40363	7.5436
H	-0.35934	0.15503	9.31984
H	-2.51405	0.59164	5.59757
H	-2.49149	0.60299	8.09674
Zn	-0.00006	0.00106	0.00005

Cartesian Coordinates of DFT optimized $\alpha\alpha$ -1-Zn(NEt₃)-dist

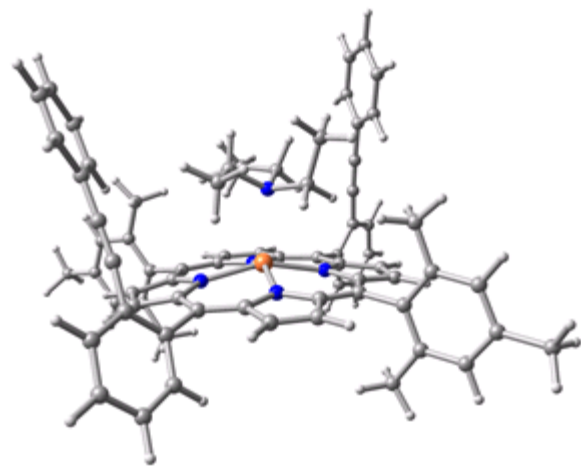


N	1.07832	-1.79462	-0.98562
N	-1.75013	-1.04861	-1.00186
N	1.80661	1.01559	-0.5895
C	2.4506	-1.95679	-0.80217
C	2.77412	-3.37962	-0.81732
C	1.59401	-4.0644	-0.98989
C	0.52776	-3.07058	-1.07962
H	3.76624	-3.78947	-0.69179
H	1.4514	-5.13482	-1.02654
C	-0.85124	-3.37633	-1.175
C	3.39406	-0.92461	-0.5838
C	-3.32186	-2.75774	-1.14862
C	-4.01614	-1.57733	-1.02739
C	-3.03157	-0.50466	-0.92941
C	-1.90032	-2.42784	-1.11842
H	-3.72772	-3.7551	-1.23703
H	-5.08747	-1.43834	-0.99793
C	-3.35256	0.86368	-0.76646
C	1.94779	2.37802	-0.33815
C	3.35661	2.68484	-0.10897
C	4.0488	1.50008	-0.19157
C	3.07669	0.45017	-0.48127
H	3.75275	3.66735	0.10366
H	5.10899	1.34071	-0.05528
C	-2.74358	3.29433	-0.33958
C	-1.56083	3.98059	-0.19604
C	-0.47877	3.02147	-0.39791
C	-2.40425	1.9046	-0.62957
H	-3.74903	3.67699	-0.23694
H	-1.42828	5.02515	0.04647
C	0.89737	3.32256	-0.26389
C	-1.22455	-4.82891	-1.30798
C	-1.7055	-5.58405	-0.19595
C	-2.03534	-6.95366	-0.37474
C	-1.8946	-7.57247	-1.62516
C	-1.41483	-6.83031	-2.7221
C	4.83195	-1.32806	-0.35891
C	5.27974	-1.63205	0.95672
C	6.62317	-2.0047	1.15889
C	7.08048	-1.7807	-1.20207
C	5.74169	-1.40349	-1.44417
H	6.95872	-2.23441	2.16928
C	1.26314	4.75402	0.02821
C	1.53841	5.19378	1.35784
C	1.86821	6.55566	1.58686
C	1.92776	7.47061	0.5257
C	1.65427	7.03821	-0.78675
C	1.32391	5.69086	-1.02252
C	-4.81255	1.23155	-0.65902
C	-5.46808	1.16092	0.60134

C	-6.83057	1.50786	0.6896
C	-7.56751	1.9226	-0.4391
C	-6.90025	1.98918	-1.6767
C	-5.53532	1.65146	-1.80501
H	-7.32531	1.45384	1.65842
H	-7.44876	2.31005	-2.56074
C	-1.08339	-5.47342	-2.55352
H	7.77228	-1.8354	-2.04097
H	-0.71145	-4.89927	-3.39827
H	-2.39844	-7.51816	0.47983
H	-1.30062	-7.30117	-3.69534
H	1.11144	5.35512	-2.03409
H	1.69751	7.74031	-1.61573
H	2.07387	6.87896	2.6037
N	-1.01858	1.77027	-0.68386
C	7.54192	-2.08644	0.092
H	2.18337	8.50987	0.71726
H	-2.15326	-8.62164	-1.74508
C	4.33459	-1.55968	2.14408
H	3.91663	-0.55183	2.26479
H	3.48449	-2.24366	2.02261
H	4.85254	-1.82356	3.07286
C	5.30234	-1.08282	-2.86263
H	4.50042	-1.75545	-3.19452
H	4.91428	-0.05868	-2.93768
H	6.13868	-1.18151	-3.56375
C	-4.72241	0.72312	1.85084
H	-4.38095	-0.31743	1.77222
H	-3.82942	1.33809	2.02111
H	-5.36324	0.8004	2.73623
C	-4.86792	1.74204	-3.16714
H	-4.02017	2.43972	-3.1521
H	-4.47513	0.76781	-3.4862
H	-5.57708	2.08649	-3.92828
C	-9.03775	2.28304	-0.31724
H	-9.62613	1.43335	0.05635
H	-9.18843	3.11439	0.38474
H	-9.45874	2.58021	-1.28454
C	8.98342	-2.49621	0.33763
H	9.5104	-1.75329	0.95159
H	9.03934	-3.45538	0.87116
H	9.53446	-2.60543	-0.60339
C	1.48259	4.28433	2.46325
C	-1.85267	-4.98807	1.09838
C	-1.98987	-4.47835	2.20576
C	1.44592	3.50154	3.40702
C	1.4078	2.55214	4.47964
C	1.21925	1.17157	4.20483
C	1.56165	2.96871	5.82744
C	1.18628	0.23751	5.25257
H	1.10272	0.84816	3.17374
C	1.52863	2.02888	6.87037
H	1.7062	4.0241	6.04299
C	1.34136	0.66066	6.58837
H	1.04212	-0.81677	5.02987
H	1.64919	2.36005	7.89919
H	1.31746	-0.0661	7.39686
C	-2.1514	-3.84129	3.47902
C	-2.55023	-4.58477	4.62016
C	-1.91886	-2.44686	3.61433
C	-2.71263	-3.94885	5.86159
H	-2.72973	-5.65212	4.52149
C	-2.08217	-1.81773	4.85889
H	-1.61576	-1.87409	2.74179
C	-2.48021	-2.56427	5.98657
H	-3.01977	-4.52857	6.72891
H	-1.90182	-0.74959	4.94999
H	-2.60784	-2.07311	6.94826
C	-0.34303	1.05847	-4.44822
H	-1.37112	1.20709	-4.10413
N	0.20595	-0.12855	-3.70208
C	-0.49327	-1.39951	-4.13024

H	-0.2038	-2.17344	-3.41084
C	1.69357	-0.29705	-3.89097
H	2.18672	0.55047	-3.40802
H	1.97786	-1.18824	-3.32205
C	2.21378	-0.43048	-5.34271
H	1.9696	0.44543	-5.95564
H	3.30767	-0.51866	-5.31566
H	1.82845	-1.32109	-5.85245
C	-2.02624	-1.31946	-4.2134
H	-2.4236	-2.32877	-4.38179
H	-2.46254	-0.94084	-3.28742
H	-2.36231	-0.69079	-5.04631
H	-0.11771	-1.7124	-5.11946
H	-0.39203	0.83226	-5.52942
C	0.43521	2.3666	-4.2427
H	1.4324	2.33939	-4.69672
H	-0.1217	3.18732	-4.71441
H	0.54467	2.59949	-3.18154
Zn	0.04333	0.02512	-1.22312

Cartesian Coordinates of DFT optimized $\alpha\alpha$ -1-Zn(NEt₃)-prox

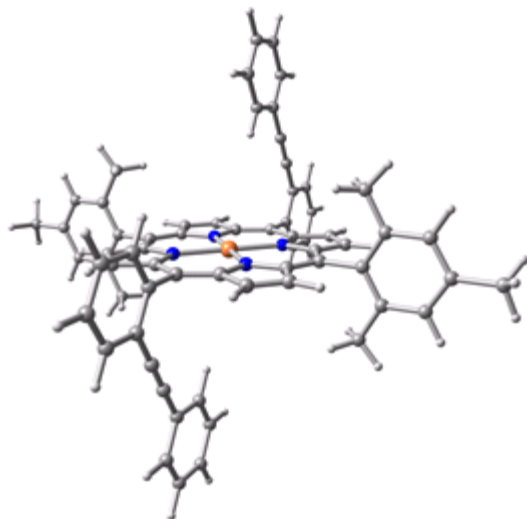


N	1.56203	0.47388	0.84451
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C	2.33462	-0.35006	1.65941
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H	4.18777	0.03824	2.89782
C	2.06436	-1.70508	1.96754
C	1.59691	2.92665	0.32587
C	0.62335	-3.8073	1.90214
C	-0.58274	-4.12956	1.3255
C	-1.04101	-2.95246	0.59616
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H	1.24902	-4.43908	2.51552
H	-1.11769	-5.06658	1.38704
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C	0.38115	2.99817	-0.39424
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H	0.25573	5.21325	-0.82318
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C	-4.22649	-0.30655	-1.7806
C	-2.98575	0.39236	-1.45937
C	-2.75887	-1.71539	-0.74651
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C	4.19754	-3.03844	2.51063
C	5.01294	-3.68953	3.47552
C	4.65591	-3.70764	4.83079
C	3.46823	-3.07396	5.24615
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C	2.04151	4.98898	1.73185
C	2.73417	6.19693	1.95282
C	3.99201	5.89249	-0.08646
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C	-3.91584	2.69495	-3.76835
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C	-5.90045	3.9041	-2.15235
C	-4.85755	3.16338	-1.56462

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H	-3.88446	-6.88465	-1.93922
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H	5.9267	-4.17387	3.14211
H	3.18189	-3.07715	6.29491
H	-4.81257	3.05446	-0.48404
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C	5.73263	-1.90492	-2.07591
C	6.67247	-4.31667	-3.18378
H	6.05323	-5.23095	-1.31893
C	6.28884	-1.91741	-3.36553
H	5.37561	-0.97662	-1.63777
C	6.76011	-3.12174	-3.92567
H	7.03546	-5.24872	-3.6103
H	6.35973	-0.99112	-3.93079
H	7.19147	-3.1286	-4.92372
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C	1.66869	-3.1792	-1.90219
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H	3.03525	-1.73619	-2.71473
H	1.02203	-1.5499	-4.32889
C	-0.54642	-0.06612	-4.15287
H	0.01994	0.72872	-4.65168
H	-1.19316	-0.53605	-4.90582
H	-1.18857	0.38808	-3.39558
Zn	-0.08127	-0.11993	-0.35589

Cartesian Coordinates of DFT optimized $\alpha\beta$ -1-Zn

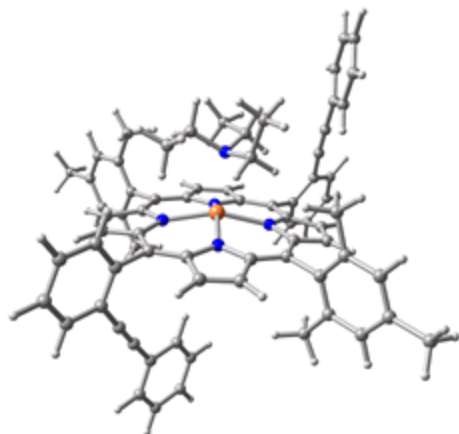


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H	-4.4621	-1.66522	2.34137
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C	-0.79034	-3.40092	0.03673
C	-2.36549	3.20646	1.73202
C	-1.32976	3.95012	1.23531
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C	-2.07439	1.80361	1.40083
H	-3.23967	3.55461	2.26338
H	-1.19322	5.02113	1.28352
C	0.79636	3.414	-0.03953
C	2.08042	-1.7904	-1.40341
C	2.37079	-3.19303	-1.73605
C	1.33516	-3.93681	-1.23929
C	0.40667	-2.99441	-0.59813
H	3.24444	-3.54103	-2.26839
H	1.19837	-5.00776	-1.28829
C	2.9395	2.91212	-1.32604
C	3.53586	1.76059	-1.80556
C	2.69218	0.63896	-1.45886
C	1.7077	2.54124	-0.66689
H	3.30188	3.9262	-1.40844
H	4.46813	1.67844	-2.34425
C	2.9318	-0.71733	-1.75463
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C	-0.66583	-5.69555	1.11417
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H	-5.31173	1.42987	5.72919
H	3.25882	-0.88145	-4.4374
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N	1.59968	1.15818	-0.77376
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H	-7.46284	1.84768	4.51858
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H	1.11084	-4.6869	1.86274
H	-0.35265	-4.32198	2.77323
H	0.43676	-5.89957	2.96903
C	-2.41521	-4.57769	-2.14101
H	-3.06677	-3.76788	-1.78724
H	-1.58601	-4.10308	-2.68166
H	-2.98509	-5.18233	-2.85538
C	2.43512	4.58636	2.13008
H	1.61025	4.09937	2.66601
H	3.09534	3.78564	1.7719
H	2.99781	5.19118	2.84983
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C	5.50908	-1.23612	0.84583
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C	4.29981	-1.00776	2.99082
C	6.71893	-1.36601	3.00823
C	4.29946	-0.97481	4.39441
H	3.37378	-0.8849	2.43581
C	6.71064	-1.33195	4.4119
H	7.64964	-1.51641	2.46756
C	5.50253	-1.1363	5.11096
H	3.36465	-0.82379	4.92884
H	7.64127	-1.45706	4.96038
H	5.49866	-1.11029	6.19803
C	-5.53214	1.16495	-2.27466
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C	-4.32851	0.93361	-2.99156
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H	-7.6621	1.52784	-2.45482
C	-4.33669	0.88906	-4.3948
H	-3.40251	0.79386	-2.44051
C	-5.53948	1.07355	-5.10627
H	-7.66896	1.44741	-4.947
H	-3.40867	0.71156	-4.9329
H	-5.54222	1.03863	-6.19309

Zn	-0.01082	-0.02923	-0.09239
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Cartesian Coordinates of DFT optimized $\alpha\beta$ -1-Zn(NEt₃)



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N	-0.56695	1.81617	-0.80235
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C	3.60016	1.03994	1.99044
C	2.63586	0.08576	1.46551
H	3.66376	3.2408	1.80091
H	4.4504	0.78386	2.60562
C	2.64459	-1.29349	1.75376
C	1.25841	3.18629	0.23155
C	1.60925	-3.60545	1.69733
C	0.45708	-4.13327	1.16712
C	-0.23675	-3.05466	0.48148
C	1.63591	-2.19205	1.35142
H	2.36798	-4.11506	2.27278
H	0.09809	-5.15024	1.23262
C	-1.47944	-3.20156	-0.16601
C	-1.71825	2.13371	-1.5207
C	-1.7761	3.57263	-1.7253
C	-0.68063	4.11745	-1.09977
C	0.07441	3.02114	-0.51469
H	-2.56505	4.0892	-2.25219
H	-0.4065	5.15985	-1.02532
C	-3.43992	-2.29674	-1.48341
C	-3.78193	-1.06465	-1.98482
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H	-4.67198	-0.79549	-2.53456
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C	3.73211	-1.82064	2.64979
C	5.0351	-2.13209	2.16513
C	6.00928	-2.64059	3.06602
C	5.70758	-2.83209	4.42165
C	4.42058	-2.51918	4.90201
C	1.73183	4.5917	0.50502
C	1.22194	5.28755	1.63635
C	1.66943	6.59871	1.89231
C	3.09664	6.53673	-0.05709
C	2.67496	5.2209	-0.34628
H	1.27866	7.12665	2.76102
C	-3.86016	1.77596	-2.7532
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C	-3.70014	1.93493	-4.14445
C	-2.15195	-4.54977	-0.11114

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C	-3.67147	-6.10215	1.00202
C	-3.43722	-7.08635	0.01914
C	-2.55042	-6.77672	-1.02967
C	-1.90292	-5.52483	-1.10995
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H	-2.3561	-7.52022	-1.80083
C	3.44837	-2.02114	4.01698
H	3.82117	7.01473	-0.7142
H	2.45382	-1.77857	4.38193
H	6.99869	-2.87774	2.68464
H	4.1768	-2.6608	5.9518
H	-2.75113	1.65772	-4.59702
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H	6.46552	-3.21968	5.09778
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H	3.78615	3.59676	-1.27549
H	2.44403	4.19812	-2.25356
H	3.9318	5.15454	-2.11156
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H	-2.42245	-3.46954	2.5297
H	-3.8188	-2.91616	1.61939
H	-4.00621	-4.22706	2.79951
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H	-1.27282	-4.36809	-2.84214
H	0.0644	-5.04519	-1.90726
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H	-5.20834	-8.33432	0.19086
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C	-4.91783	1.21278	4.09839
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H	-8.16212	2.29946	4.25524
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C	6.25636	-1.66792	-1.71695
C	7.11458	-2.63799	-2.29728
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C	7.57853	-2.48241	-3.61352
H	7.4082	-3.50413	-1.71037
C	6.34744	-0.38882	-3.80553
H	5.2318	0.21241	-2.04727
C	7.19774	-1.35849	-4.37371
H	8.23527	-3.23344	-4.04589
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H	2.66908	1.00793	-1.6229
C	2.74624	0.55468	-3.7354
H	2.20849	0.9773	-4.55827
H	3.71075	1.01283	-3.66663
H	2.86152	-0.49814	-3.88768
C	1.25804	-2.85193	-1.65173
H	1.88207	-3.56211	-1.1506
H	0.42651	-2.60355	-1.02582
H	0.90127	-3.27444	-2.56776
H	2.60892	-1.7112	-2.87044
H	0.76438	-0.80474	-4.12597
C	-0.74456	0.53708	-3.39272
H	-0.33138	1.2212	-4.10417
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