Supporting Information

Double-decker bis(tetradiazepinoporphyrazinato) rare earth complexes: crucial role of intramolecular hydrogen bonding

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Table S1. Yields and MALDI-TOF/TOF mass spectrometric data for compounds **2a–g**

Compound		Yield, %	Mass $[M+H]^+$	
			calculated [a]	found
2a	$C_{216}H_{224}LuN_{32}$	85	3444.814	3444.775
2b	$C_{216}H_{224}ErN_{32}$	65	3436.805	3436.963
2c	$C_{216}H_{224}DyN_{32}$	69	3432.801	3433.047
2d	$C_{216}H_{224}EuN_{32}$	75	3422.793	3423.041
2e	$C_{216}H_{224}NdN_{32}$	80	3413.784	3414.124
2f	$C_{216}H_{224}CeN_{32}$	55	3408.771	3408.771
2g	$C_{216}H_{224}LaN_{32}$	83	3408.779	3409.169

[a] The value corresponds to the most abundant isotopic peak of the protonated molecular ion $[M+H]^+$, M = $[^{tBuPh}DzPz]_2LnH$ or $[^{tBuPh}DzPz]_2Ln$ for **2a–e, 2g** and **2f**, respectively.

High-resolution mass spectra

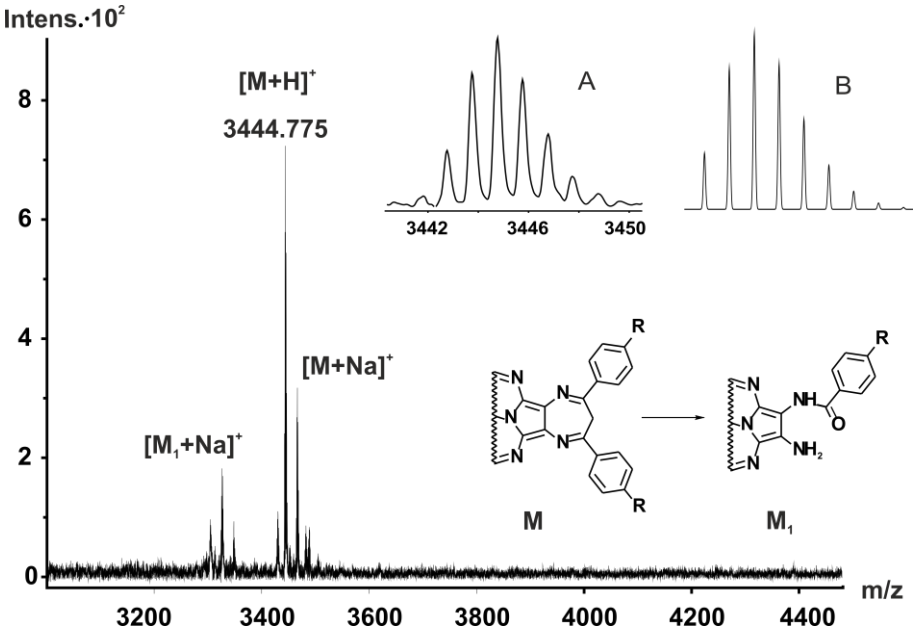


Fig. S1 MALDI-TOF/TOF mass spectrum of [$^{t\text{BuPh}}$DzPz]$_2$Lu (**2a**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).

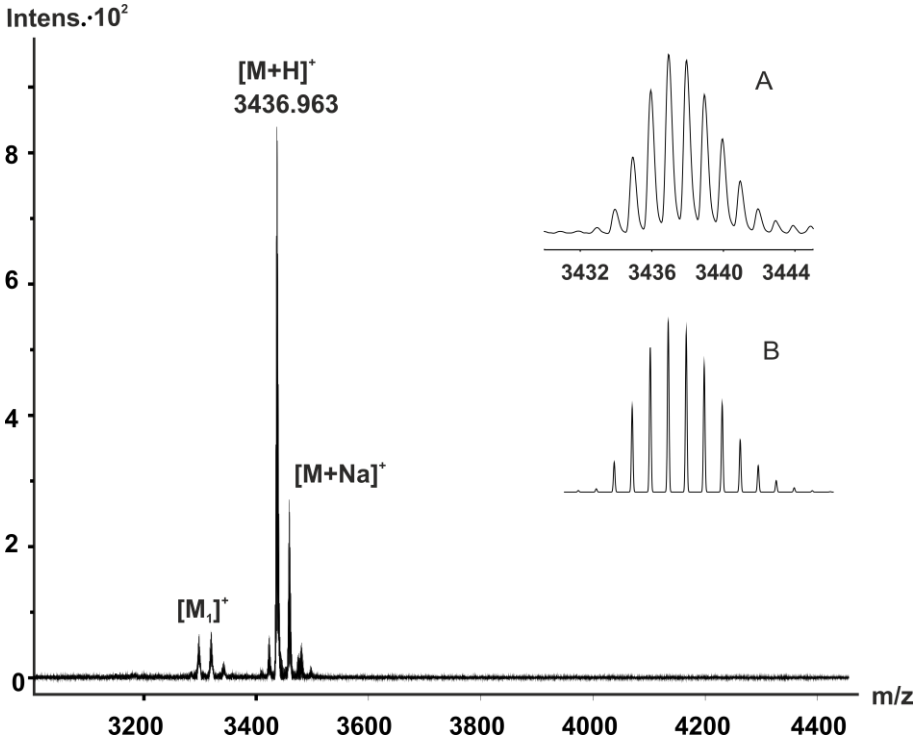


Fig. S2 MALDI-TOF/TOF mass spectrum of [$^{t\text{BuPh}}$DzPz]$_2$Er (**2b**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).

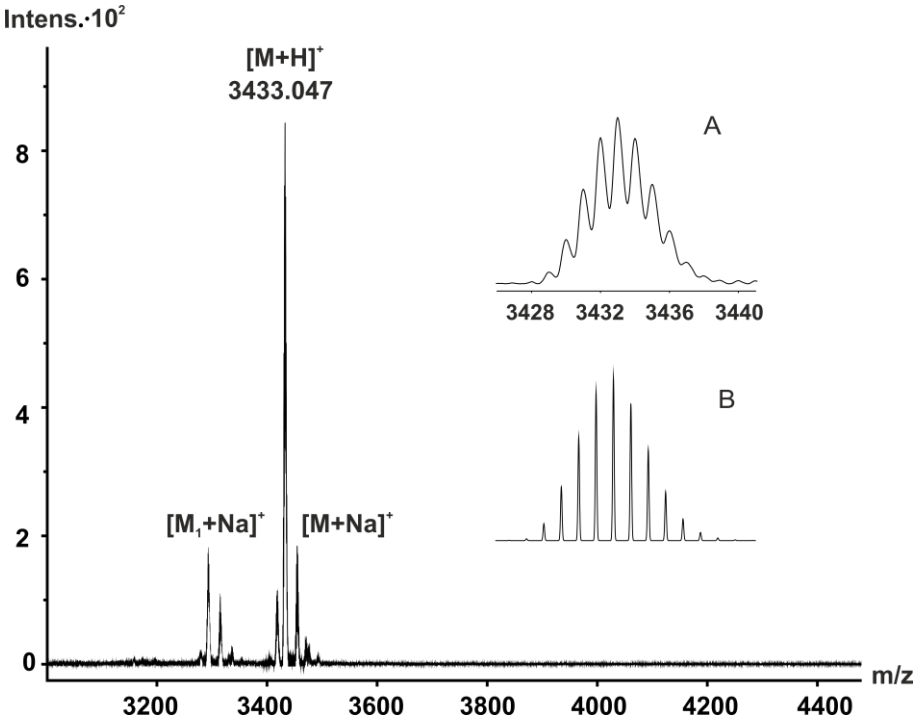


Fig. S3 MALDI-TOF/TOF mass spectrum of [^{tBuPh}DzPz]$_2$Dy (**2c**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).

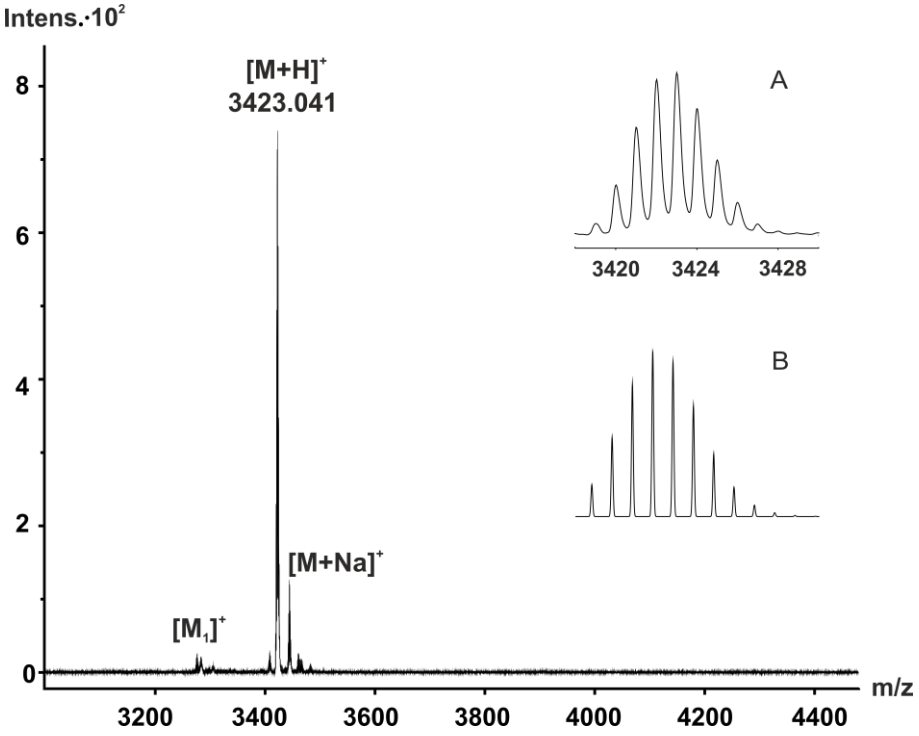


Fig. S4 MALDI-TOF/TOF mass spectrum of [^{tBuPh}DzPz]$_2$Eu (**2d**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).

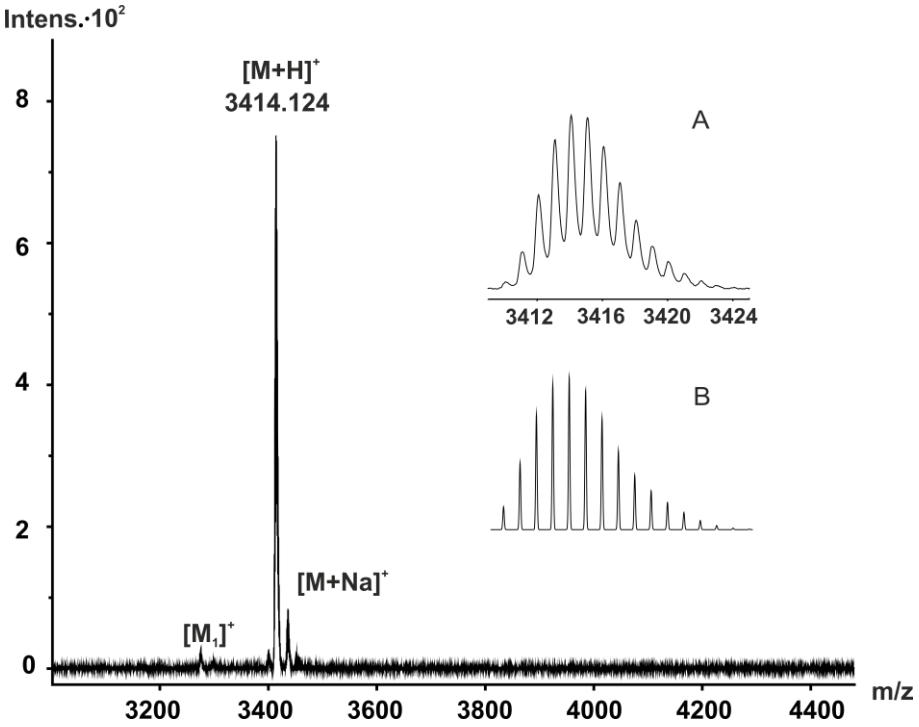


Fig. S5 MALDI-TOF/TOF mass spectrum of [$^{t\text{BuPh}}$DzPz]$_2$Nd (**2e**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).[1]

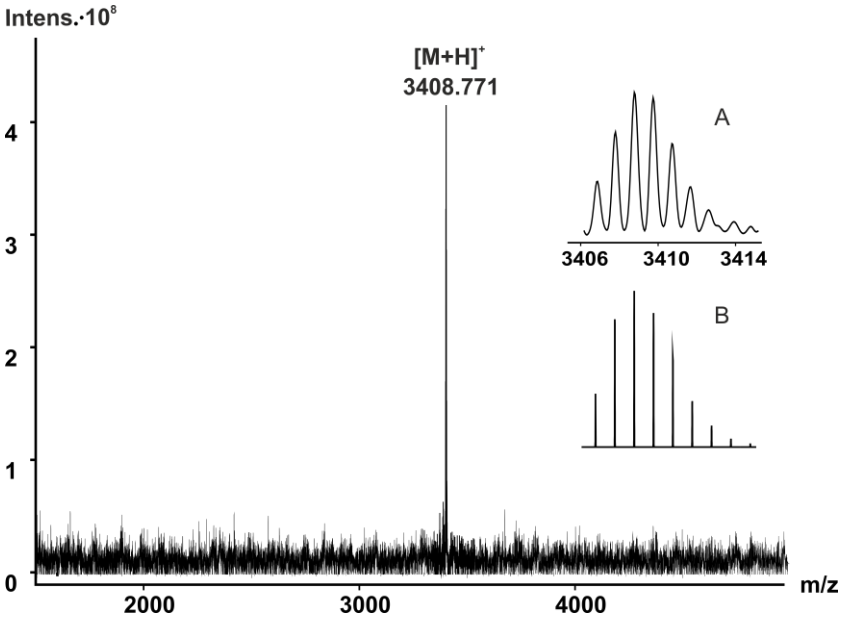


Fig. S6 MALDI-TOF/TOF mass spectrum of [$^{t\text{BuPh}}$DzPz]$_2$Ce (**2f**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).[2]

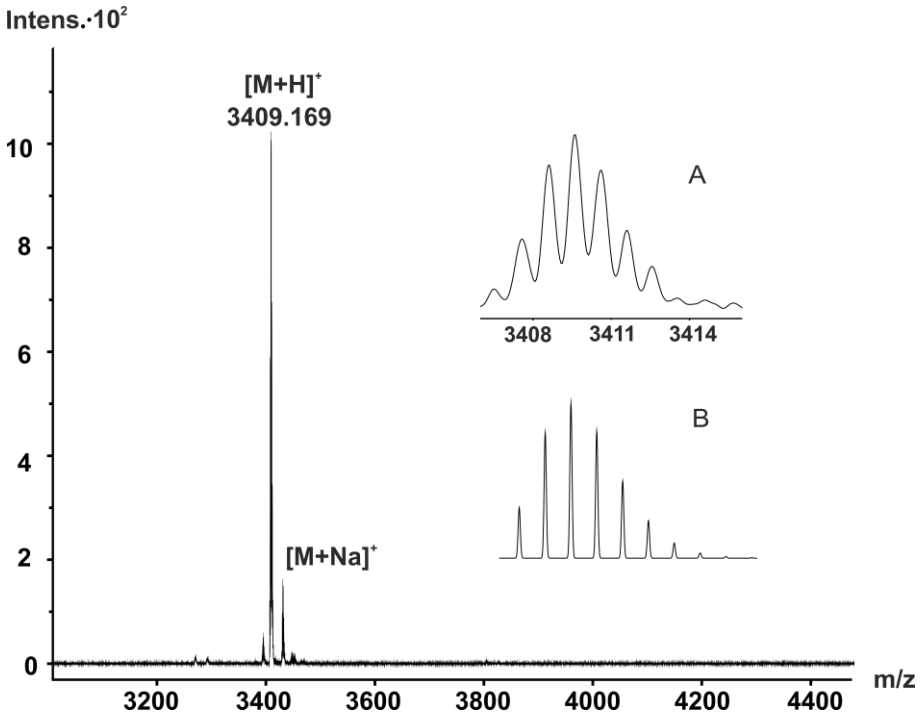
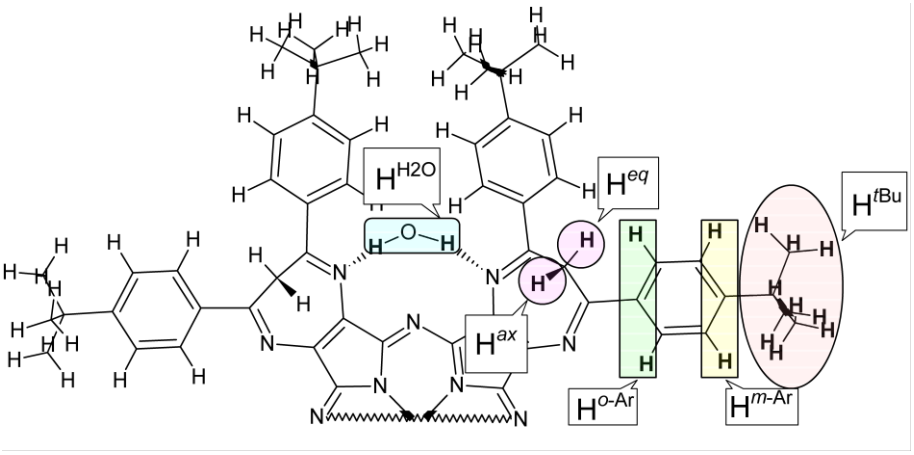


Fig. S7 MALDI-TOF/TOF mass spectrum of [$^{t\text{BuPh}}$DzPz]$_2$La (**2g**). Inset: isotopic pattern for the molecular ion (A) and simulated MS pattern of the molecular ion (B).[1]

^{1}H NMR spectra



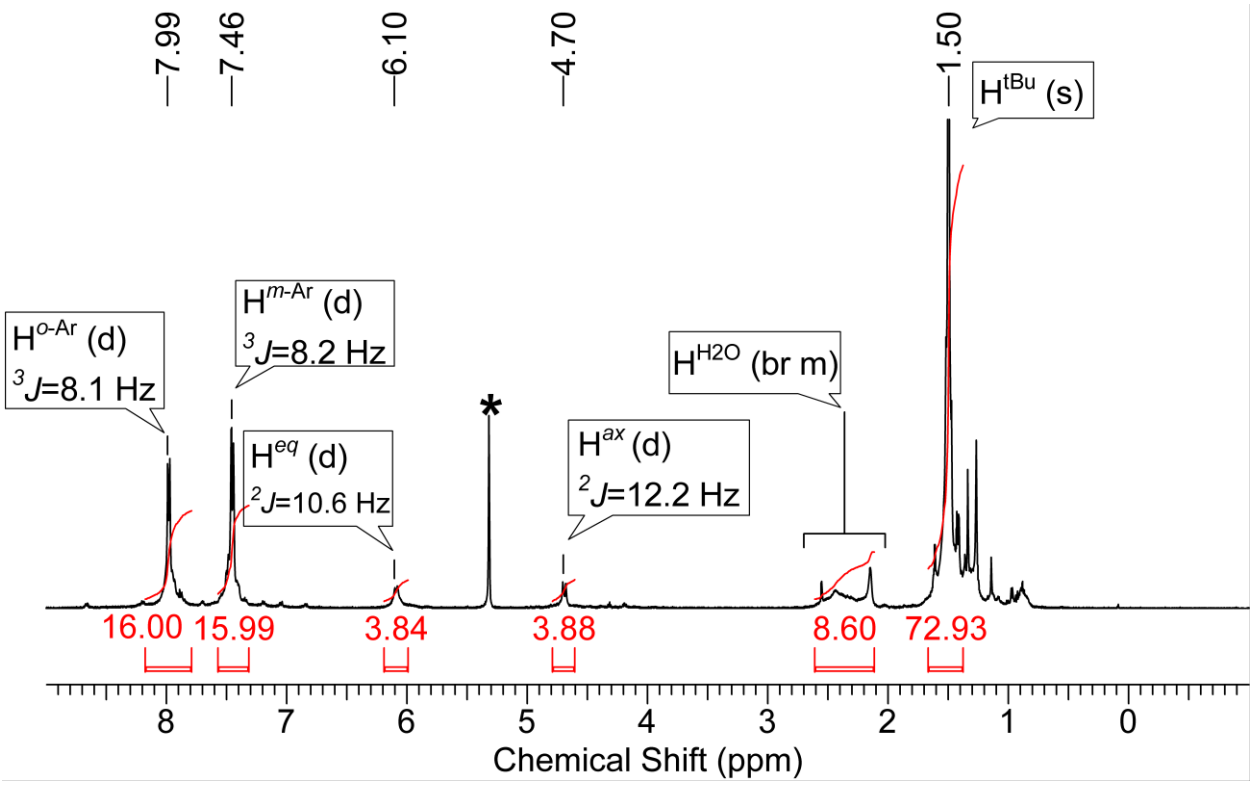


Fig. S8 ^{1}H NMR spectrum of **1** in CD_2Cl_2.

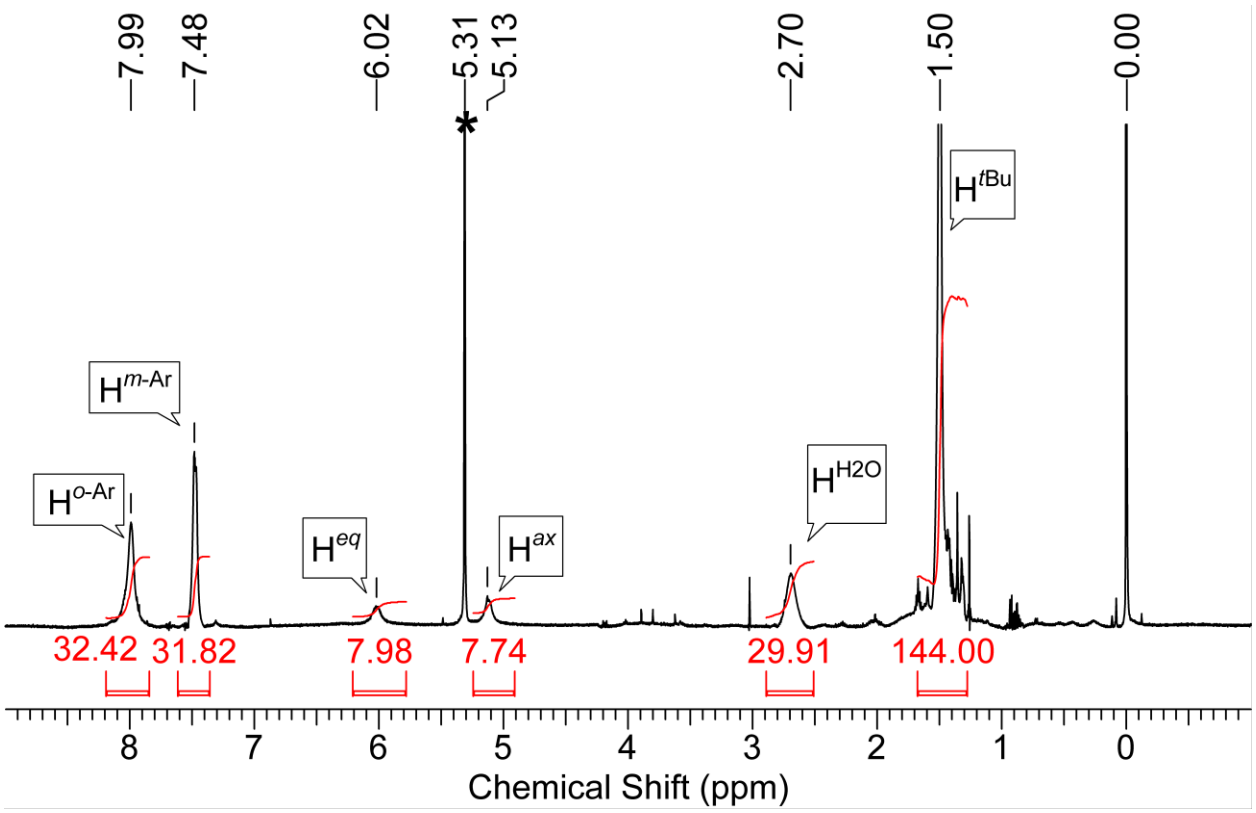


Fig. S9 ^{1}H NMR spectrum of **2a** in CD_2Cl_2.

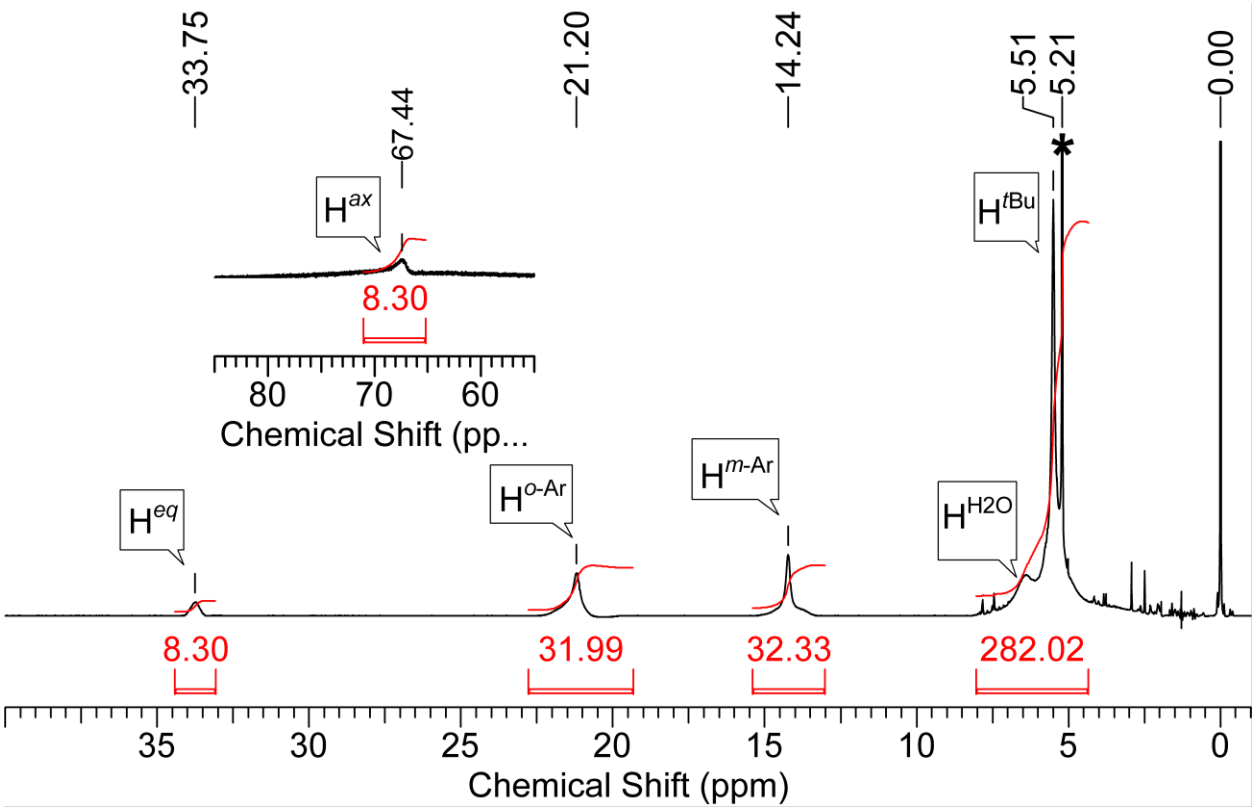


Fig. S10 ^{1}H NMR spectrum of **2b** in CD_2Cl_2.

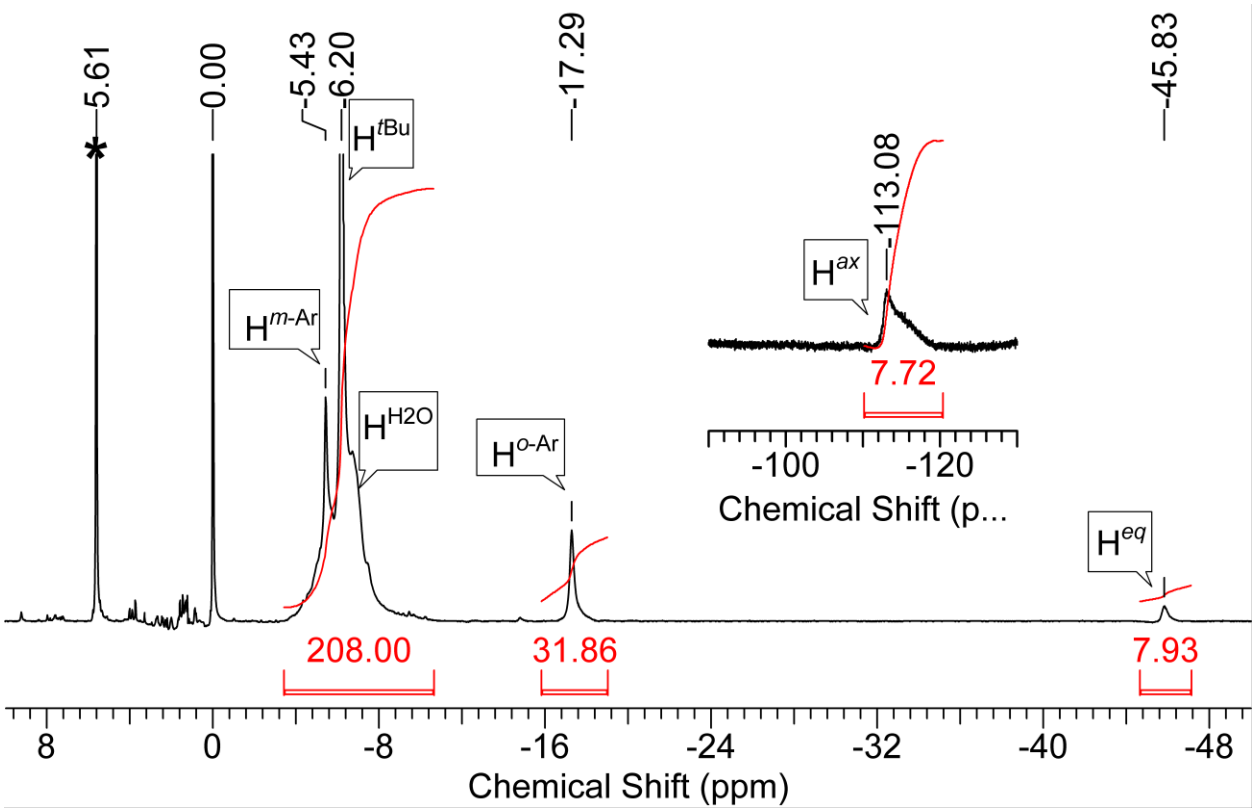


Fig. S11 ^{1}H NMR spectrum of **2c** in CD_2Cl_2.

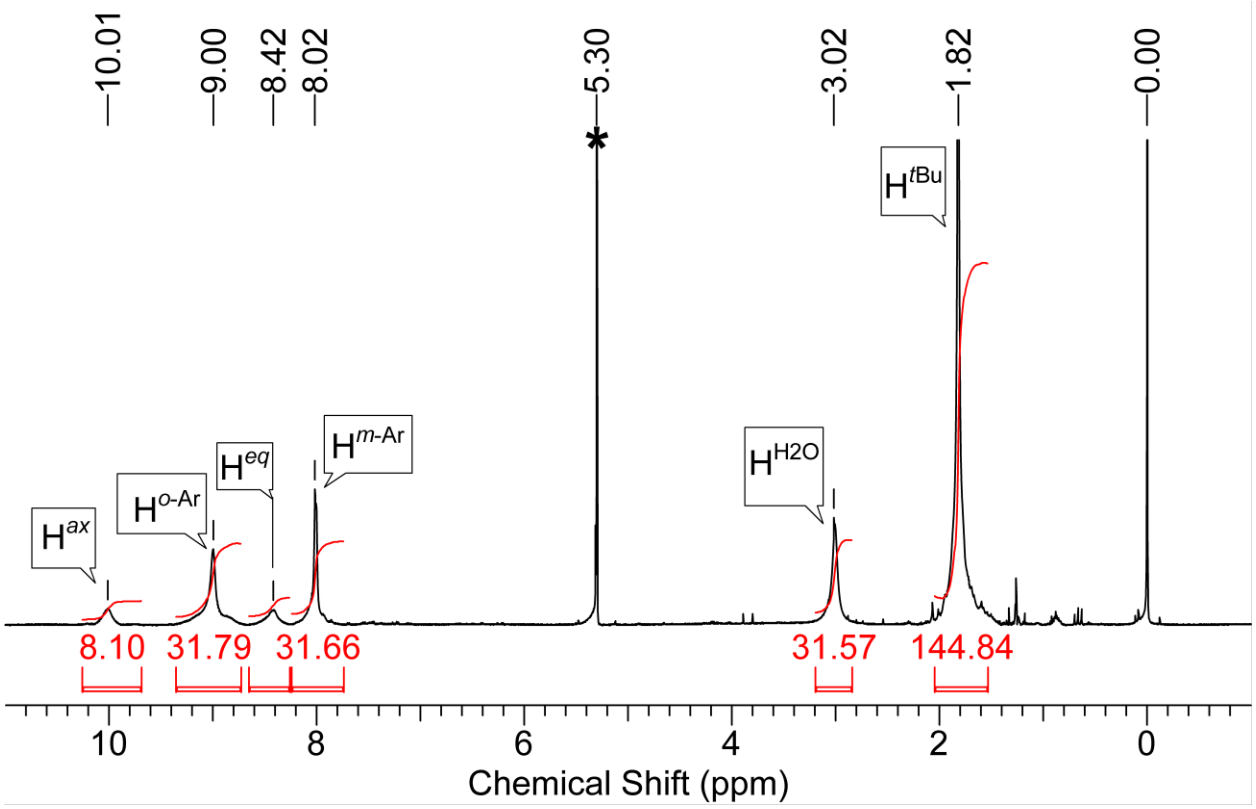


Fig. S12 ^{1}H NMR spectrum of **2d** in CD_2Cl_2.

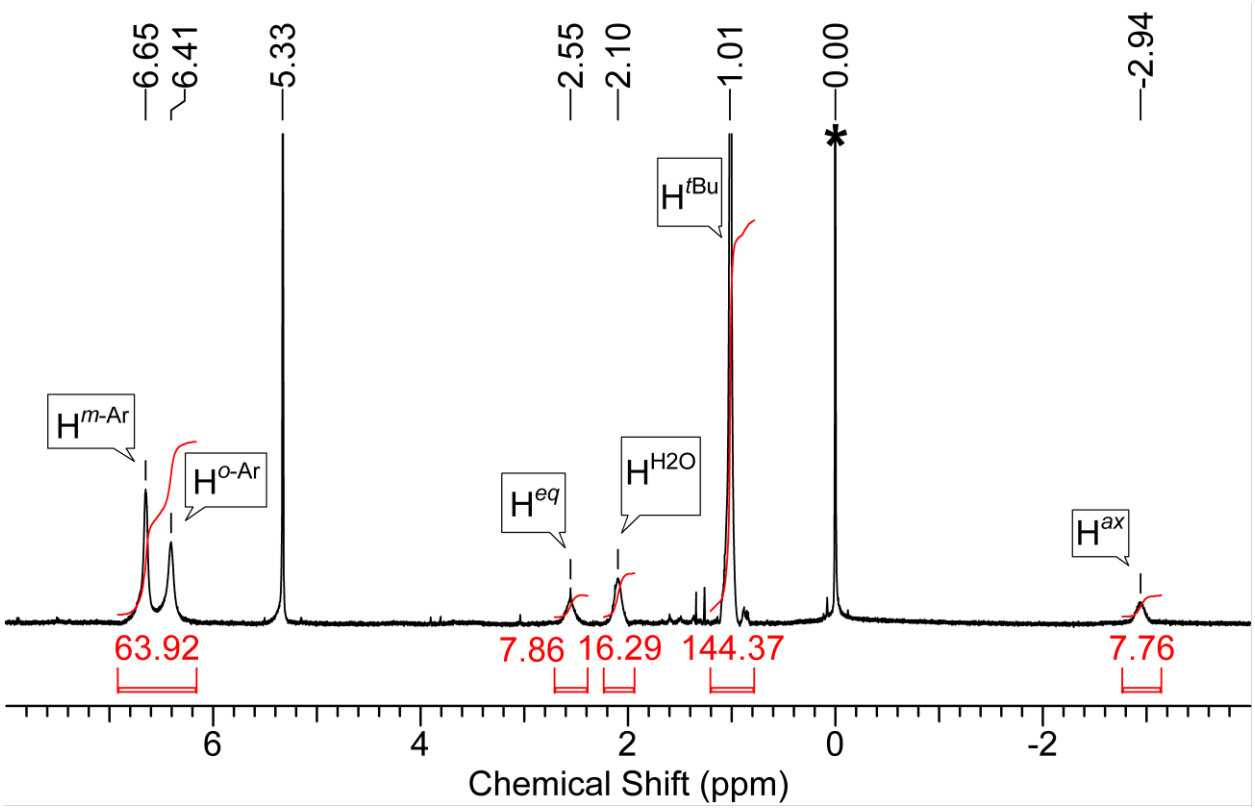


Fig. S13 ^{1}H NMR spectrum of **2e** in CD_2Cl_2.[1]

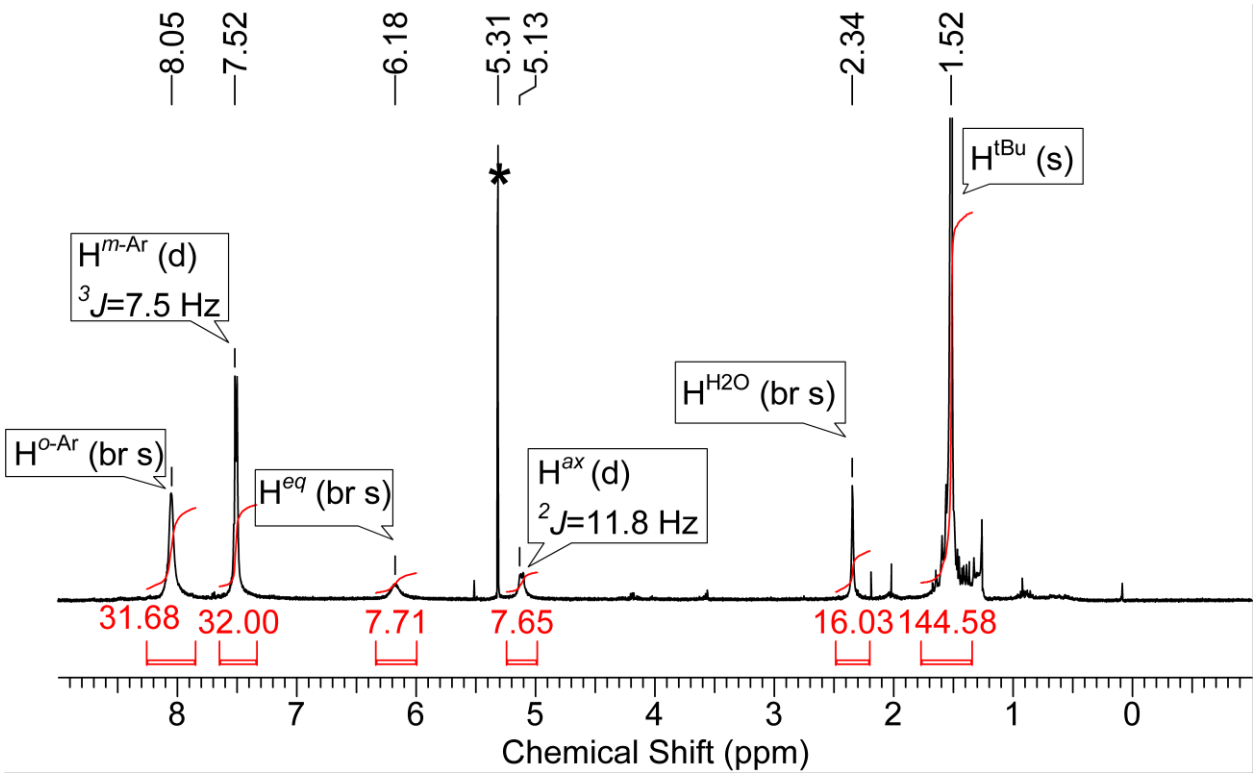


Fig. S14 ^{1}H NMR spectrum of **2f** in CD_2Cl_2.[2]

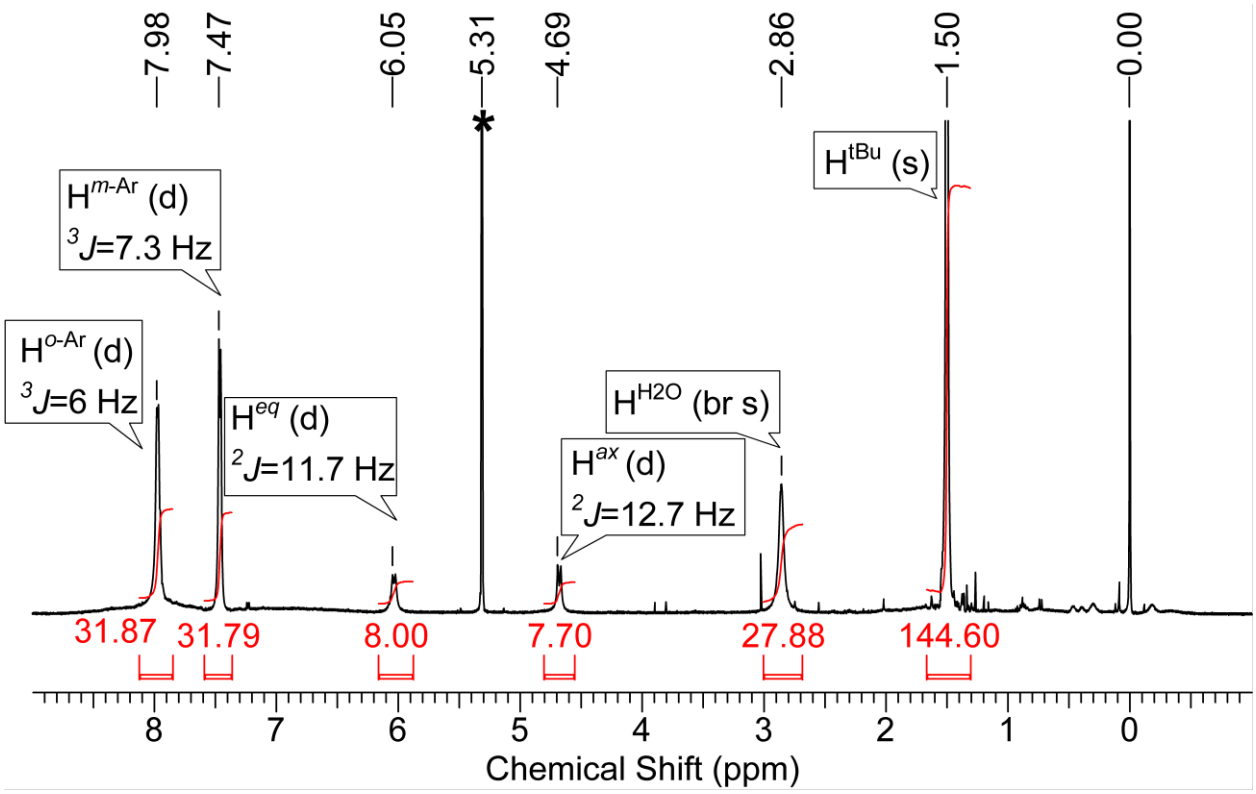


Fig. S15 ^{1}H NMR spectrum of **2g** in CD_2Cl_2.[1]

^{13}C NMR spectra

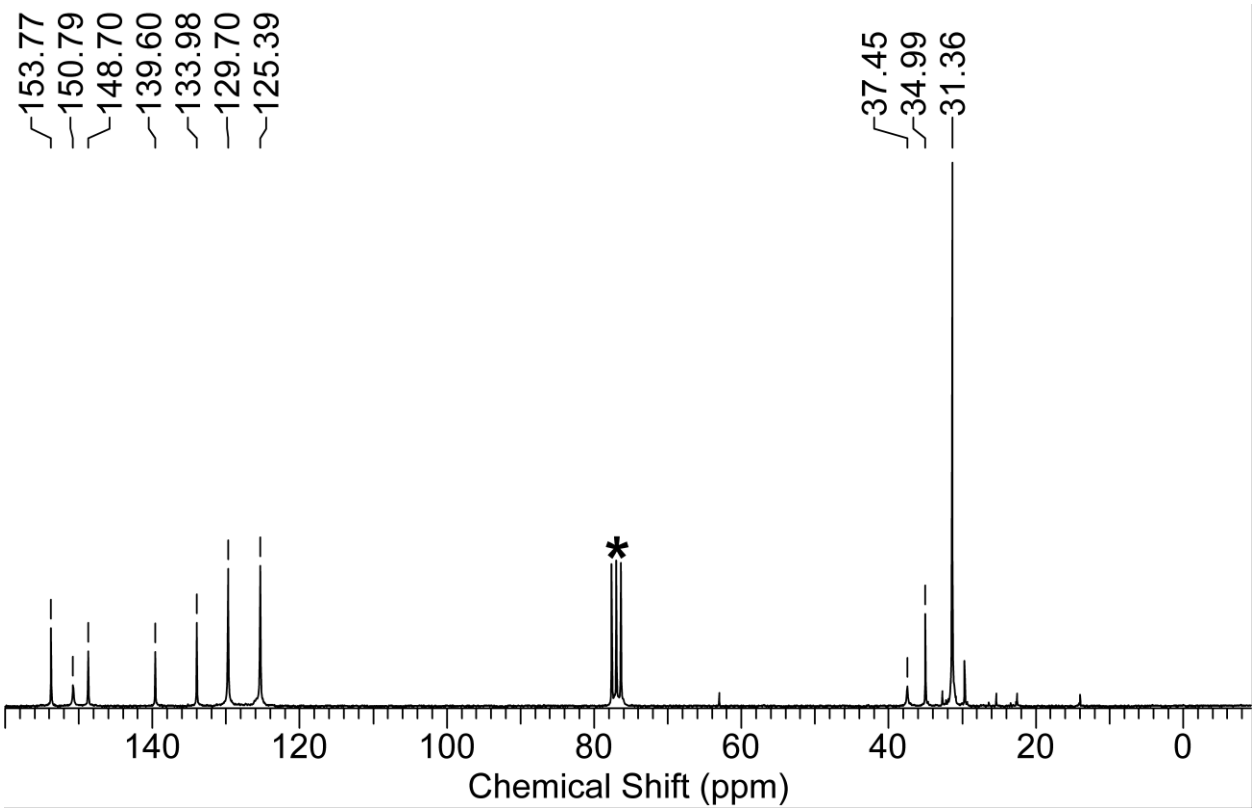


Fig. S16 ^{13}C NMR spectrum of **1** in $CDCl_3$.

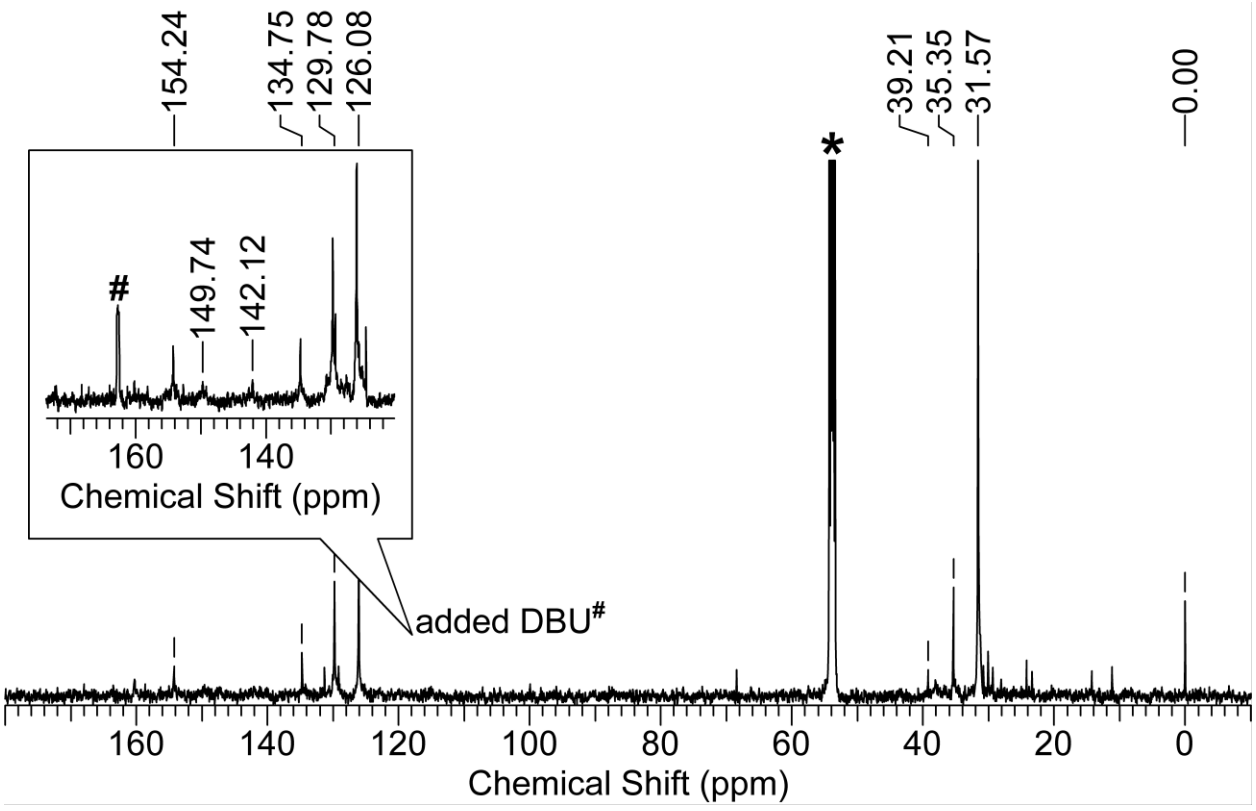


Fig. S17 ^{13}C NMR spectrum of **2a** in CD_2Cl_2.

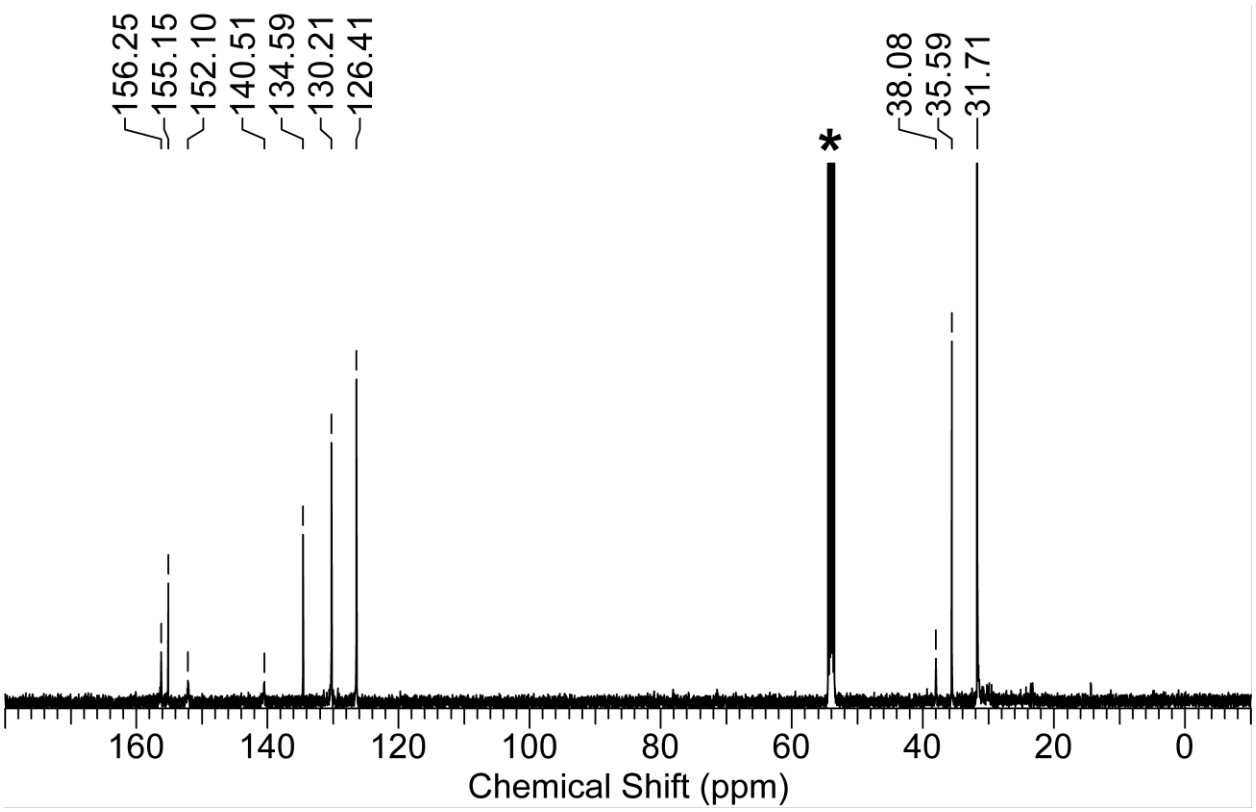


Fig. S18 ^{13}C NMR spectrum of **2f** in CD_2Cl_2.[2]

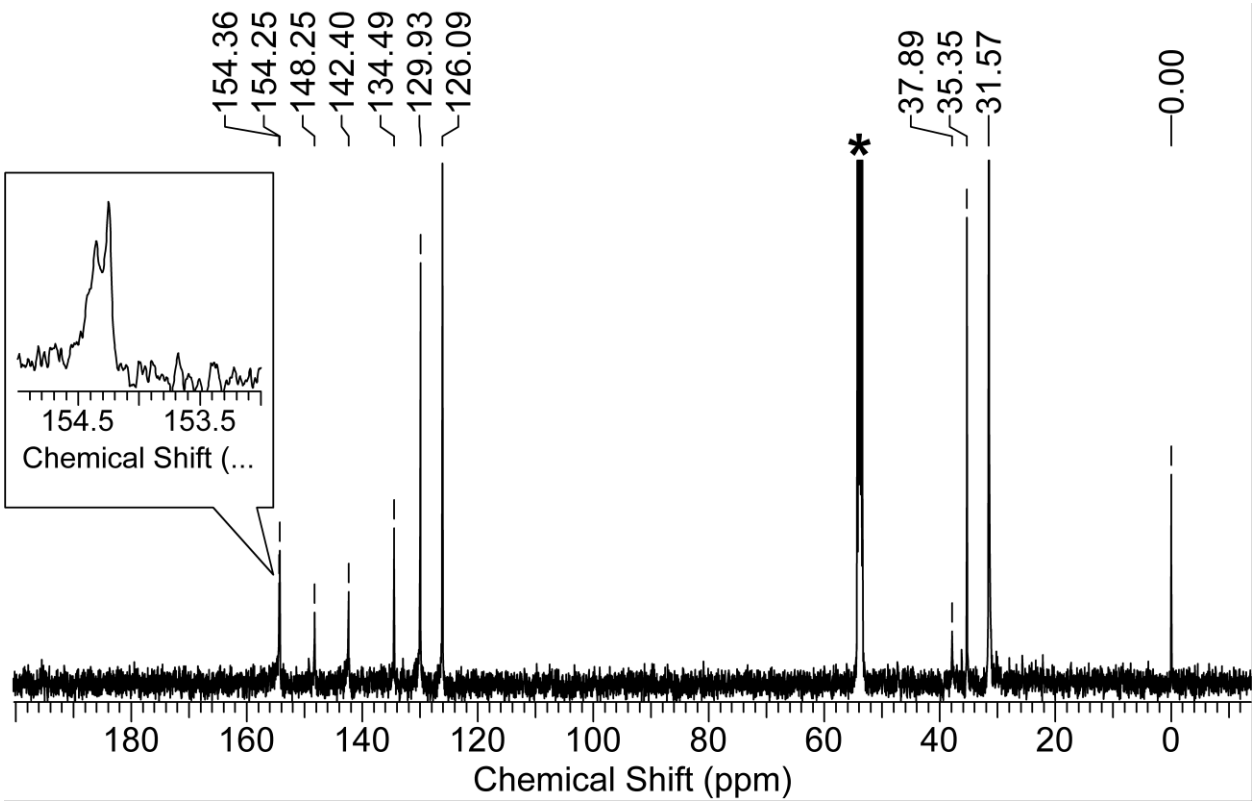


Fig. S19 ^{13}C NMR spectrum of **2g** in CD_2Cl_2.[1]

Two-dimensional NMR spectra

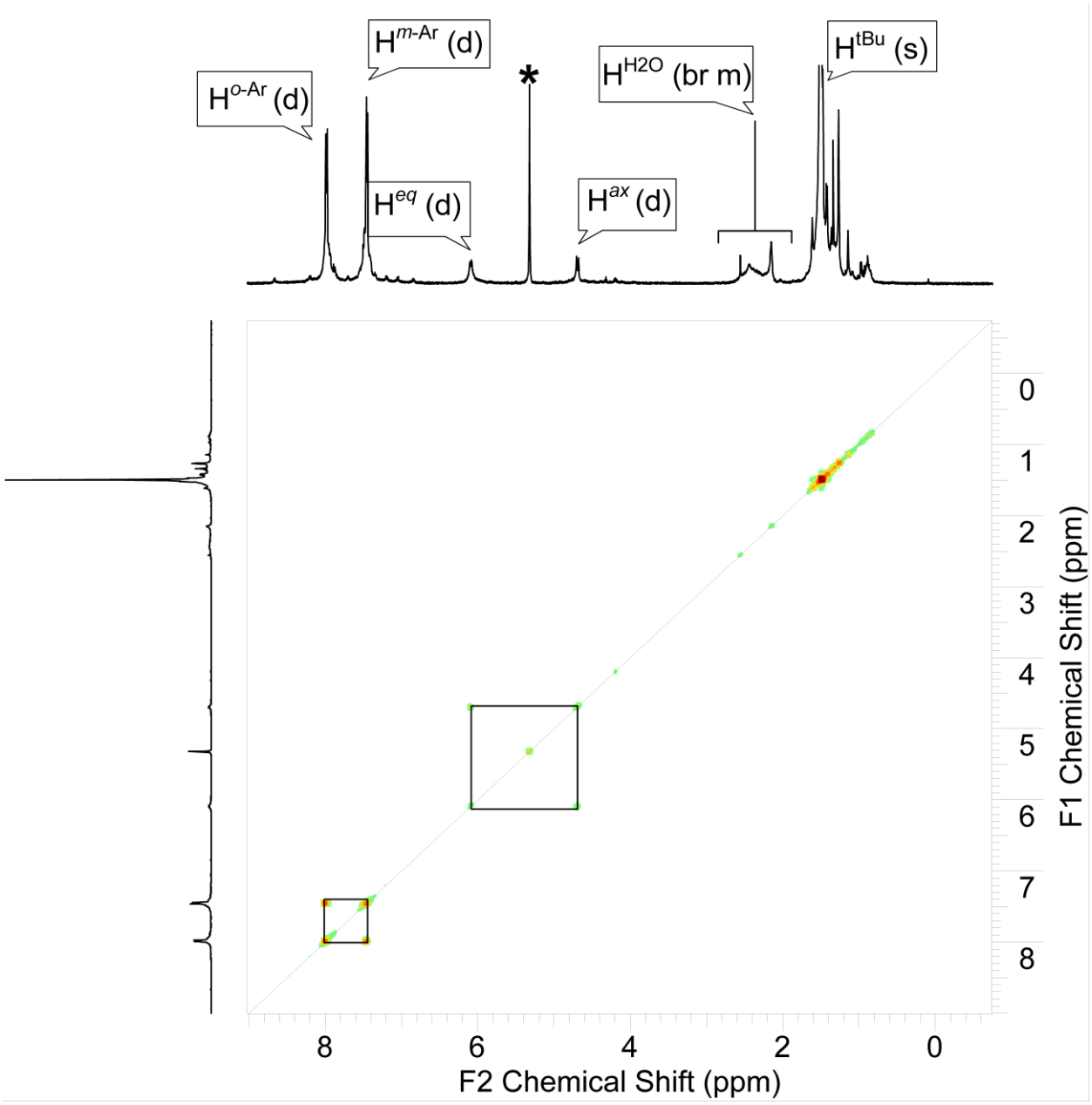


Fig. S20 ^{1}H-^{1}H COSY of **1** in CD_2Cl_2.

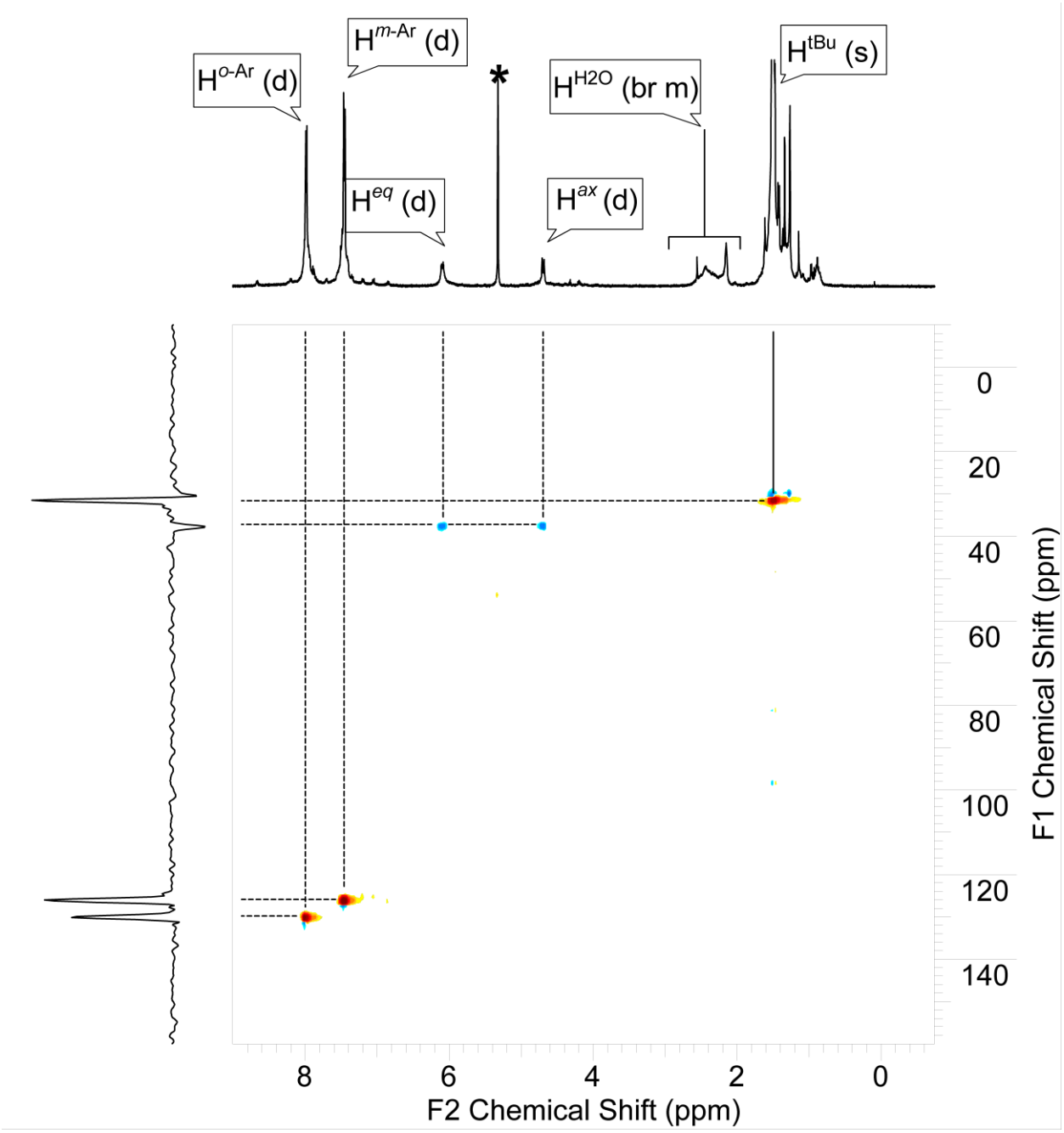


Fig. S21 ^{1}H-^{13}C HSQC of **1** in CD_2Cl_2.

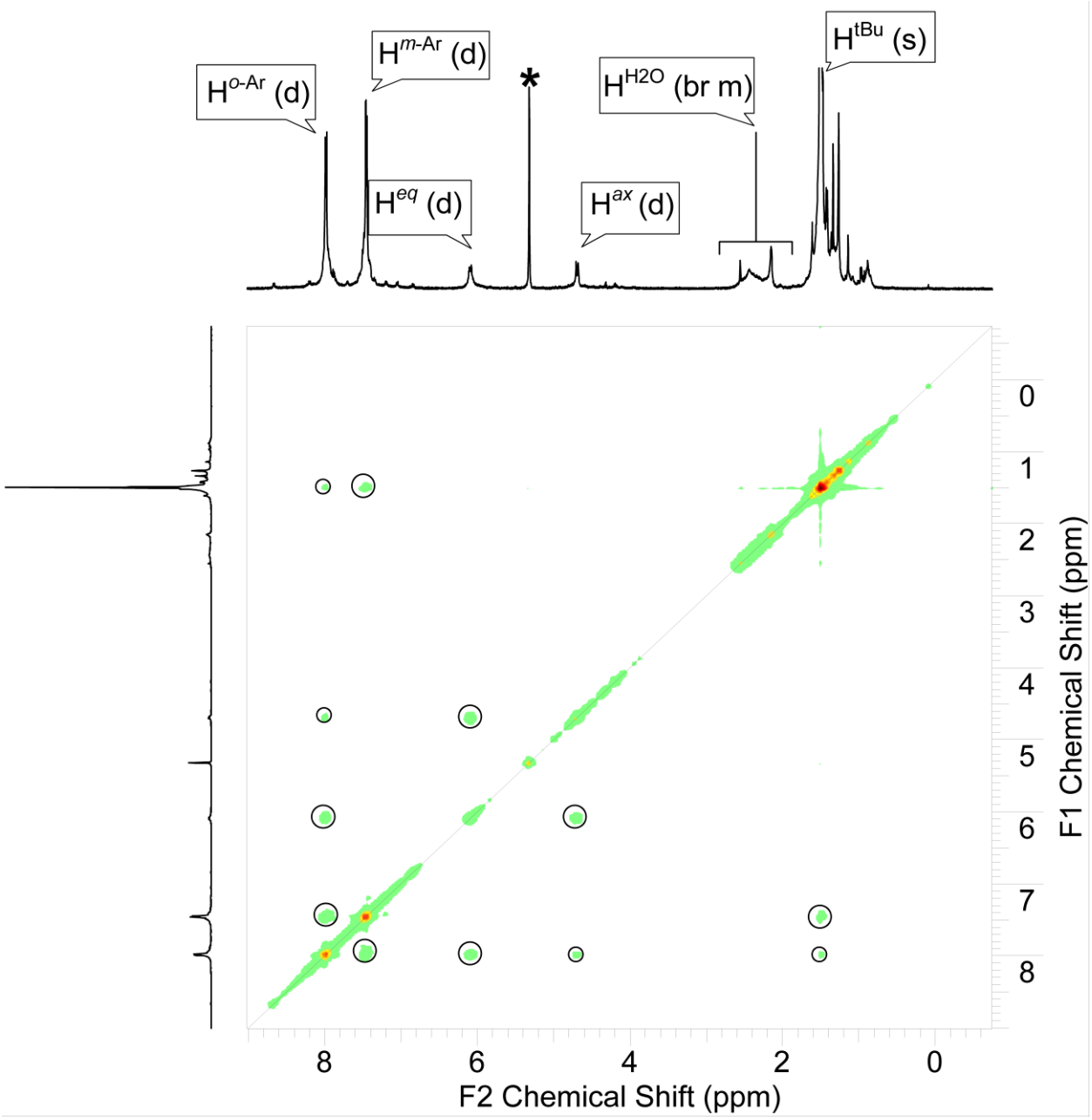


Fig. S22 ^{1}H-^{1}H NOESY of **1** in CD_2Cl_2.

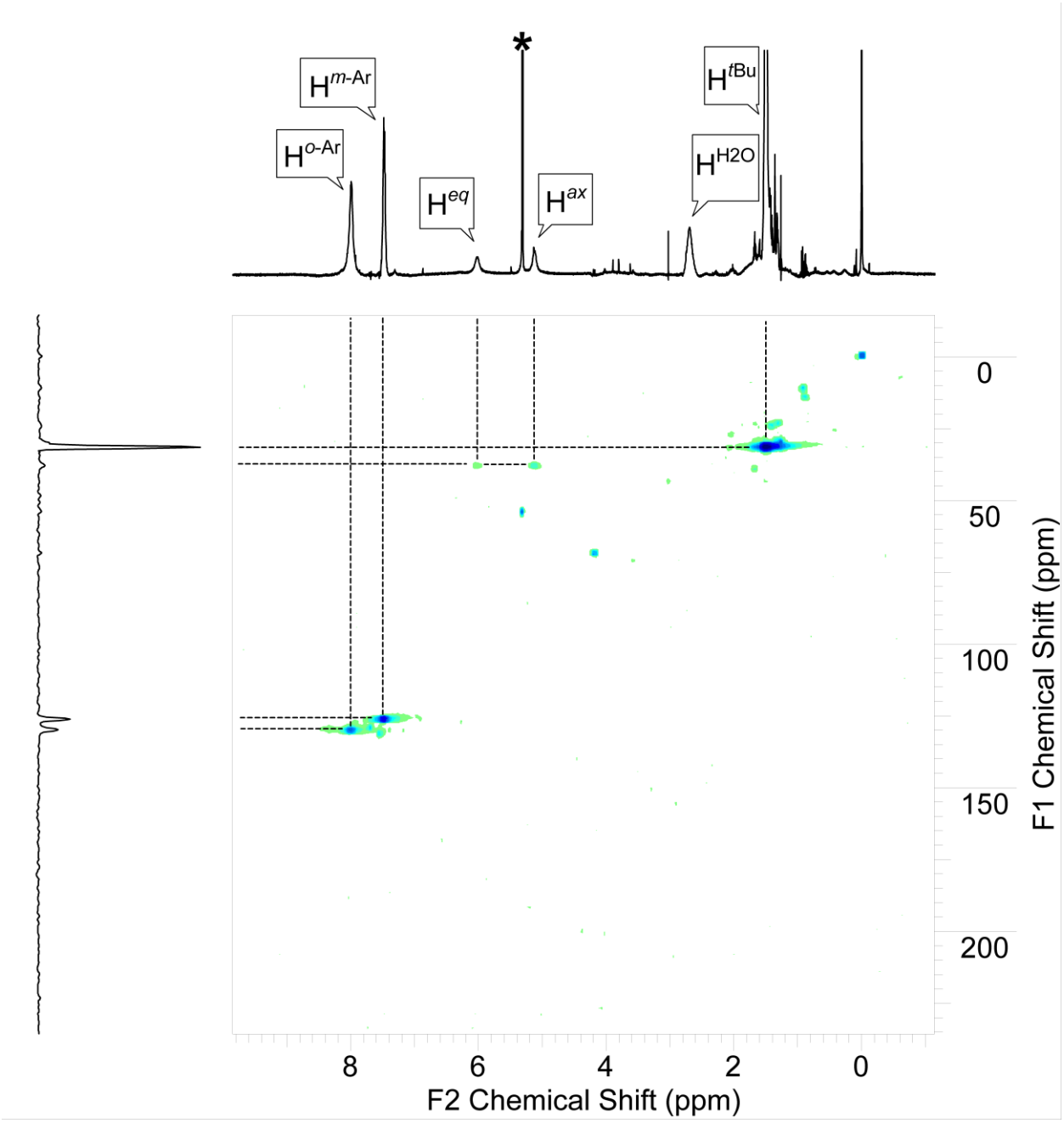


Fig. S23 ^{1}H-^{13}C HMQC of **2a** in CD_2Cl_2.

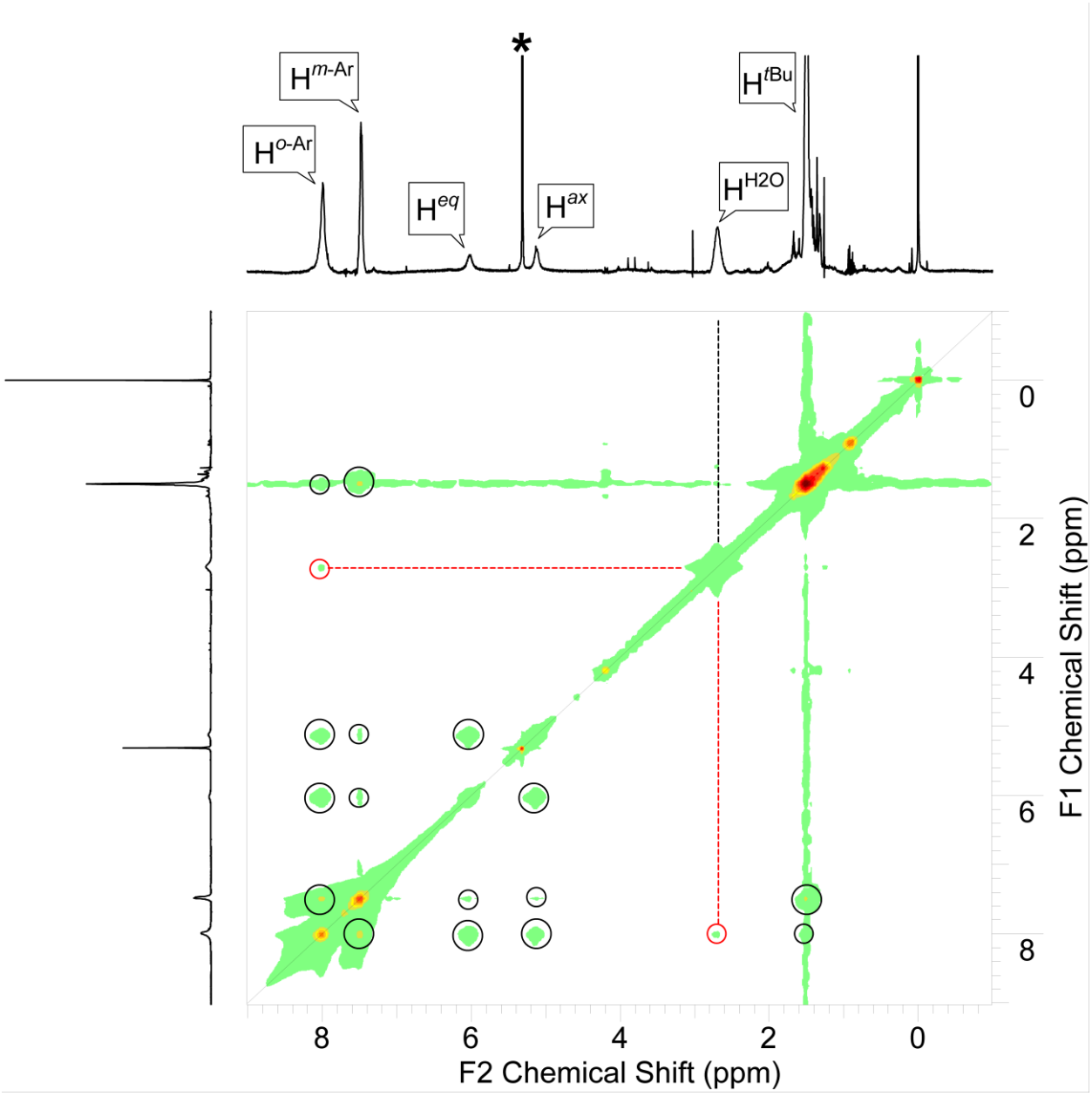


Fig. S24 ^{1}H-^{1}H NOESY of **2a** in CD_2Cl_2.

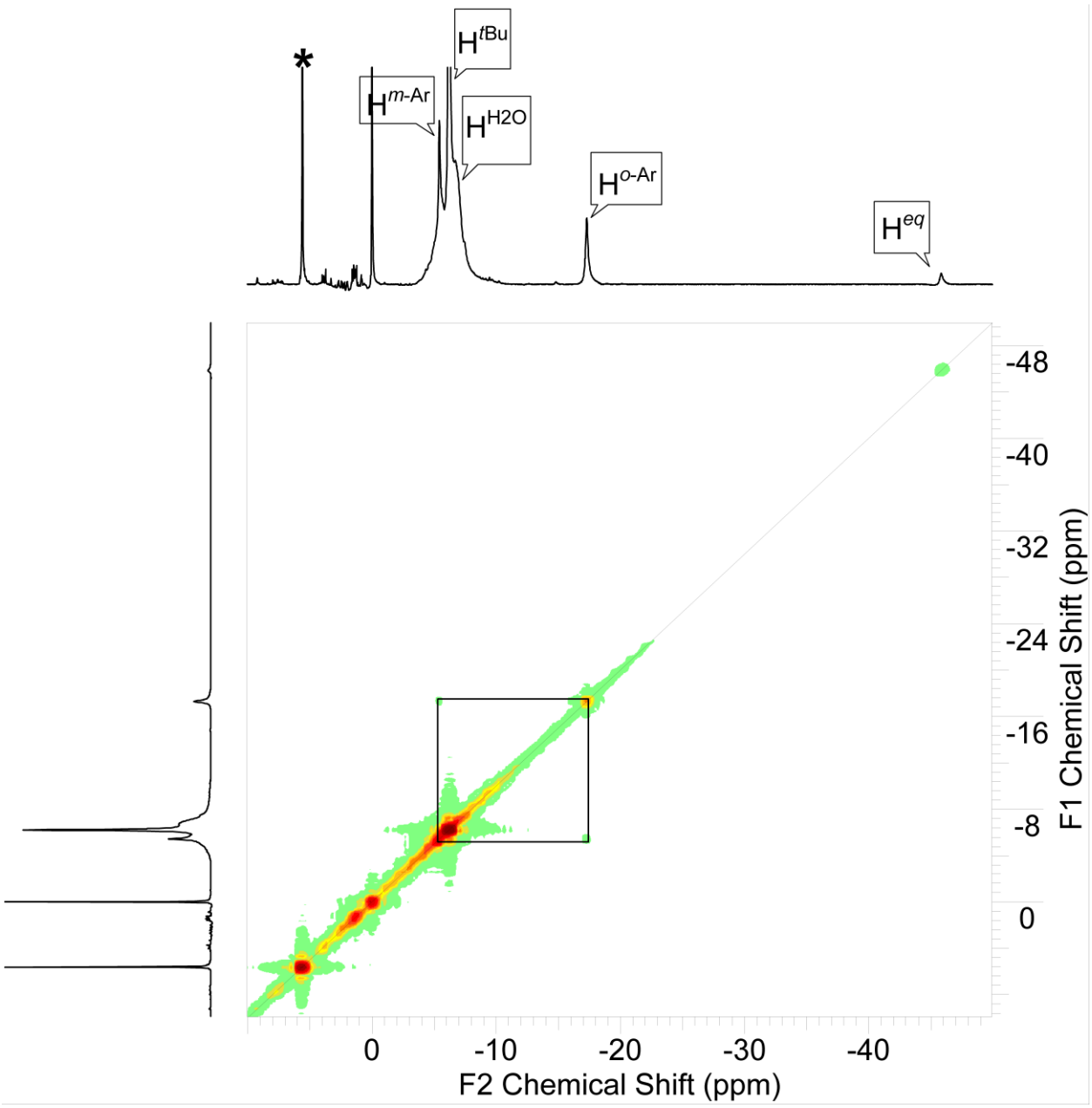


Fig. S25 ^{1}H-^{1}H COSY NMR spectrum of **2c** in CD_2Cl_2.

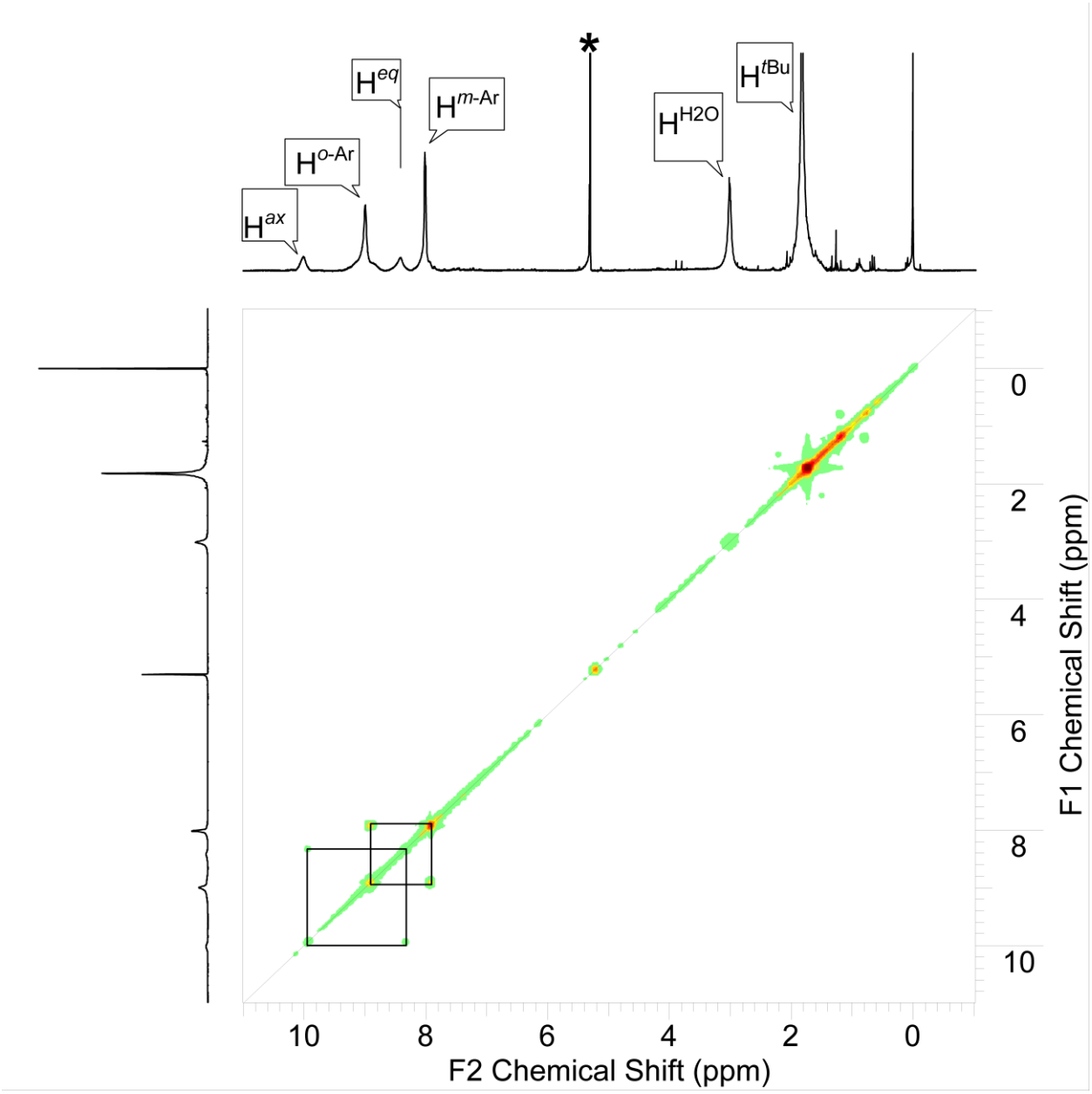


Fig. S26 ^{1}H-^{1}H COSY NMR spectrum of **2d** in CD_2Cl_2.

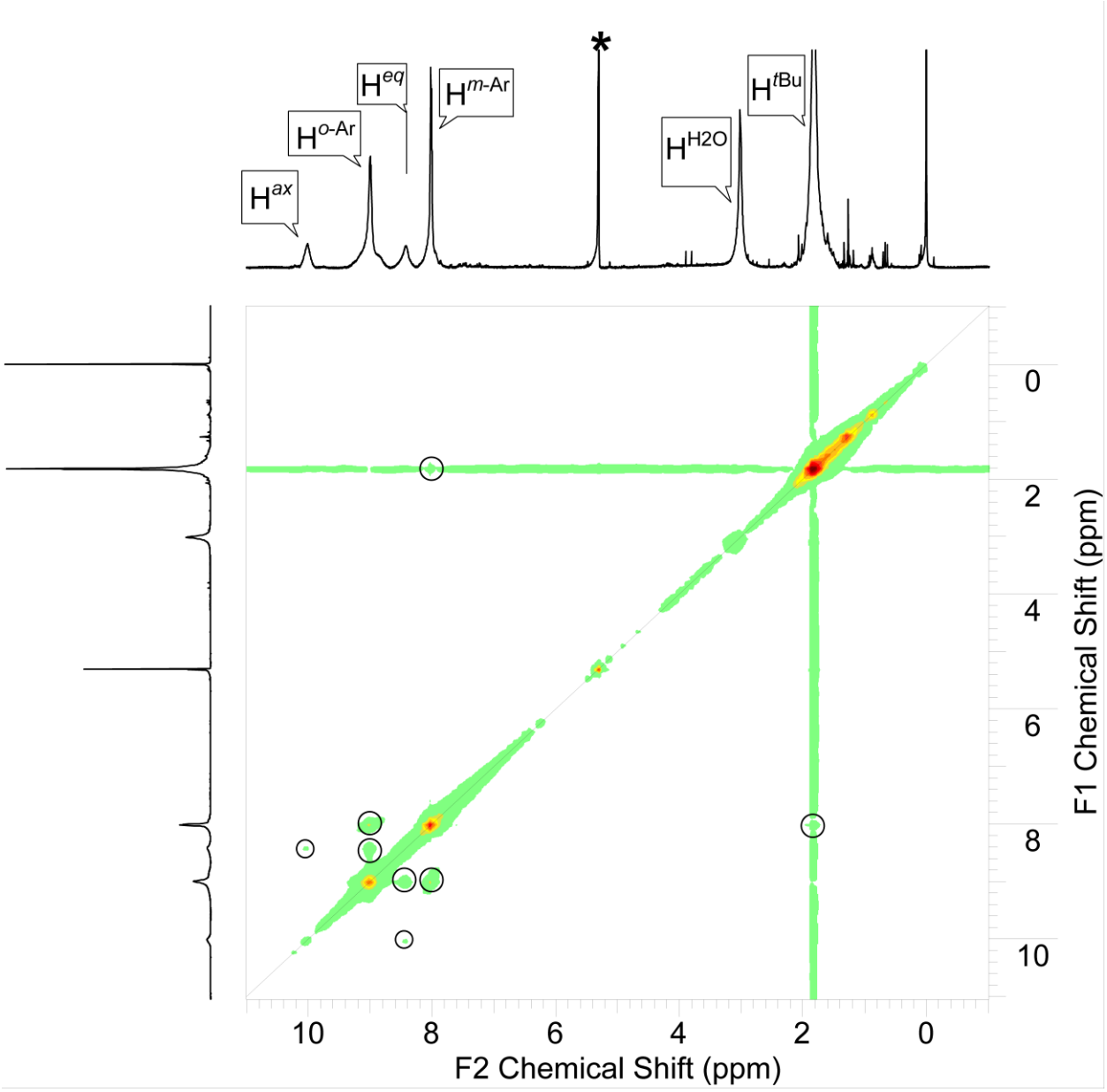


Fig. S27 ^{1}H-^{1}H NOESY NMR spectrum of **2d** in CD_2Cl_2.

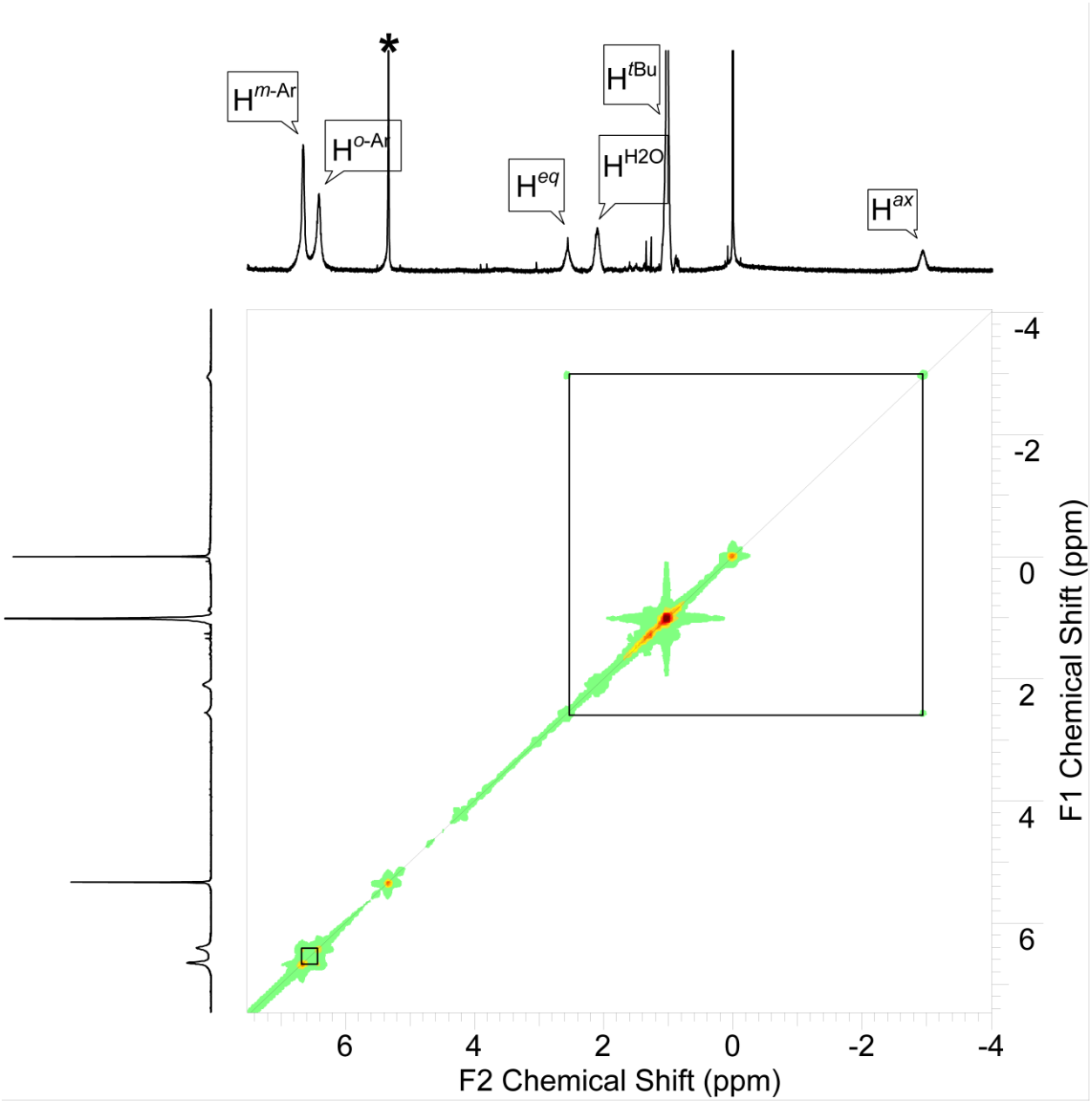


Fig. S28 ^{1}H-^{1}H COSY NMR spectrum of **2e** in CD_2Cl_2.[1]

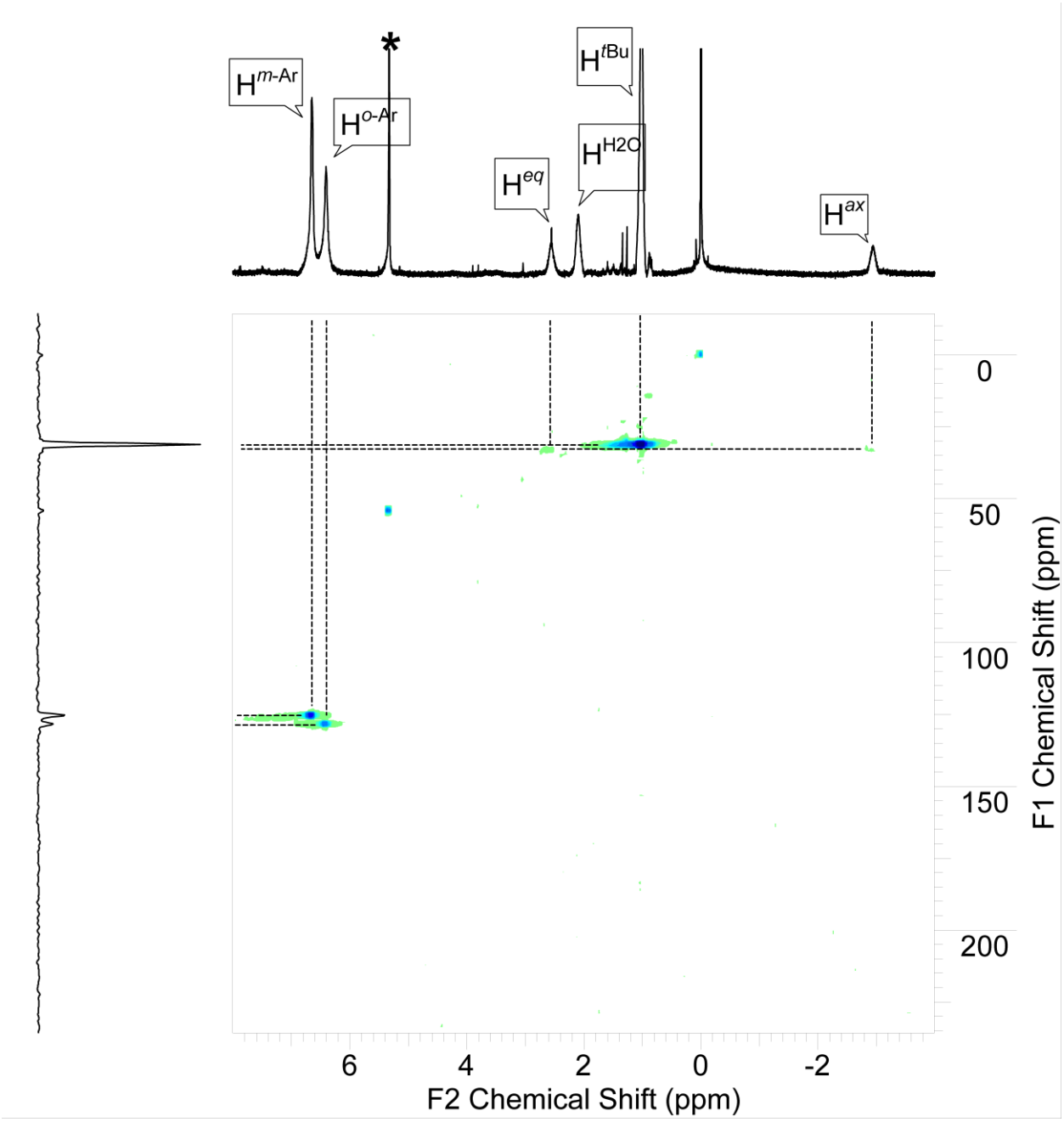


Fig. S29 ^{1}H-^{13}C HMQC spectrum of **2e** in CD_2Cl_2.

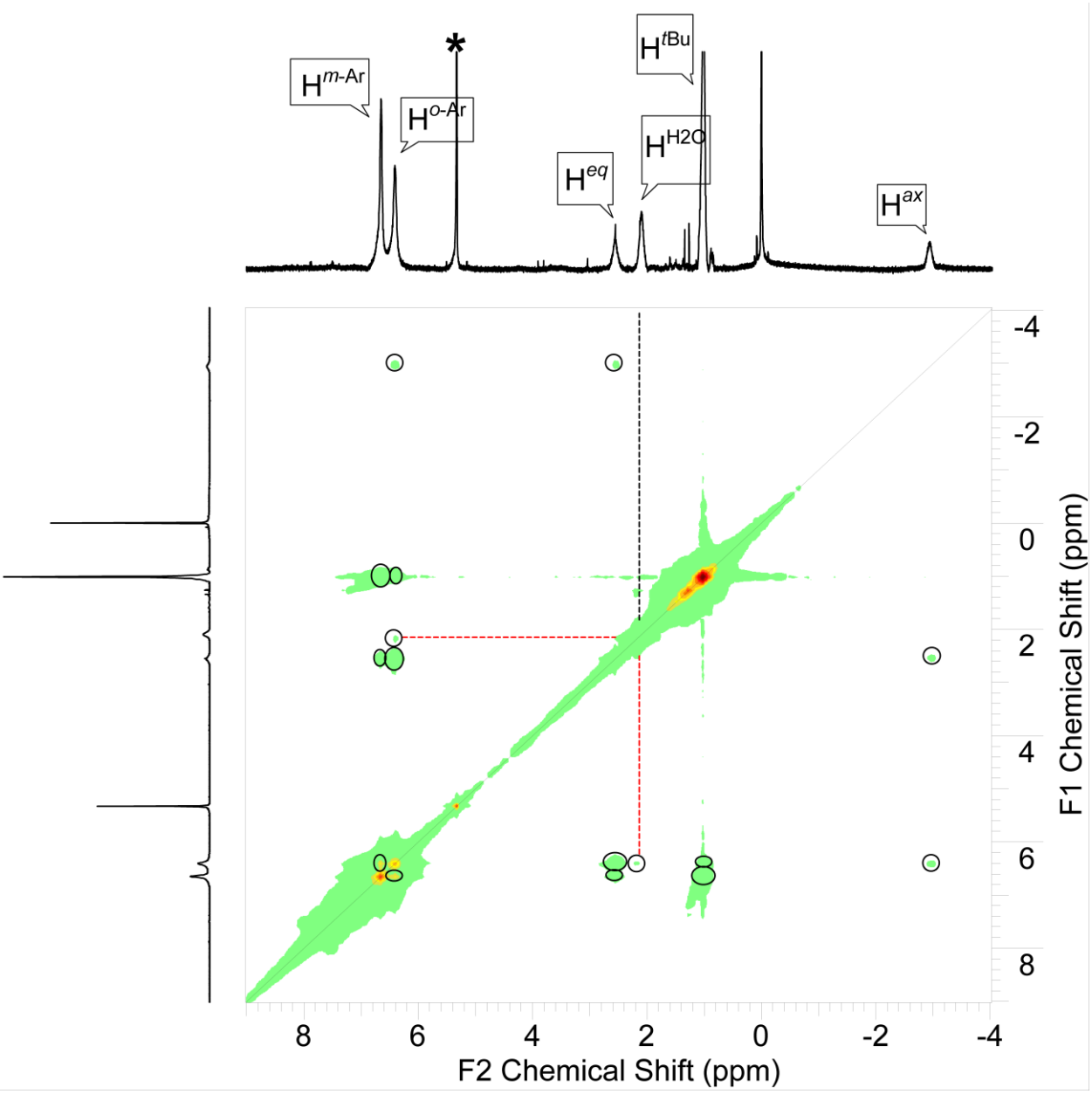


Fig. S30 ^{1}H-^{1}H NOESY NMR spectrum of **2e** in CD_2Cl_2.[1]

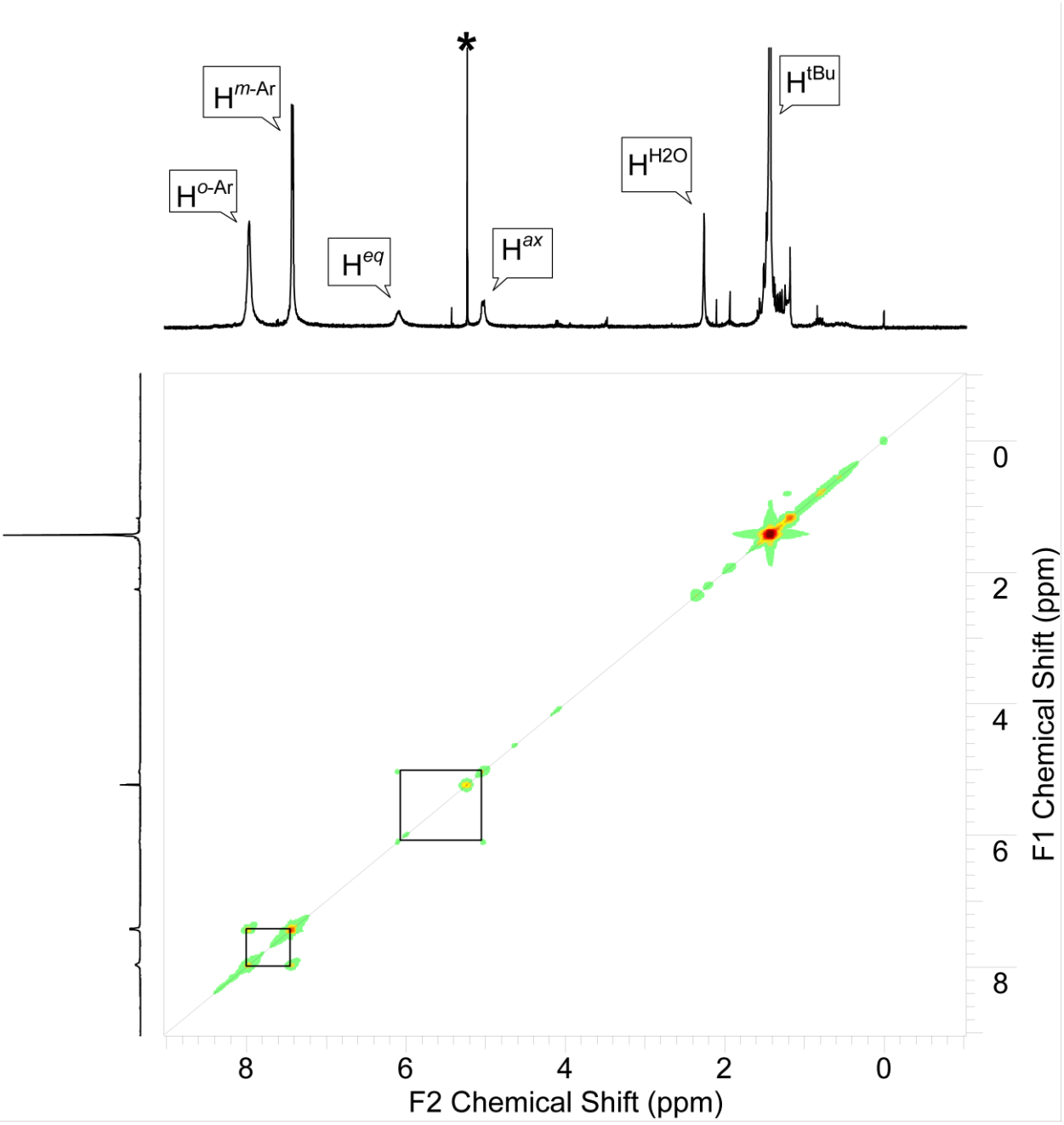


Fig. S31 ^{1}H-^{1}H COSY spectrum of **2f** in CD_2Cl_2.[2]

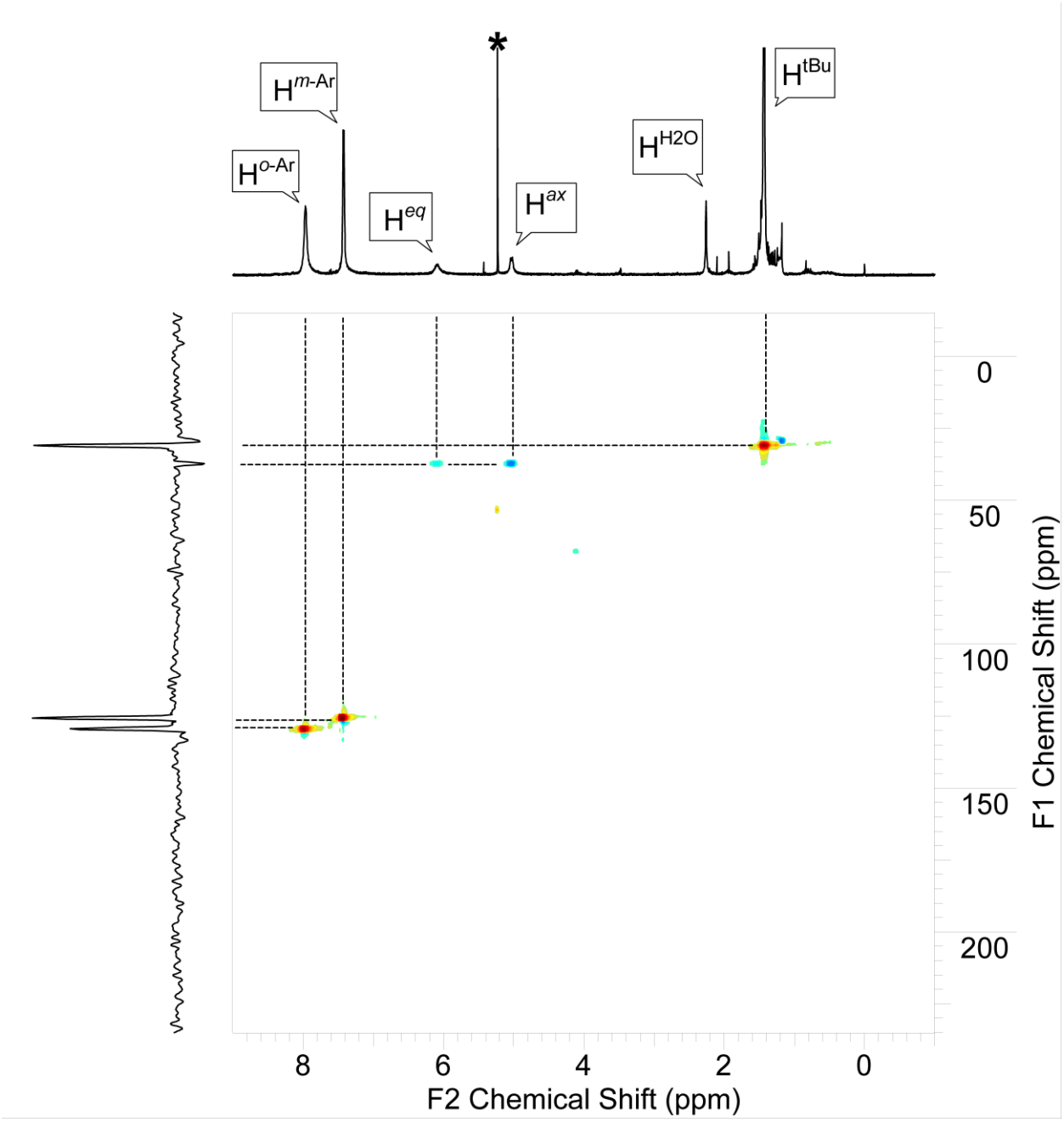


Fig. S32 ^{1}H-^{13}C HSQC spectrum of **2f** in CD_2Cl_2.[2]

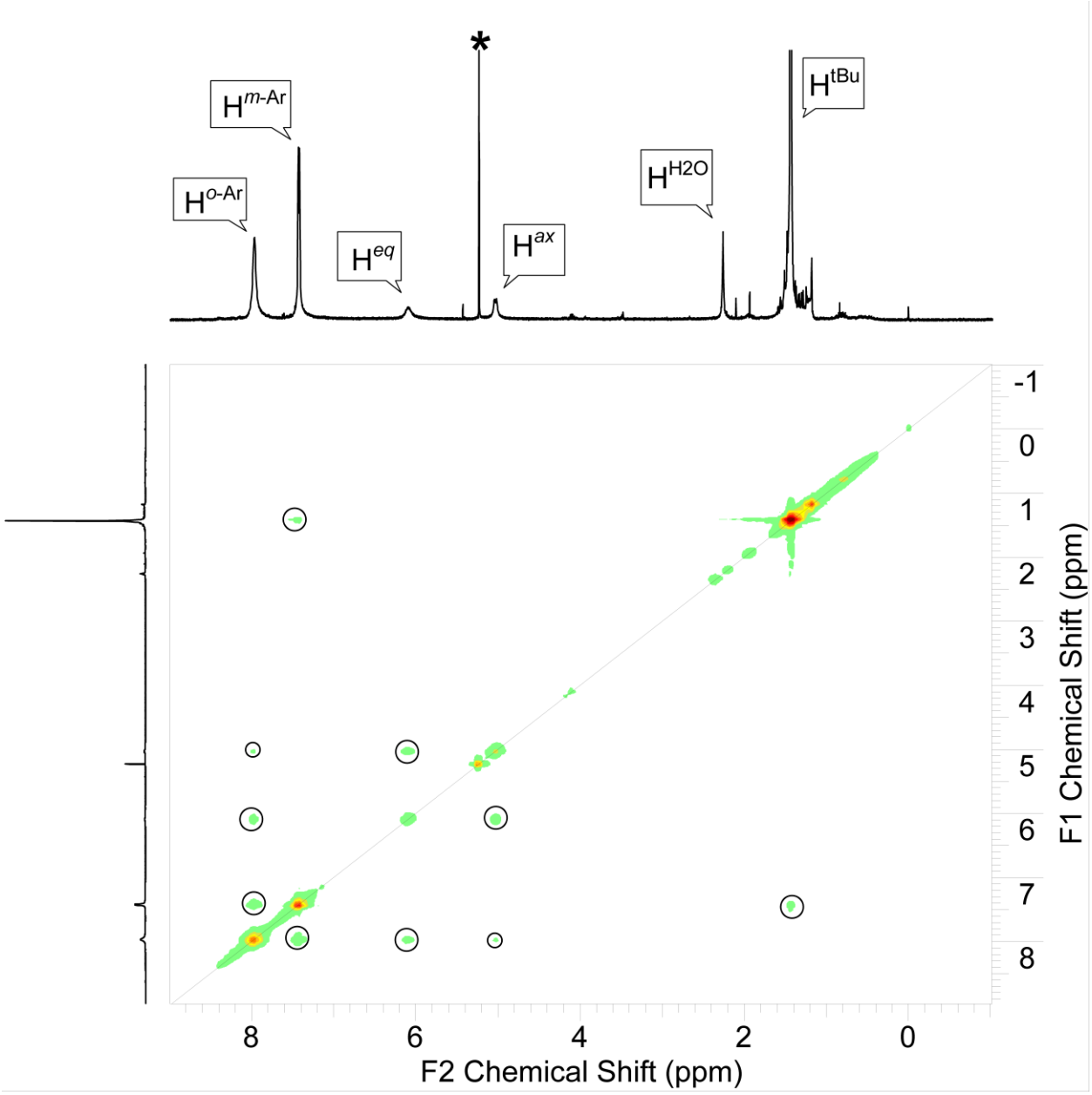


Fig. S33 ^{1}H-^{1}H NOESY NMR spectrum of **2f** in CD_2Cl_2.

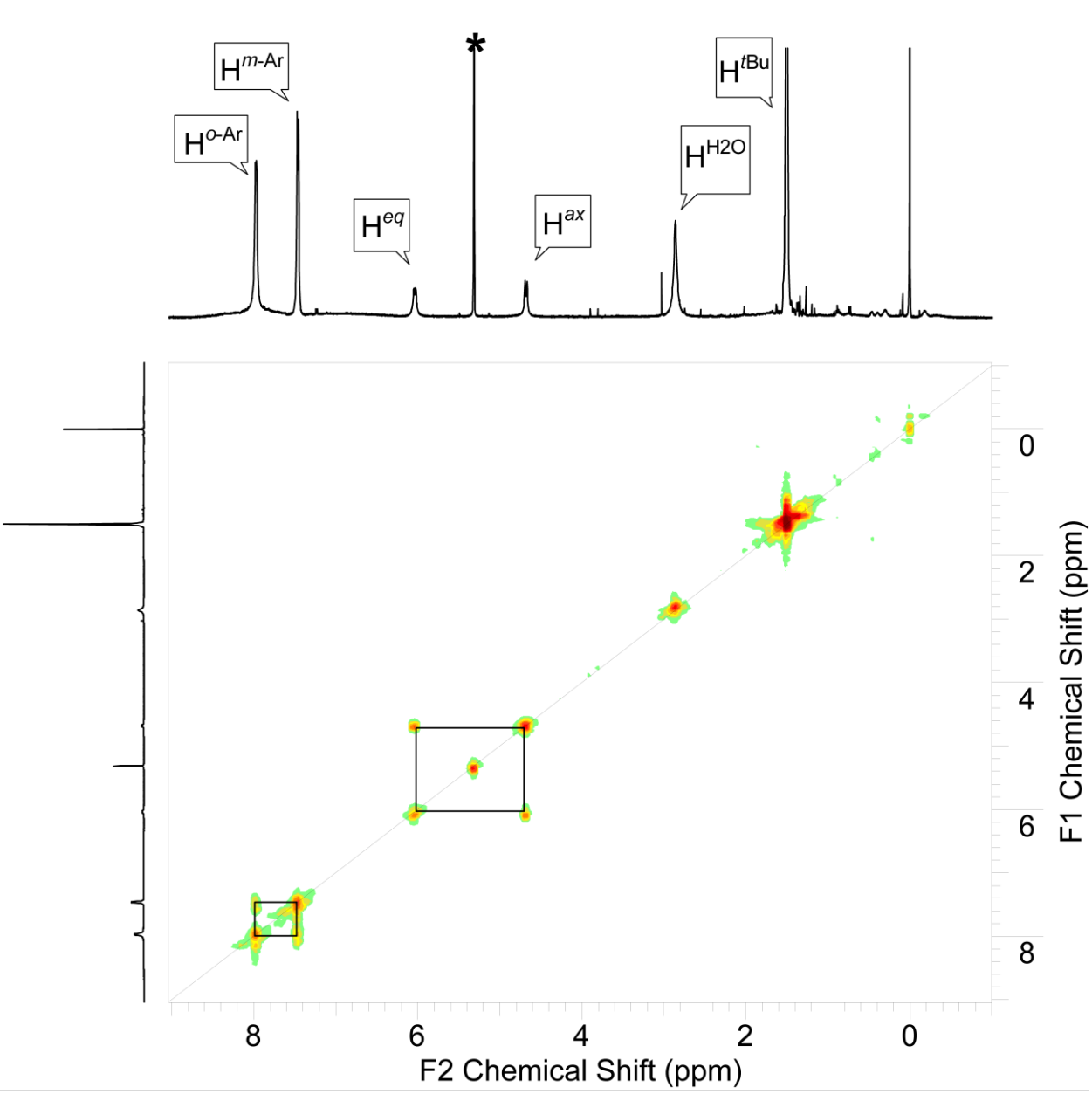


Fig. S34 ^{1}H-^{1}H COSY NMR spectrum of **2g** in CD_2Cl_2.[1]

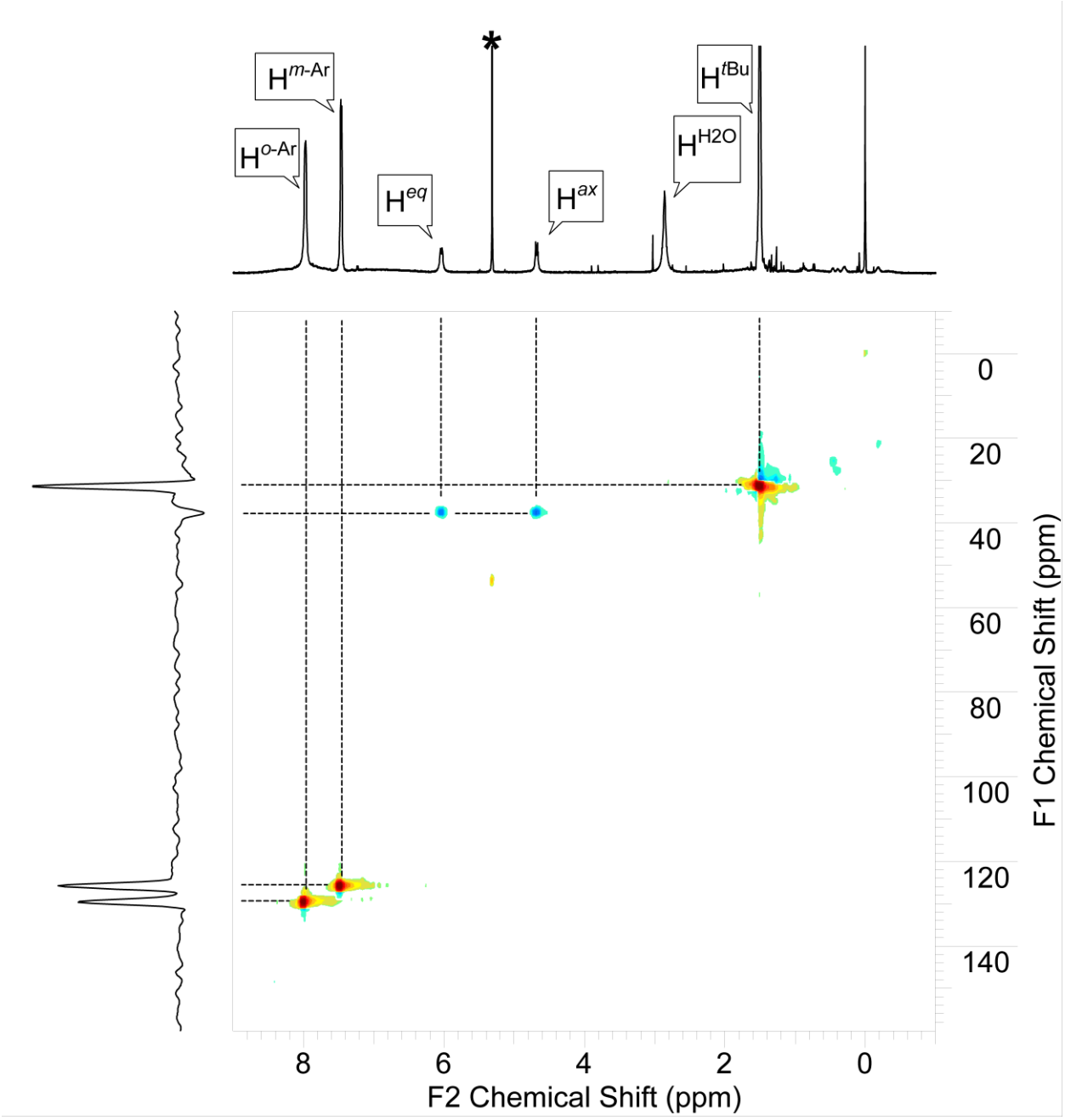


Fig. S35 ^{1}H-^{13}C HSQC NMR spectrum of **2g** in CD_2Cl_2.[1]

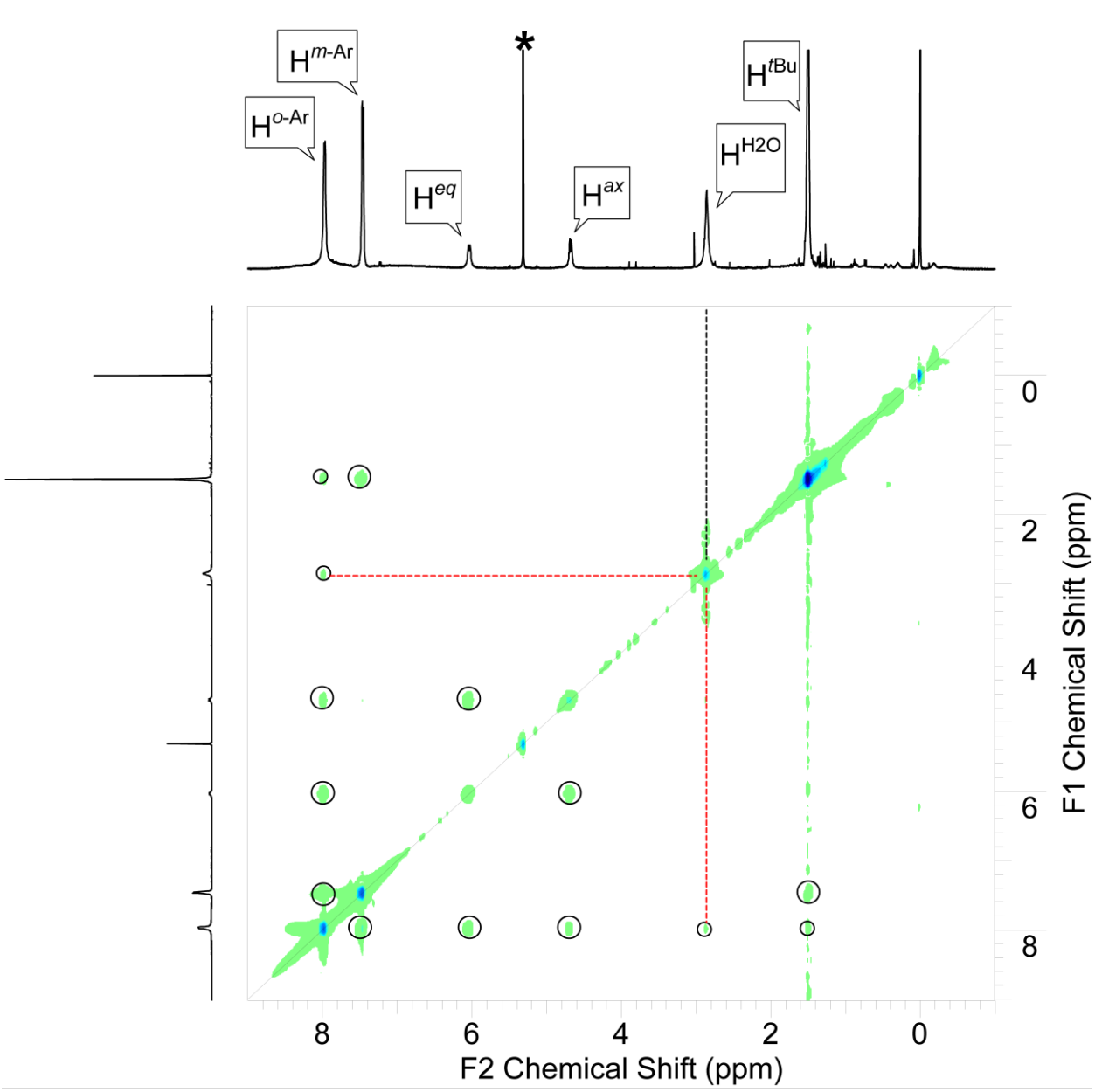


Fig. S36 ^{1}H-^{1}H NOESY NMR spectrum of **2g** in CD_2Cl_2.[1]

Table S2. Data from DOSY NMR experiments in CD_2Cl_2

Compound	Self-diffusion coefficients ($m^2 \cdot s^{-1}$)
1	$8.8 \cdot 10^{-10}$
2f	$7.8 \cdot 10^{-10}$
2g	$8.1 \cdot 10^{-10}$
2a	$7.6 \cdot 10^{-10}$

UV-vis and fluorescence data for ligand 1

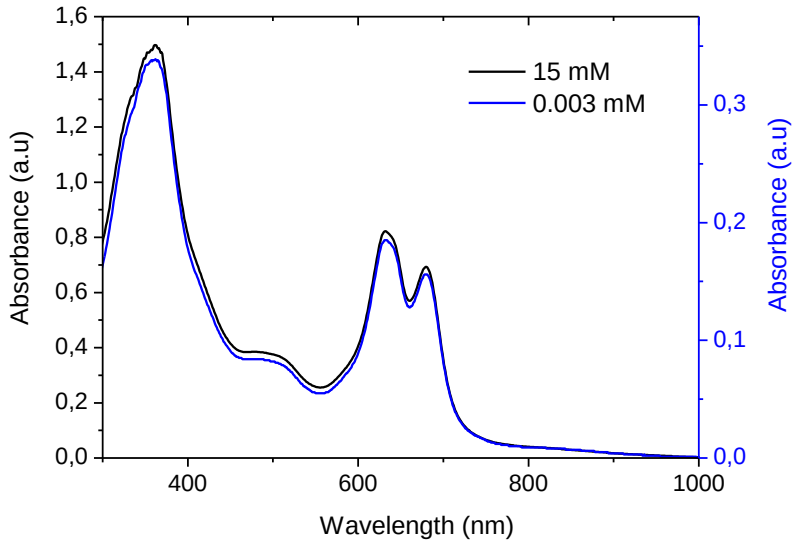


Fig. S37 The absorption spectra of ligand **1** at different concentrations (for NMR and UV-Vis, respectively) in CH_2Cl_2.

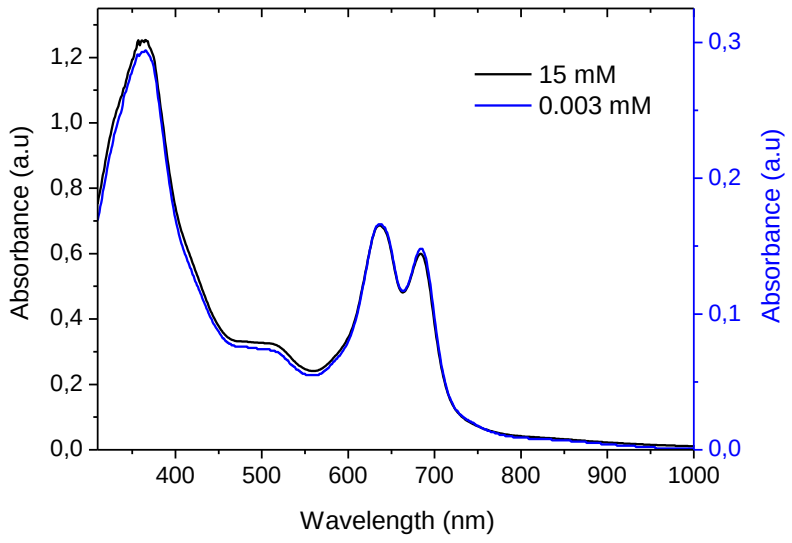
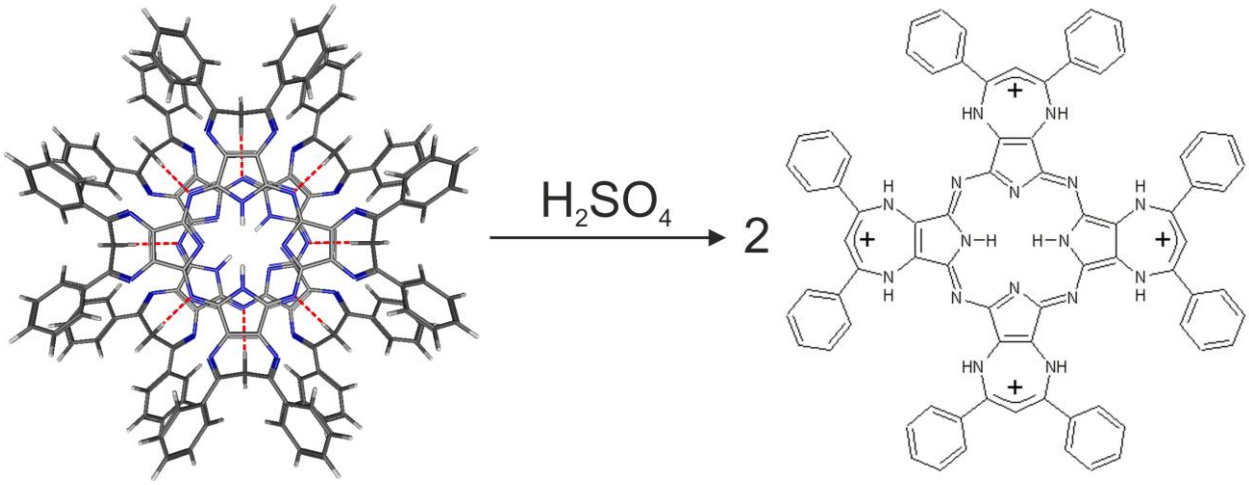


Fig. S38 The absorption spectra of ligand **1** at different concentrations (for NMR and UV-Vis, respectively) in pyridine.

Scheme S1



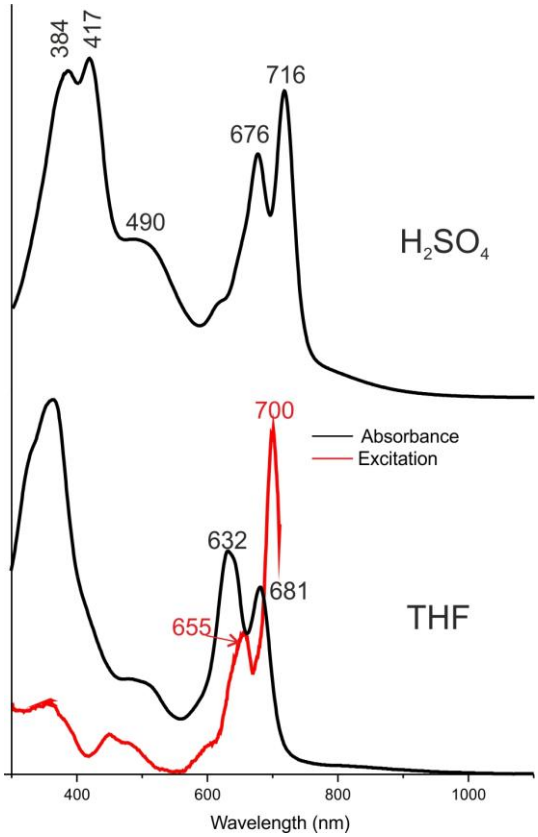


Fig. S39 The absorption (black) and excitation (red) spectra of ligand **1** in THF and sulfuric acid.

As shown in Figure 39 the spectrum in THF (DCM, Py) corresponds to H-type dimer, while the spectrum in sulfuric acid can be regarded as that of monomer. The diazepine moieties are protonated by the action of sulfuric acid, becoming planar, which results in the dissociation of the dimer to the monomers (Scheme S1). Taking into account that excitation spectrum is of the same nature as that in sulfuric acid a very weak observed fluorescence is due to a small admixture of monomer. Thus, the ligand predominantly (>95%) exists as H-type dimer even at concentration of 10^{-6} mol L^{-1}.

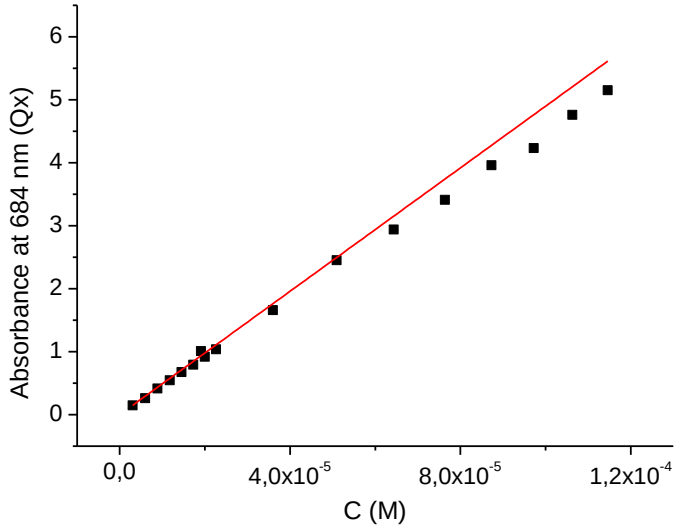


Fig. S40 Absorbance at 684 nm *vs.* concentration plot for the ligand in pyridine. Line corresponds to the theoretical values, squares are experimental results.

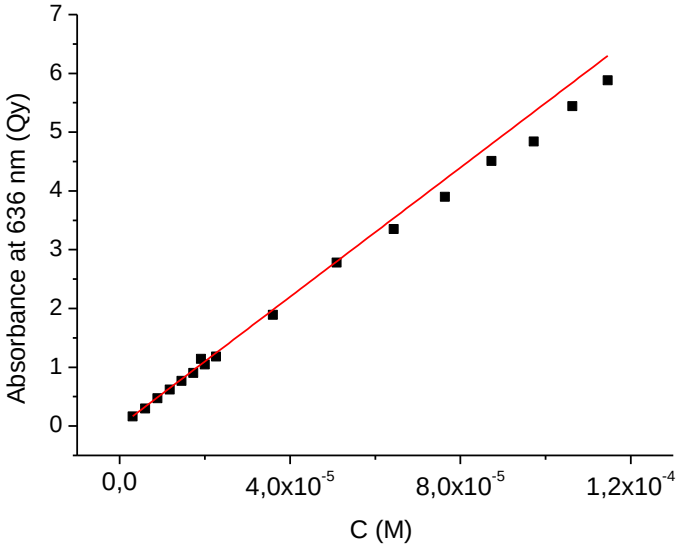


Fig. S41 Absorbance at 636 nm *vs.* concentration plot for the ligand in pyridine. Line corresponds to the theoretical values, squares are experimental results.

Since during the transition from monomer to dimer the decrease in the Q_x-band and increase in the Q_y-band should be observed, the deviation from the Lambert-Beer law at concentration above $5 \cdot 10^{-5}$ mol L^{-1} (Figs. S40 and S41) can be interpreted as an aggregation which is not associated with the dimer-monomer equilibrium.

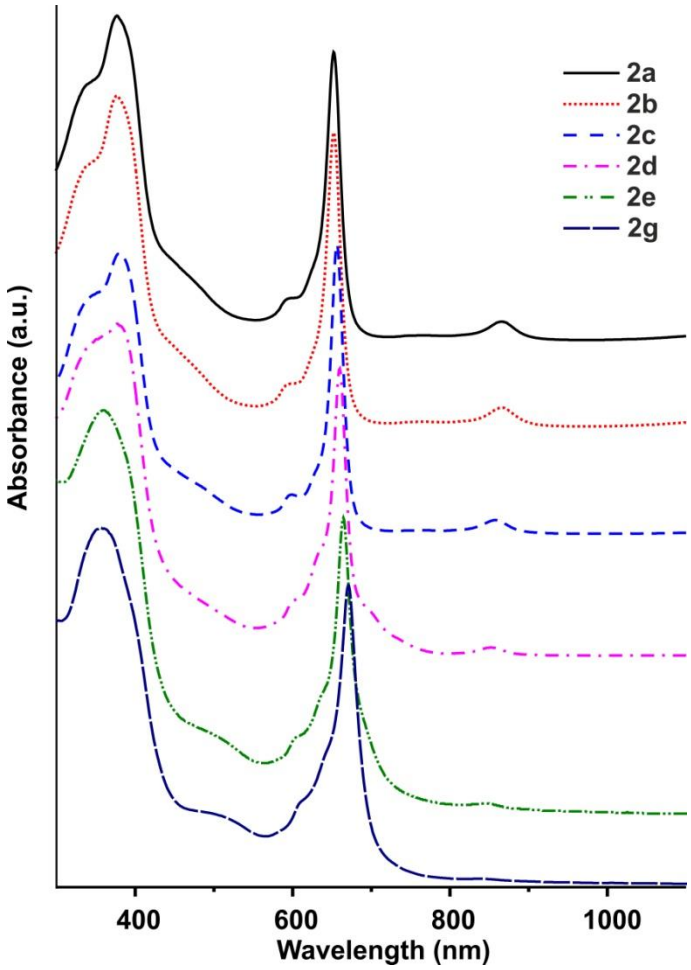


Fig. S42 UV-vis spectra of neutral forms of complexes $[^{t\text{BuPh}}\text{DzPz}]_2\text{Ln}^{\text{III}}$ in CH_2Cl_2.

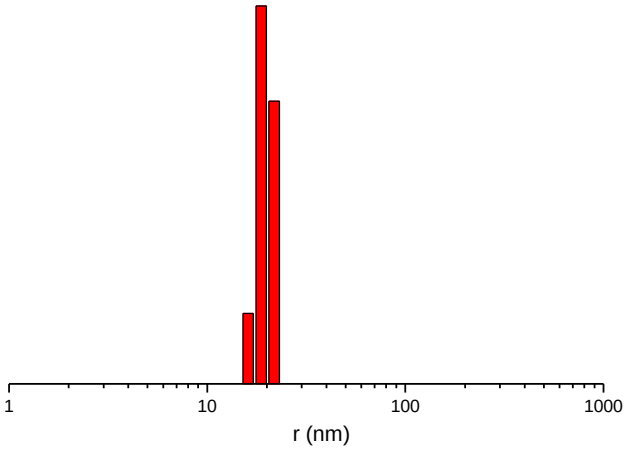


Fig. S43 Results of DLS measurements for **2a** in CH_2Cl_2 at 296 K; R_h = 21 nm.

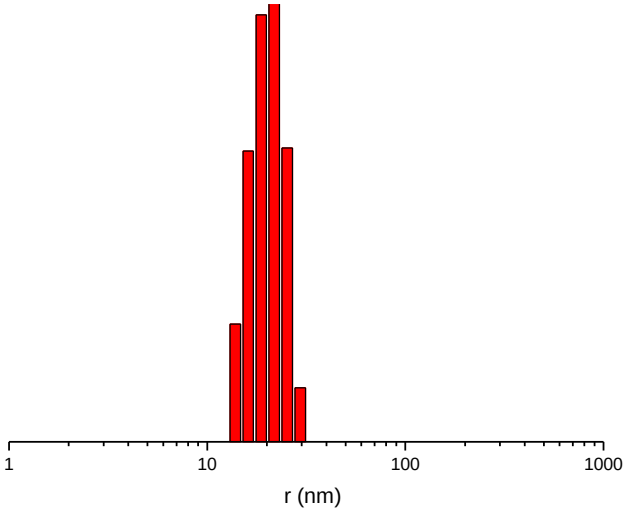


Fig. S44 Results of DLS measurements for **2d** in CH_2Cl_2 at 296 K; R_h = 22 nm.

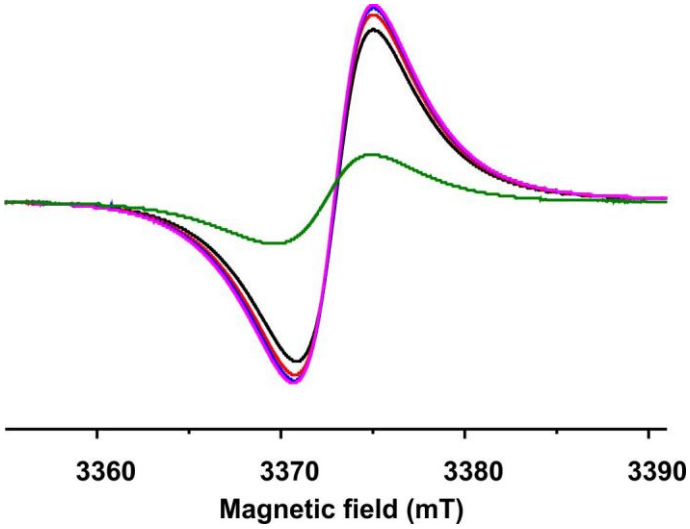


Fig. S45 ESR changes observed for the neutral form of **2g** in solid state.

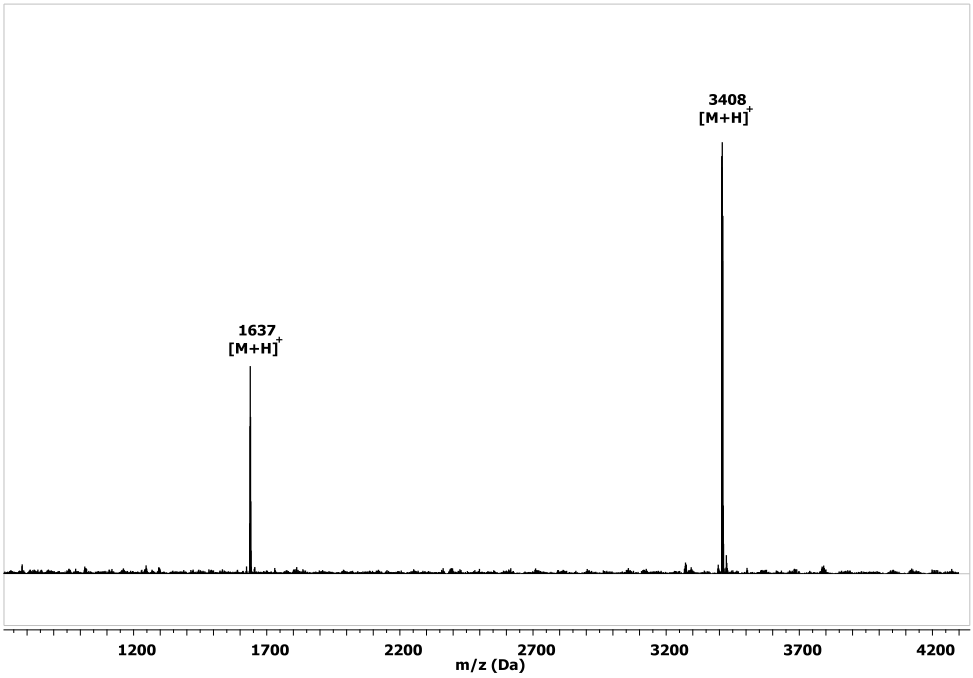


Fig. S46 MALDI-TOF mass spectrum of the neutral form of **2g** after storage in CH_2Cl_2.

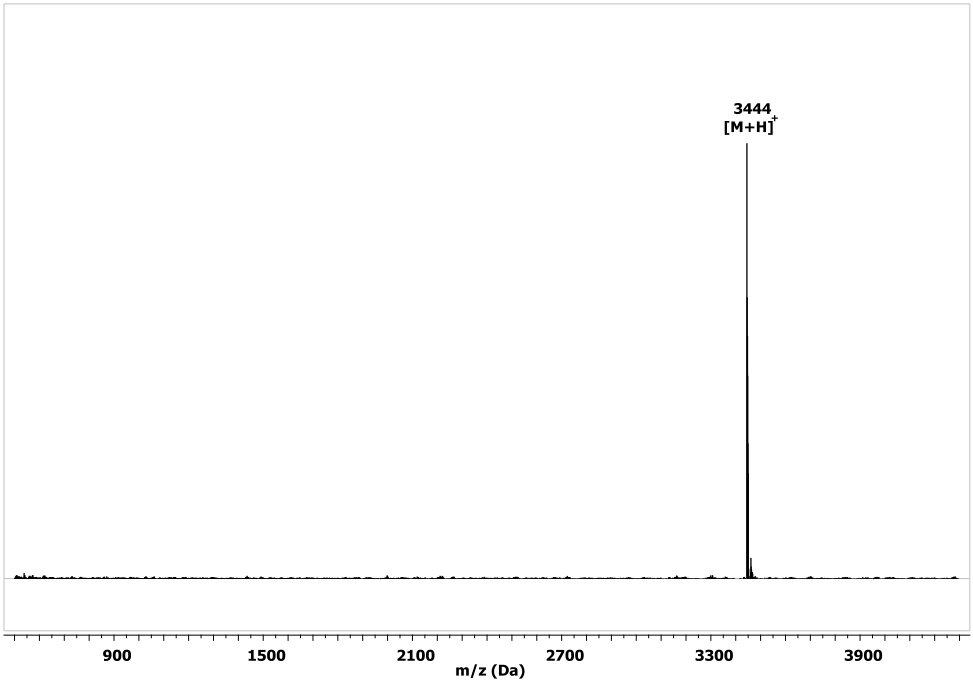


Fig. S47 MALDI-TOF mass spectrum of the neutral form of **2a** after storage in CH_2Cl_2.

Thermal analysis details

According to evolved gas analysis (mass-spectrometry) the removal of physically adsorbed water takes place until 100 °C (m/z 17 and 18) and thereafter the dehydration of crystalline water occurs (Fig. S48). The smooth mass loss in the range of 200–350 °C under inert atmosphere presumably relates to recyclization of diazepine into pyrazine and imidazole with emission of CH_2 (at C6 atom in diazepine cycle) forming CH_2=CH_2 (m/z 28) (Fig. S49). According to quantum chemical calculations water is most likely confined between nitrogen atoms of neighboring diazepine fragments of one deck. Situated closely (less than 3.5 Å) to C6 atom it is able to interact with evolved radical resulting in CO formation (m/z 28) (Figs. S48 and S49). The presence of particles with m/z 106 and 119 in MS above 350 °C can be considered as the confirmation of suggested recyclization process. The decomposition of the macrocycle proceeds in two steps: in 350–450 °C elimination of *tert*-butylphenyl substituents occurs (m/z 133 и 134, fragmented into *tert*-butyl, m/z 57 and 58, and benzene, m/z 77 and 78) and in 450–650 °C porphyrazine ring cracks. Degradation products, containing carbon and nitrogen, react with metal forming presumably the mixture of carbon and nitrogen containing lanthanide compounds as evidenced by a residual weight of ca. 40%.

Under oxidation atmosphere complex decomposition begins already at ca. 250 °C followed by active elimination and combustion of *tert*-butylphenyl substituents (m/z 27, 28, 44, 57, 58). Next are the destruction of macrocycle (m/z 13, 15, 16, 26–29) and gradual oxidation of diazepine and porphyrazine nitrogen atoms together with the elimination of water (360–460 °C, m/z 18 and 44). Within 420–520 °C one can see clearly two-stepped oxidation of carbon skeleton residues (m/z 12, 44). Finally, lanthanide oxide stable up to end temperature (1000 °C) is formed.

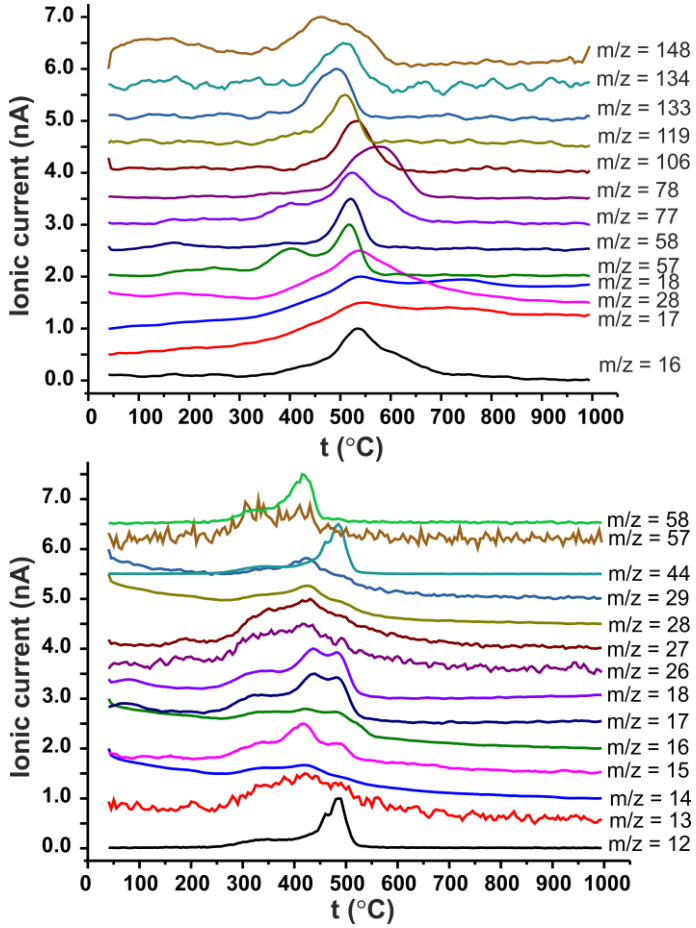


Fig. S48 Ion current curves for **2a** heated in an argon atmosphere (top) and **2g** heated in an air atmosphere (bottom).

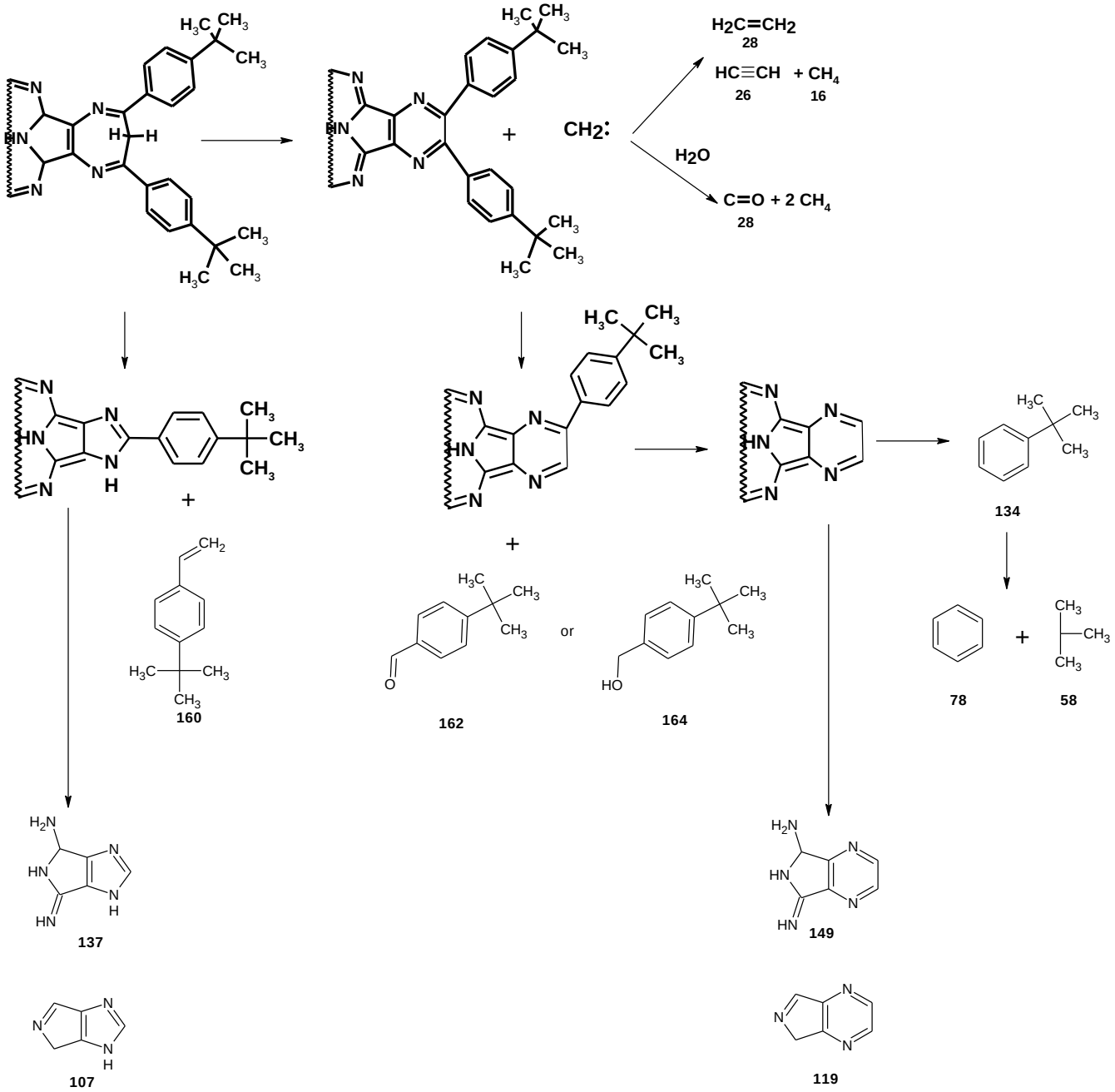


Fig. S49 Possible scheme of thermal degradation of the double-deckers based on TG-MS data.

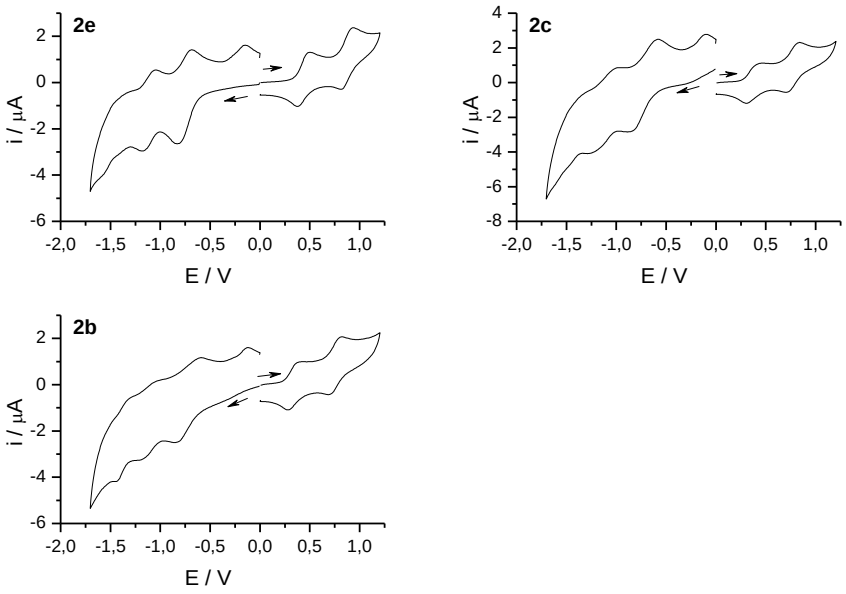


Fig. S50 CV of **2b**, **2c**, **2e** (0.5-1.0 mM, *o*-DCB, 0.15 M $TBABF_4$, scan rate of 0.1 V/s). $E_{1/2}(Fc^+/Fc)$ = 0.64 V.

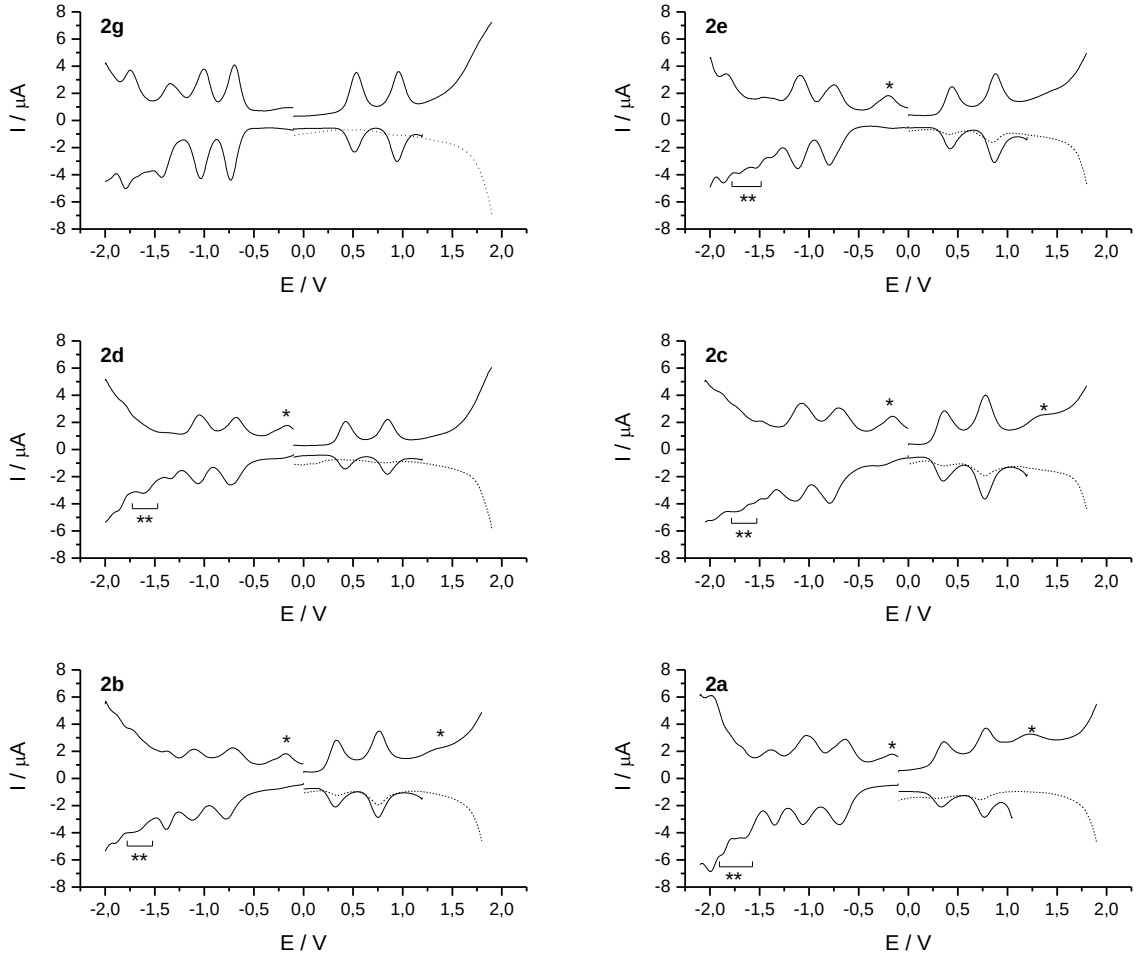


Fig. S51 SWVA of **2a–g** (0.5-1.0 mM, *o*-DCB, 0.15 M $TBABF_4$, frequency of 10 Hz; amplitude of 50 mV; step potential of 5 mV). $E_{1/2}(Fc^+/Fc)$ = 0.64 V. Designations: *- peak of background; ** - irregular weakly reversible peaks, probably, owing to traces of contaminants in the samples.

DFT calculations

Table S3. Cartesian coordinates (Angstrom) of ligand **1** without H_2O

N	-0.743662	1.787163	1.636945
N	0.743284	-1.787166	1.636989
N	-0.743217	-1.787291	-1.636903
N	0.743770	1.786982	-1.636945
N	-1.870985	-0.772191	1.653054
N	1.870628	0.772222	1.652909
N	-1.870578	0.772039	-1.652886
N	1.871093	-0.772326	-1.653032
N	-3.128203	1.303992	1.595604
N	3.127843	-1.303961	1.595561
N	-3.127788	-1.304124	-1.595481
N	3.128317	1.303851	-1.595601
N	1.287377	3.129085	1.628874
N	-1.287743	-3.129069	1.628976
N	1.287819	-3.129189	-1.628911
N	-1.287293	3.128896	-1.628891
N	-3.429834	4.243464	1.488459
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C	10.177245	1.378668	0.907792
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H	9.084621	6.490506	0.461766
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H	7.979501	-8.251385	2.242325
H	-7.978764	-8.252125	-2.243245
H	7.979080	8.252192	-2.243044
H	-0.198629	11.478333	2.279794
H	0.198781	-11.478393	2.279240
H	-0.199730	-11.478517	-2.280024
H	0.198252	11.478129	-2.279703
H	-8.243763	8.011523	-2.273678
H	8.245489	-8.010761	-2.274045
H	-8.245781	-8.010048	2.275585
H	8.244346	8.011165	2.274172
H	-11.510783	-0.281402	2.234017
H	11.510353	0.281217	2.234688
H	-11.510359	0.281130	-2.234407
H	11.510907	-0.281716	-2.234000

Table S4. Cartesian coordinates (Angstrom) of ligand **1** with H_2O

O	-5.392710	2.735877	2.506967
O	-5.594001	-2.760558	-2.832725
O	5.592942	2.762933	-2.832860
O	5.393339	-2.734898	2.506107
O	2.660276	5.408880	2.534161
O	2.791645	-5.597099	-2.971508
O	-2.792636	5.598014	-2.973068
O	-2.658457	-5.407687	2.534715
N	-0.702754	1.798561	0.947603
N	-0.674370	-1.802391	-2.283200
N	0.673828	1.803049	-2.283129
N	0.702817	-1.799119	0.947362
N	-1.886544	-0.737775	0.940667
N	-1.879906	0.725829	-2.295789
N	1.879338	-0.725108	-2.294953
N	1.886480	0.737261	0.940813
N	-3.086814	1.369219	1.048918
N	-3.063517	-1.393297	-2.202421
N	3.062980	1.394010	-2.201797
N	3.086825	-1.369751	1.048865
N	1.357569	3.090605	1.068642
N	1.389718	-3.091444	-2.231152
N	-1.390296	3.092148	-2.231628
N	-1.357487	-3.091102	1.068174
N	-3.336717	4.321480	1.200555
N	-3.304427	-4.310488	-1.912246
N	3.303623	4.311237	-1.910926
N	3.336715	-4.321924	1.201744
N	-0.399583	5.399453	1.342749
N	-0.345347	-5.421949	-2.081700
N	0.344484	5.422602	-2.082011
N	0.399676	-5.400096	1.342256
N	-5.420711	-0.403984	1.358816
N	-5.431114	0.343309	-2.055090
N	5.430628	-0.342679	-2.055696
N	5.420581	0.403192	1.358622
N	-4.348796	3.315476	-1.961337
N	-4.333741	-3.348664	1.273936
N	4.333936	3.347937	1.274134
N	4.348154	-3.314894	-1.961113
C	-2.021815	2.176488	1.008863
C	-1.989652	-2.188004	-2.211775
C	1.989089	2.188714	-2.211319
C	2.021829	-2.177042	1.008920
C	0.027494	2.954029	1.038889
C	0.059994	-2.959167	-2.239801
C	-0.060584	2.959819	-2.239992
C	-0.027438	-2.954598	1.038479
C	-3.013722	0.049890	1.029732
C	-2.999856	-0.075247	-2.229965
C	2.999332	0.075956	-2.229380
C	3.013626	-0.050439	1.029711
C	-2.218824	2.064490	-2.235108

C	-2.205034	-2.080444	1.023391
C	2.205049	2.079931	1.023648
C	2.218233	-2.063761	-2.234436
C	-2.165018	3.647735	1.048175
C	-2.119935	-3.649330	-2.043393
C	2.119217	3.650065	-2.042873
C	2.165080	-3.648276	1.048492
C	-0.844375	4.144234	1.094999
C	-0.803151	-4.144443	-2.085788
C	0.802421	4.145093	-2.085709
C	0.844433	-4.144827	1.094731
C	-4.165453	-0.848046	1.103879
C	-4.154247	0.806648	-2.085408
C	4.153739	-0.805982	-2.085249
C	4.165392	0.847449	1.103826
C	-3.667752	2.139238	-2.070257
C	-3.663646	-2.179986	1.079460
C	3.663677	2.179403	1.079534
C	3.667234	-2.138555	-2.069906
C	-2.301927	6.232666	0.055684
C	-2.129726	-5.925603	-0.491144
C	2.127994	5.926233	-0.490445
C	2.302910	-6.233207	0.056297
C	-5.931844	2.154752	-0.492700
C	-6.296061	-2.358218	0.171878
C	6.295930	2.357300	0.171624
C	5.932691	-2.154368	-0.493845
C	-3.413742	5.593190	0.861803
C	-3.344263	-5.455250	-1.261889
C	3.343082	5.455802	-1.260226
C	3.414123	-5.593693	0.863277
C	-1.118909	6.440994	0.986504
C	-1.019497	-6.347455	-1.440605
C	1.018266	6.348095	-1.440588
C	1.119313	-6.441553	0.986386
C	-6.351909	1.018296	-1.410208
C	-6.467966	-1.135405	1.055674
C	6.467943	1.134401	1.055307
C	6.351835	-1.017803	-1.411608
C	-5.483804	3.355830	-1.299072
C	-5.613242	-3.443224	0.981135
C	5.613482	3.442199	0.981352
C	5.483513	-3.355538	-1.299480
C	-4.566022	6.391818	1.319806
C	-4.595663	-6.234432	-1.260542
C	4.594619	6.234750	-1.257417
C	4.566353	-6.391903	1.322059
C	-0.735787	7.777001	1.476191
C	-0.615952	-7.756517	-1.577603
C	0.615356	7.757288	-1.578168
C	0.736180	-7.777496	1.476260
C	-7.788018	-0.722756	1.566938
C	-7.756965	0.589889	-1.508704
C	7.756815	-0.589305	-1.511049
C	7.787992	0.721443	1.566273
C	-6.281143	4.594681	-1.327502
C	-6.377792	-4.598222	1.487378
C	6.378433	4.596572	1.488347

C	6.280118	-4.594890	-1.327521
C	0.495680	7.950935	2.161842
C	0.604958	-8.078679	-2.226395
C	-0.606156	8.080148	-2.225509
C	-0.495514	-7.951573	2.161508
C	-5.294034	5.991874	2.468600
C	-5.566015	-6.023582	-2.271611
C	5.565467	6.024872	-2.268198
C	5.294013	-5.991056	2.470769
C	-6.093119	5.532493	-2.373258
C	-5.905718	-5.318706	2.613948
C	5.906779	5.315961	2.615786
C	6.090657	-5.533712	-2.372119
C	-7.928069	0.537671	2.206320
C	-8.070875	-0.654223	-2.115707
C	8.070014	0.654851	-2.118296
C	7.928056	-0.539409	2.204857
C	-4.960941	7.570187	0.642077
C	-4.871716	-7.177512	-0.238728
C	4.870192	7.176697	-0.234430
C	4.961978	-7.570347	0.644895
C	-8.805882	1.364765	-0.957007
C	-8.932286	-1.543520	1.430588
C	8.932249	1.542256	1.430157
C	8.806272	-1.363788	-0.959817
C	-1.558529	8.909023	1.266683
C	-1.389588	-8.804540	-1.022496
C	1.390968	8.805065	-1.025320
C	1.559481	-8.909277	1.267703
C	-7.218980	4.888711	-0.306260
C	-7.589306	-5.006957	0.879536
C	7.589867	5.005631	0.880592
C	7.219004	-4.888273	-0.307039
C	0.885970	9.218348	2.606023
C	1.037062	-9.407793	-2.294756
C	-1.036387	9.409846	-2.295196
C	-0.885197	-9.218899	2.606521
C	-6.367440	6.761529	2.932172
C	-6.760141	-6.755132	-2.274155
C	6.759588	6.756430	-2.269439
C	6.367879	-6.759808	2.934734
C	-6.846367	6.712135	-2.411542
C	-6.635853	-6.398622	3.122906
C	6.637207	6.395244	3.125649
C	6.843577	-6.713578	-2.410091
C	-9.174808	0.958043	2.679337
C	-9.394028	-1.108248	-2.145370
C	9.392946	1.109469	-2.148486
C	9.174888	-0.960088	2.677356
C	-6.036798	8.335451	1.109181
C	-6.066908	-7.907549	-0.246812
C	6.065429	7.906687	-0.241192
C	6.038219	-8.334799	1.112466
C	-10.129667	0.909745	-1.003111
C	-10.177157	-1.120990	1.917873
C	10.177197	1.119373	1.916937
C	10.129838	-0.908180	-1.006406
C	-1.166669	10.174233	1.725304

C	-0.956792	-10.134028	-1.106458
C	0.959880	10.135033	-1.110468
C	1.168194	-10.174364	1.727172
C	-7.968765	6.070834	-0.349218
C	-8.316434	-6.088304	1.393277
C	8.317327	6.086316	1.395271
C	7.968376	-6.070666	-0.349612
C	-6.736899	7.941484	2.261414
C	-7.010296	-7.707760	-1.269341
C	7.009293	7.707969	-1.263487
C	6.738110	-7.939821	2.264480
C	0.058045	10.336530	2.392508
C	0.260874	-10.440694	-1.736464
C	-0.258002	10.442541	-1.739631
C	-0.056609	-10.336810	2.394155
C	-7.794607	6.979935	-1.406996
C	-7.848890	-6.781799	2.521790
C	7.850152	6.778794	2.524567
C	7.792925	-6.980660	-1.406402
C	-10.305869	0.131504	2.539461
C	-10.427994	-0.331381	-1.590013
C	10.427435	0.333054	-1.593466
C	10.305953	-0.133501	2.537763
H	-0.925121	-0.377403	0.868836
H	-0.909575	0.384535	-2.324761
H	0.909093	-0.383565	-2.323730
H	0.924971	0.377102	0.869048
H	-5.049599	1.799469	0.085359
H	-5.651536	-2.104058	-0.700302
H	5.650850	2.103205	-0.700151
H	5.051365	-1.799359	0.085785
H	-2.000291	5.536426	-0.757791
H	-1.749638	-5.051520	0.082752
H	1.747363	5.052161	0.083089
H	2.002176	-5.536347	-0.756940
H	-5.075407	1.822977	2.310122
H	-5.226400	-1.844896	-2.784182
H	5.225431	1.847268	-2.783856
H	5.074893	-1.822445	2.308841
H	-3.329683	4.849728	-2.592837
H	-3.231240	-4.769520	2.026466
H	3.232084	4.769713	2.026061
H	3.328367	-4.847870	-2.592632
H	-4.743592	3.293009	1.989714
H	-4.822549	-3.304996	-2.504837
H	4.821392	3.307127	-2.504720
H	4.744138	-3.292824	1.989809
H	1.750569	5.110979	2.291970
H	1.874402	-5.238380	-2.894280
H	-1.875424	5.239108	-2.896935
H	-1.749353	-5.108548	2.291800
H	-6.715722	2.403076	0.235338
H	-7.254323	-2.694984	-0.250375
H	7.254047	2.694045	-0.251006
H	6.717851	-2.402655	0.232801
H	-2.620456	7.167182	-0.429417
H	-2.368673	-6.713831	0.235654
H	2.366458	6.714550	0.236397

H	2.621593	-7.167582	-0.429011
H	1.162906	7.091157	2.324786
H	1.239150	-7.275230	-2.630374
H	-1.243235	7.277475	-2.626604
H	-1.163602	-7.092223	2.323536
H	-5.005749	5.073486	3.002073
H	-5.370180	-5.282347	-3.060708
H	5.370036	5.284403	-3.058107
H	5.004926	-5.072659	3.003794
H	-5.352397	5.320928	-3.158931
H	-4.960824	-5.020455	3.091862
H	4.961990	5.017118	3.093541
H	5.348924	-5.323080	-3.157066
H	-7.054428	1.198928	2.309863
H	-7.264666	-1.287063	-2.516613
H	7.263352	1.286959	-2.519403
H	7.054369	-1.200725	2.308052
H	-8.591007	2.339587	-0.496395
H	-8.855270	-2.533128	0.959853
H	8.855172	2.532085	0.959892
H	8.592016	-2.338627	-0.498941
H	-4.458559	7.865940	-0.291143
H	-4.173058	-7.302573	0.602992
H	4.171147	7.300917	0.607107
H	4.459977	-7.866800	-0.288297
H	-2.524903	8.805634	0.755059
H	-2.346951	-8.583981	-0.528994
H	2.348619	8.583923	-0.532610
H	2.525977	-8.805723	0.756357
H	-7.323693	4.217223	0.560121
H	-7.943971	-4.512381	-0.036815
H	7.944253	4.511793	-0.036263
H	7.324942	-4.215930	0.558522
H	1.851217	9.333245	3.126446
H	1.996670	-9.639412	-2.786043
H	-1.996389	9.642079	-2.785431
H	-1.850609	-9.333968	3.126604
H	-6.914987	6.440736	3.833400
H	-7.500179	-6.583799	-3.073696
H	7.500019	6.585880	-3.068787
H	6.915262	-6.438261	3.835791
H	-6.693938	7.427668	-3.236570
H	-6.256672	-6.941272	4.004028
H	6.258348	6.937105	4.007391
H	6.690130	-7.429798	-3.234336
H	-9.262859	1.944149	3.164229
H	-9.619843	-2.085291	-2.603635
H	9.618171	2.086510	-2.607042
H	9.263018	-1.946502	3.161607
H	-6.338293	9.242324	0.560553
H	-6.271904	-8.622811	0.565691
H	6.270171	8.620903	0.572299
H	6.340304	-9.241753	0.564300
H	-10.931670	1.524503	-0.564847
H	-11.054756	-1.778811	1.807268
H	11.054818	1.777209	1.806606
H	10.932289	-1.522684	-0.568610
H	-1.825880	11.040986	1.554503

H	-1.571061	-10.934416	-0.664440
H	1.575936	10.935174	-0.670480
H	1.827896	-11.040900	1.557133
H	-8.679471	6.293316	0.462567
H	-9.250137	-6.400267	0.898602
H	9.250952	6.398638	0.900671
H	8.679923	-6.292546	0.461602
H	-7.578058	8.550522	2.632876
H	-7.949536	-8.285594	-1.275082
H	7.948524	8.285829	-1.268204
H	7.579556	-8.548238	2.636305
H	0.367733	11.333720	2.746707
H	0.608288	-11.486234	-1.787898
H	-0.604090	11.488470	-1.792106
H	-0.365803	-11.333861	2.749179
H	-8.388556	7.908431	-1.439887
H	-8.426245	-7.628541	2.929065
H	8.427788	7.625003	2.932556
H	8.386421	-7.909457	-1.438961
H	-11.287352	0.463631	2.916476
H	-11.468652	-0.696249	-1.610423
H	11.467918	0.698408	-1.614156
H	11.287493	-0.465888	2.914402

Table S5. Cartesian coordinates (Angstrom) of La complex **2g**

N	-1.408119	1.408342	1.645796
N	1.408277	-1.408301	1.645692
N	-0.000050	-1.993285	-1.463846
N	-0.000004	1.993318	-1.463911
N	-1.408198	-1.408383	1.645728
N	1.408357	1.408394	1.645719
N	-1.993329	-0.000193	-1.463754
N	1.993265	0.000215	-1.463968
N	-3.390209	0.000027	1.668433
N	3.390364	-0.000008	1.668489
N	-2.396366	-2.396566	-1.506460
N	2.396322	2.396596	-1.506503
N	0.000137	3.390493	1.668146
N	0.000052	-3.390468	1.668084
N	2.396392	-2.396161	-1.506720
N	-2.396429	2.396182	-1.506720
N	-4.818475	2.631290	1.591802
N	4.818622	-2.631210	1.592209
N	-1.544021	-5.270080	-1.485145
N	1.544056	5.270036	-1.485156
N	-2.631156	4.818622	1.591352
N	2.631262	-4.818602	1.591602
N	1.544840	-5.269455	-1.486003
N	-1.544798	5.269567	-1.485884
N	-4.818567	-2.631200	1.591748
N	4.818736	2.631114	1.592003
N	-5.269871	-1.544623	-1.485421
N	5.269801	1.544593	-1.485421
N	-5.269746	1.544365	-1.485609

N	5.269683	-1.544265	-1.485463
N	-2.631545	-4.818637	1.591041
N	2.631694	4.818660	1.591368
C	-2.764314	1.183320	1.668331
C	2.764466	-1.183287	1.668348
C	-1.117583	-2.791789	-1.500454
C	1.117539	2.791814	-1.500496
C	-1.183137	2.764548	1.668144
C	1.183311	-2.764501	1.668140
C	1.117649	-2.791501	-1.500700
C	-1.117696	2.791544	-1.500690
C	-2.764370	-1.183302	1.668283
C	2.764522	1.183309	1.668333
C	-2.791694	-1.117810	-1.500492
C	2.791627	1.117840	-1.500575
C	-2.791687	1.117415	-1.500627
C	2.791635	-1.117396	-1.500656
C	-1.183266	-2.764607	1.668025
C	1.183448	2.764614	1.668125
C	-3.477646	2.475703	1.580433
C	3.477808	-2.475661	1.580622
C	-0.709142	-4.211524	-1.435976
C	0.709120	4.211535	-1.435968
C	-2.475560	3.477813	1.580273
C	2.475735	-3.477777	1.580429
C	0.709576	-4.211281	-1.436269
C	-0.709601	4.211336	-1.436206
C	-3.477749	-2.475650	1.580324
C	3.477919	2.475636	1.580501
C	-4.211467	-0.709532	-1.436104
C	4.211382	0.709568	-1.436058
C	-4.211437	0.709175	-1.436196
C	4.211364	-0.709134	-1.436109
C	-2.475720	-3.477841	1.580068
C	2.475914	3.477845	1.580288
C	-4.549472	4.549324	0.087970
C	4.549971	-4.549481	0.088676
C	0.001113	-6.482735	-0.019836
C	-0.000952	6.482740	-0.019752
C	-6.482411	0.000035	-0.019568
C	6.482548	0.000071	-0.019557
C	-4.549658	-4.548859	0.087436
C	4.550053	4.549040	0.088041
C	-5.378728	3.666619	1.007664
C	5.379057	-3.666599	1.008382
C	-1.203876	-6.418778	-0.944044
C	1.204013	6.418747	-0.944021
C	-3.666590	5.378783	1.007318
C	3.666735	-5.378887	1.007757
C	1.205512	-6.418315	-0.944797
C	-1.205334	6.418413	-0.944713
C	-6.418533	-1.204678	-0.944104
C	6.418477	1.204820	-0.944082
C	-5.378833	-3.666435	1.007437
C	5.379139	3.666377	1.007905
C	-6.418435	1.204691	-0.944202
C	6.418382	-1.204744	-0.944032
C	-3.667071	-5.378525	1.006864

C	3.667225	5.378655	1.007316
C	-6.801898	3.934267	1.297254
C	6.802231	-3.933960	1.298211
C	-1.999851	-7.611543	-1.295214
C	2.000018	7.611466	-1.295288
C	-3.933913	6.802109	1.296414
C	3.933712	-6.802283	1.296807
C	2.001792	-7.610665	-1.296707
C	-2.001512	7.610842	-1.296580
C	-6.801863	-3.934437	1.297394
C	6.802271	3.933952	1.297743
C	-7.611214	-2.000835	-1.295134
C	7.611013	2.001188	-1.295161
C	-7.610988	2.001021	-1.295261
C	7.610776	-2.001288	-1.295168
C	-3.935223	-6.801638	1.296247
C	3.935112	6.801823	1.296657
C	-3.167904	7.452737	2.297620
C	3.167433	-7.452804	2.297874
C	2.980696	-7.502751	-2.317866
C	-2.980124	7.503148	-2.318042
C	-7.452018	3.169289	2.299569
C	7.452389	-3.167917	2.299702
C	-2.977503	-7.505038	-2.317709
C	2.977718	7.504821	-2.317721
C	-7.503895	2.979496	-2.316908
C	7.503295	-2.980176	-2.316385
C	-3.171120	-7.451964	2.299091
C	3.170749	7.452096	2.299337
C	-7.451872	-3.169753	2.300002
C	7.452456	3.168208	2.299439
C	-7.504381	-2.979142	-2.316966
C	7.503851	2.979811	-2.316660
C	-7.553039	4.912462	0.606220
C	7.553416	-4.912671	0.607974
C	-1.839045	-8.857520	-0.647677
C	1.839140	8.857543	-0.647964
C	-8.857403	-1.839591	-0.648129
C	8.857339	1.839939	-0.648420
C	-7.552997	-4.912658	0.606394
C	7.553350	4.912691	0.607428
C	-4.912704	7.552926	0.605885
C	4.912245	-7.553343	0.606170
C	1.840069	-8.857573	-0.651213
C	-1.839984	8.857606	-0.650758
C	-8.857293	1.839791	-0.648474
C	8.857204	-1.840113	-0.648609
C	-4.913055	-7.552544	0.604447
C	4.912847	7.552870	0.604867
C	-3.387979	8.798948	2.605786
C	3.387137	-8.799102	2.605928
C	3.756384	-8.606362	-2.686678
C	-3.755744	8.606823	-2.686813
C	-8.797991	3.389895	2.608416
C	8.798434	-3.388023	2.608543
C	-3.752816	-8.609131	-2.685900
C	3.752969	8.608894	-2.686100
C	-8.607720	3.755249	-2.684967

C	8.606908	-3.756281	-2.684319
C	-3.392152	-8.797935	2.607652
C	3.391521	8.798126	2.607829
C	-8.797721	-3.390671	2.609173
C	8.798444	3.388575	2.608366
C	-8.608342	-3.754724	-2.684985
C	8.607633	3.755674	-2.684614
C	-8.902534	5.131499	0.916229
C	8.902985	-5.131230	0.918008
C	-2.617558	-9.963220	-1.017740
C	2.617624	9.963211	-1.018183
C	-9.962978	-2.618364	-1.018027
C	9.962732	2.619001	-1.018246
C	-8.902370	-5.132002	0.916720
C	8.902865	5.131492	0.917527
C	-5.131263	8.902641	0.915272
C	5.130381	-8.903163	0.915391
C	2.618969	-9.962795	-1.021898
C	-2.618807	9.962893	-1.021411
C	-9.962720	2.618768	-1.018385
C	9.962422	-2.619440	-1.018403
C	-5.132536	-8.902029	0.914188
C	5.132023	8.902429	0.914494
C	-9.529313	4.378391	1.922125
C	9.529731	-4.377246	1.923258
C	-3.571673	-9.847910	-2.041269
C	3.571850	9.847738	-2.041589
C	-4.377190	9.529912	1.920134
C	4.376108	-9.530303	1.920185
C	3.574484	-9.846027	-2.043948
C	-3.573993	9.846359	-2.043794
C	-9.846771	3.573867	-2.040920
C	9.846154	-3.574783	-2.040670
C	-4.380433	-9.528962	1.920736
C	4.379695	9.529297	1.920917
C	-9.529012	-4.379247	1.922966
C	9.529663	4.377742	1.922922
C	-9.847300	-3.573255	-2.040790
C	9.846741	3.574169	-2.040711
H	-5.575898	0.000083	0.633428
H	5.576131	0.000027	0.633566
H	-3.895773	-3.895038	-0.538855
H	3.896136	3.895345	-0.538332
H	-3.895721	3.895471	-0.538432
H	3.896274	-3.895667	-0.537798
H	0.001008	-5.576405	0.633389
H	-0.000799	5.576391	0.633455
H	-7.376923	0.000137	0.626927
H	7.377227	0.000016	0.626700
H	-5.168996	-5.167797	-0.583683
H	5.169488	5.167988	-0.582985
H	-5.168716	5.168438	-0.583079
H	5.169370	-5.168583	-0.582246
H	0.001683	-7.377530	0.626255
H	-0.001431	7.377517	0.626363
H	-2.400886	6.862027	2.821871
H	2.400541	-6.861929	2.822122
H	3.104590	-6.525288	-2.808535

H	-3.103887	6.525786	-2.808948
H	-6.861016	2.402908	2.824426
H	6.861454	-2.400791	2.823542
H	-3.100854	-6.528232	-2.809836
H	3.100987	6.527988	-2.809817
H	-6.526904	3.102998	-2.808629
H	6.526124	-3.103850	-2.807693
H	-2.404826	-6.861238	2.824385
H	2.404507	6.861265	2.824589
H	-6.860928	-2.403277	2.824785
H	6.861578	2.401186	2.823494
H	-6.527467	-3.102723	-2.808818
H	6.526817	3.103415	-2.808259
H	-8.968816	-1.119583	0.175260
H	8.968953	1.119635	0.174691
H	-7.092386	-5.497815	-0.201448
H	7.092557	5.498588	-0.199769
H	-7.092264	5.497893	-0.201332
H	7.092639	-5.498639	-0.199178
H	-1.119655	-8.968562	0.176324
H	1.119642	8.968720	0.175916
H	-5.498909	7.091710	-0.200853
H	5.498449	-7.092249	-0.200636
H	1.119325	-8.969823	0.171412
H	-1.119544	8.969672	0.172159
H	-8.968897	1.119583	0.174710
H	8.968985	-1.119701	0.174382
H	-5.497561	-7.091723	-0.203757
H	5.497440	7.092111	-0.203310
H	-2.788622	9.285923	3.393332
H	2.787516	-9.286032	3.393301
H	4.507017	-8.504230	-3.488607
H	-4.506066	8.504891	-3.489056
H	-9.284657	2.791096	3.396573
H	9.285028	-2.788663	3.396322
H	-4.502233	-8.508190	-3.489112
H	4.502603	8.507786	-3.489089
H	-8.506228	4.505560	-3.487276
H	8.505172	-4.506759	-3.486444
H	-2.794337	-9.284625	3.396538
H	2.793455	9.284807	3.396530
H	-9.284257	-2.792169	3.397636
H	9.285077	2.789376	3.396243
H	-8.507089	-4.504808	-3.487535
H	8.506130	4.505976	-3.486931
H	-9.471175	5.892540	0.357983
H	9.471554	-5.892999	0.360682
H	-2.481595	-10.922536	-0.492998
H	2.481721	10.922567	-0.493498
H	-10.922442	-2.482088	-0.493640
H	10.922313	2.482689	-0.494086
H	-9.470956	-5.893187	0.358614
H	9.471368	5.893239	0.360102
H	-5.892987	9.470960	0.357632
H	5.891898	-9.471670	0.357659
H	2.482333	-10.922833	-0.498660
H	-2.482259	10.922846	-0.497991
H	-10.922253	2.482574	-0.494101

H	10.922115	-2.483111	-0.494453
H	-5.893496	-9.470416	0.355569
H	5.892885	9.470935	0.355864
H	-10.589233	4.556800	2.168153
H	10.589799	-4.555054	2.169080
H	-4.179318	-10.720542	-2.332804
H	4.179330	10.720395	-2.333395
H	-4.554988	10.590106	2.165427
H	4.553652	-10.590546	2.165457
H	4.182347	-10.718303	-2.336092
H	-4.181869	10.718666	-2.335818
H	-10.719256	4.181684	-2.332538
H	10.718403	-4.183064	-2.332024
H	-4.559000	-10.588959	2.166319
H	4.558092	10.589324	2.166500
H	-10.588870	-4.557812	2.169150
H	10.589676	4.555780	2.168820
H	-10.719860	-4.181015	-2.332299
H	10.719134	4.182227	-2.332100
La	0.000054	0.000038	0.087626

Table S6. Cartesian coordinates (Angstrom) of Lu complex **2a**

N	-1.387755	1.387765	1.350093
N	1.387573	-1.387763	1.350150
N	-0.000008	-1.964770	-1.358027
N	0.000011	1.964806	-1.358100
N	-1.387776	-1.387753	1.350127
N	1.387580	1.387731	1.350177
N	-1.964748	-0.000037	-1.358104
N	1.964803	0.000059	-1.357981
N	-3.377944	0.000010	1.512827
N	3.377759	-0.000050	1.513014
N	-2.388730	-2.388808	-1.524311
N	2.388774	2.388803	-1.524324
N	-0.000091	3.377992	1.512764
N	-0.000139	-3.377992	1.512841
N	2.388782	-2.388665	-1.524354
N	-2.388722	2.388731	-1.524522
N	-4.800865	2.605839	1.544202
N	4.800632	-2.606120	1.544325
N	-1.549953	-5.239831	-1.560071
N	1.550263	5.239634	-1.560398
N	-2.606417	4.800811	1.543845
N	2.605909	-4.800808	1.544329
N	1.550462	-5.239428	-1.560510
N	-1.550159	5.239722	-1.560423
N	-4.800888	-2.605881	1.544181
N	4.800667	2.605841	1.544654
N	-5.239662	-1.550186	-1.560444
N	5.239647	1.550278	-1.560253
N	-5.239543	1.550247	-1.560586
N	5.239692	-1.550113	-1.560288
N	-2.606376	-4.800807	1.543952
N	2.606135	4.800749	1.544299

C	-2.743832	1.171282	1.468514
C	2.743675	-1.171332	1.468638
C	-1.111724	-2.769042	-1.480485
C	1.111755	2.769000	-1.480589
C	-1.171380	2.743901	1.468436
C	1.171132	-2.743861	1.468579
C	1.111774	-2.768886	-1.480582
C	-1.111734	2.769005	-1.480674
C	-2.743850	-1.171273	1.468583
C	2.743657	1.171234	1.468729
C	-2.768954	-1.111790	-1.480566
C	2.768998	1.111806	-1.480446
C	-2.768927	1.111716	-1.480677
C	2.769018	-1.111678	-1.480455
C	-1.171410	-2.743881	1.468548
C	1.171188	2.743852	1.468583
C	-3.460498	2.461748	1.477028
C	3.460275	-2.461854	1.477210
C	-0.706026	-4.188766	-1.491956
C	0.706164	4.188729	-1.492155
C	-2.461965	3.460452	1.476892
C	2.461654	-3.460457	1.477174
C	0.706272	-4.188625	-1.492109
C	-0.706129	4.188747	-1.492187
C	-3.460516	-2.461750	1.477151
C	3.460304	2.461715	1.477402
C	-4.188693	-0.706163	-1.492135
C	4.188735	0.706217	-1.491882
C	-4.188654	0.706132	-1.492204
C	4.188753	-0.706079	-1.491910
C	-2.461975	-3.460434	1.477071
C	2.461756	3.460393	1.477246
C	-4.592659	4.591824	0.118479
C	4.592148	-4.592379	0.118929
C	0.000682	-6.489318	-0.129193
C	0.000103	6.489291	-0.129258
C	-6.489456	0.000160	-0.129570
C	6.489641	0.000096	-0.129386
C	-4.592405	-4.591740	0.118313
C	4.592503	4.591977	0.119097
C	-5.387060	3.659124	1.022953
C	5.386662	-3.659550	1.023175
C	-1.219339	-6.397236	-1.034724
C	1.219989	6.397079	-1.034960
C	-3.659996	5.386590	1.022673
C	3.659344	-5.386879	1.023242
C	1.220388	-6.396944	-1.035118
C	-1.219779	6.397134	-1.034959
C	-6.397164	-1.219783	-1.035198
C	6.397216	1.219962	-1.035104
C	-5.386978	-3.659140	1.022756
C	5.386870	3.659159	1.023487
C	-6.397061	1.220019	-1.035278
C	6.397240	-1.219768	-1.035105
C	-3.659828	-5.386583	1.022531
C	3.659675	5.386652	1.023221
C	-6.809734	3.884021	1.350055
C	6.809360	-3.884517	1.350135

C	-2.067803	-7.562626	-1.355303
C	2.068888	7.562199	-1.355359
C	-3.885268	6.809290	1.349396
C	3.884316	-6.809538	1.350364
C	2.069288	-7.561950	-1.355938
C	-2.068495	7.562374	-1.355427
C	-6.809726	-3.884044	1.349508
C	6.809576	3.883948	1.350534
C	-7.562329	-2.068521	-1.355866
C	7.562288	2.068753	-1.355995
C	-7.562133	2.068865	-1.356033
C	7.562379	-2.068449	-1.356050
C	-3.885176	-6.809284	1.349198
C	3.884726	6.809372	1.350005
C	-3.015822	7.442811	2.274810
C	3.014348	-7.442686	2.275553
C	3.129392	-7.397778	-2.284782
C	-3.128289	7.398880	-2.284735
C	-7.442726	3.014288	2.275570
C	7.442390	-3.015080	2.275897
C	-3.127478	-7.399346	-2.284784
C	3.129182	7.398364	-2.284042
C	-7.398213	3.128647	-2.285283
C	7.398605	-3.127905	-2.285700
C	-3.016133	-7.442720	2.275046
C	3.014807	7.442866	2.275000
C	-7.443133	-3.014050	2.274497
C	7.442570	3.014118	2.275956
C	-7.398452	-3.128763	-2.284599
C	7.398205	3.128779	-2.284946
C	-7.578202	4.916148	0.765415
C	7.577847	-4.916375	0.765033
C	-1.889493	-8.830731	-0.757250
C	1.890466	8.830526	-0.757825
C	-8.830721	-1.890052	-0.758481
C	8.830782	1.890476	-0.758774
C	-7.577953	-4.916301	0.764782
C	7.578122	4.915970	0.765807
C	-4.917547	7.577291	0.764400
C	4.916694	-7.577873	0.765992
C	1.890998	-8.830482	-0.758802
C	-1.890328	8.830520	-0.757424
C	-8.830471	1.890879	-0.758388
C	8.830648	-1.890625	-0.758206
C	-4.917045	-7.577406	0.763630
C	4.917109	7.577477	0.765334
C	-3.186458	8.788893	2.611441
C	3.184654	-8.788675	2.612698
C	3.969212	-8.467436	-2.609570
C	-3.967946	8.468812	-2.609076
C	-8.788698	3.184601	2.612788
C	8.788405	-3.185436	2.612929
C	-3.966888	-8.469438	-2.609237
C	3.969085	8.468142	-2.608226
C	-8.467943	3.968403	-2.610024
C	8.468424	-3.967453	-2.610684
C	-3.186829	-8.788813	2.611613
C	3.185090	8.789009	2.611550

C	-8.789305	-3.184164	2.611007
C	8.788608	3.184238	2.613004
C	-8.468252	-3.968554	-2.608997
C	8.467931	3.968484	-2.609814
C	-8.927871	5.085705	1.105216
C	8.927569	-5.085950	1.104608
C	-2.732035	-9.902742	-1.084246
C	2.733515	9.902225	-1.084553
C	-9.902446	-2.732983	-1.085429
C	9.902431	2.733340	-1.086179
C	-8.927807	-5.085685	1.103910
C	8.927866	5.085316	1.105410
C	-5.087435	8.927055	1.103615
C	5.086243	-8.927562	1.105720
C	2.733953	-9.902073	-1.086156
C	-2.733127	9.902368	-1.084295
C	-9.902129	2.733774	-1.085674
C	9.902382	-2.733344	-1.085700
C	-5.086986	-8.927181	1.102770
C	5.086637	8.927310	1.104467
C	-9.537720	4.227140	2.033845
C	9.537438	-4.227709	2.033525
C	-3.769657	-9.730464	-2.014136
C	3.771795	9.729386	-2.013602
C	-4.229044	9.537474	2.032012
C	4.227435	-9.537563	2.034024
C	3.771964	-9.728933	-2.015470
C	-3.770907	9.729864	-2.013968
C	-9.729257	3.771422	-2.015446
C	9.729670	-3.770621	-2.015913
C	-4.229063	-9.537488	2.031674
C	4.227794	9.537693	2.032468
C	-9.538099	-4.226787	2.031919
C	9.537706	4.226669	2.033971
C	-9.729582	-3.771162	-2.014587
C	9.729399	3.771224	-2.015654
H	-5.598594	0.000138	0.546109
H	5.598831	0.000102	0.546364
H	-3.966005	-3.965334	-0.562559
H	3.966239	3.965728	-0.562047
H	-3.966331	3.965522	-0.562544
H	3.965865	-3.966158	-0.562230
H	0.000702	-5.598370	0.546389
H	0.000101	5.598322	0.546286
H	-7.398293	0.000222	0.496659
H	7.398562	0.000126	0.496724
H	-5.239118	-5.238208	-0.498606
H	5.239349	5.238587	-0.497535
H	-5.239484	5.238350	-0.498263
H	5.238866	-5.239142	-0.497677
H	0.000943	-7.398094	0.497125
H	0.000138	7.398023	0.497128
H	-2.206713	6.838292	2.712875
H	2.205106	-6.837934	2.713048
H	3.266215	-6.402981	-2.735272
H	-3.264955	6.404435	-2.736050
H	-6.837854	2.205263	2.713303
H	6.837526	-2.206213	2.713934

H	-3.264325	-6.404907	-2.736058
H	3.266078	6.403748	-2.734911
H	-6.403562	3.265271	-2.736156
H	6.404006	-3.264425	-2.736718
H	-2.207256	-6.838144	2.713458
H	2.205559	6.838297	2.712736
H	-6.838482	-2.204861	2.712230
H	6.837659	2.205136	2.713712
H	-6.403753	-3.265782	-2.735248
H	6.403429	3.265627	-2.735474
H	-8.987964	-1.100122	-0.010013
H	8.988147	1.100776	-0.010080
H	-7.128715	-5.587869	0.020159
H	7.129233	5.587325	0.020768
H	-7.129287	5.587488	0.020386
H	7.128939	-5.587381	0.019689
H	-1.100024	-8.987493	-0.008182
H	1.100440	8.987748	-0.009451
H	-5.588670	7.127954	0.019431
H	5.588237	-7.128852	0.021206
H	1.101106	-8.987971	-0.010336
H	-1.100726	8.987466	-0.008538
H	-8.987710	1.101375	-0.009456
H	8.987737	-1.101465	-0.008879
H	-5.587748	-7.128158	0.018228
H	5.588597	7.128185	0.020664
H	-2.503906	9.263038	3.336956
H	2.501703	-9.262486	3.338059
H	4.785109	-8.320983	-3.337698
H	-4.783698	8.322858	-3.337466
H	-9.262397	2.501840	3.338400
H	9.262122	-2.502942	3.338779
H	-4.782463	-8.323686	-3.337864
H	4.785211	8.321937	-3.336148
H	-8.321688	4.784025	-3.338499
H	8.322289	-4.782805	-3.339484
H	-2.504642	-9.262877	3.337524
H	2.502167	9.263116	3.336743
H	-9.263337	-2.501202	3.336212
H	9.262302	2.501405	3.338551
H	-8.322037	-4.784575	-3.337034
H	8.321553	4.784297	-3.338051
H	-9.509549	5.892888	0.631473
H	9.509260	-5.892910	0.630504
H	-2.580078	-10.880062	-0.598790
H	2.581474	10.879726	-0.599485
H	-10.880024	-2.580847	-0.600548
H	10.880109	2.581357	-0.601447
H	-9.509267	-5.893003	0.630134
H	9.509590	5.892439	0.631621
H	-5.894689	9.508370	0.629553
H	5.893642	-9.509124	0.632204
H	2.581981	-10.879772	-0.601464
H	-2.581318	10.879704	-0.598824
H	-10.879663	2.582037	-0.600577
H	10.879865	-2.581734	-0.600459
H	-5.893946	-9.508575	0.628305
H	5.894029	9.508683	0.630708

H	-10.598013	4.365533	2.302858
H	10.597767	-4.366131	2.302386
H	-4.429099	-10.575999	-2.271319
H	4.431591	10.574693	-2.270628
H	-4.367660	10.597858	2.300555
H	4.365815	-10.597874	2.302973
H	4.431692	-10.574153	-2.272951
H	-4.430493	10.575295	-2.271126
H	-10.574531	4.431100	-2.272878
H	10.575014	-4.430133	-2.273537
H	-4.367691	-10.597895	2.300124
H	4.366105	10.598142	2.300914
H	-10.598582	-4.364946	2.300313
H	10.598056	4.364903	2.302844
H	-10.574877	-4.430940	-2.271696
H	10.574672	4.430859	-2.273193
Lu	-0.000047	0.000008	-0.004192

NBO analysis

Table S7. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
S7-A Ligand **1** without H_2O (see Table S3 and Figs. 1A,B)				
from unit 1 to unit 2				
595. LP (1) N^{meso} 9	/***. RY*(1) H^{ax} 189	0.11	0.97	0.009
595. LP (1) N^{meso} 9	/***. BD*(1) C 69 - H^{ax} 189	4.28	0.66	0.049
596. LP (1) N^{meso} 10	/***. RY*(1) H^{ax} 190	0.11	0.97	0.009
596. LP (1) N^{meso} 10	/***. BD*(1) C 70 - H^{ax} 190	4.28	0.66	0.049
599. LP (1) N^{meso} 13	/***. RY*(1) H^{ax} 196	0.11	0.97	0.010
599. LP (1) N^{meso} 13	/***. BD*(1) C 68 - H^{ax} 196	4.17	0.66	0.048
600. LP (1) N^{meso} 14	/***. RY*(1) H^{ax} 195	0.11	0.97	0.010
600. LP (1) N^{meso} 14	/***. BD*(1) C 67 - H^{ax} 195	4.17	0.66	0.048
from unit 2 to unit 1				
597. LP (1) N^{meso} 11	/***. RY*(1) H^{ax} 191	0.11	0.97	0.009
597. LP (1) N^{meso} 11	/***. BD*(1) C 71 - H^{ax} 191	4.28	0.66	0.049
598. LP (1) N^{meso} 12	/***. RY*(1) H^{ax} 192	0.11	0.97	0.009
598. LP (1) N^{meso} 12	/***. BD*(1) C 72 - H^{ax} 192	4.28	0.66	0.049
601. LP (1) N^{meso} 15	/***. RY*(1) H^{ax} 194	0.11	0.97	0.010
601. LP (1) N^{meso} 15	/***. BD*(1) C 66 - H^{ax} 194	4.17	0.66	0.048
602. LP (1) N^{meso} 16	/***. RY*(1) H^{ax} 193	0.11	0.97	0.010
602. LP (1) N^{meso} 16	/***. BD*(1) C 65 - H^{ax} 193	4.16	0.66	0.048

Notes to **S7-A**: units 1,2 denote $^{t\text{BuPh}}$DzPzH_2 subunits in ligand dimer **1**.

S7-B Ligand **1** with H_2O (see Table S4 and Fig. 1C)

from unit 1 to unit 9

615. LP (1) O 1	/***. RY*(1) $H^{o\text{-}Ar}$ 233	0.23	0.85	0.013
615. LP (1) O 1	/***. RY*(1) $H^{o\text{-}Ar}$ 241	0.09	1.02	0.008
615. LP (1) O 1	/***. BD*(1) C 117 - $H^{o\text{-}Ar}$ 233	0.60	0.86	0.020
615. LP (1) O 1	/***. BD*(1) C 125 - $H^{o\text{-}Ar}$ 241	0.63	0.88	0.021
616. LP (2) O 1	/***. BD*(1) C 117 - $H^{o\text{-}Ar}$ 233	0.07	0.66	0.006
616. LP (2) O 1	/***. BD*(1) C 125 - $H^{o\text{-}Ar}$ 241	2.15	0.68	0.034

from unit 9 to unit 1

635. LP (1) N^{meso} 17	/***. BD*(1) O 1 - H 205	1.54	0.65	0.029
635. LP (1) N^{meso} 17	/***. BD*(1) O 1 - H 213	0.43	0.64	0.015
643. LP (1) N^{Dz} 25	/***. RY*(1) H 213	0.20	1.02	0.013
643. LP (1) N^{Dz} 25	/***. BD*(1) O 1 - H 213	16.29	0.65	0.095
651. LP (1) N^{Dz} 33	/***. BD*(1) O 1 - H 205	2.34	0.65	0.036

from unit 1 to unit 10

616. LP (2) O 1	/***. RY*(1) H^{ax} 197	0.10	1.05	0.009
616. LP (2) O 1	/***. RY*(1) $H^{o\text{-}Ar}$ 257	0.15	0.71	0.009
616. LP (2) O 1	/***. BD*(1) C 77 – H^{eq} 221	0.41	0.65	0.015
616. LP (2) O 1	/***. BD*(1) C 141 - $H^{o\text{-}Ar}$ 257	0.12	0.65	0.008

from unit 4 to unit 9

621. LP (1) O 4	/***. RY*(1) $H^{o\text{-}Ar}$ 236	0.23	0.85	0.013
621. LP (1) O 4	/***. RY*(1) $H^{o\text{-}Ar}$ 244	0.09	1.02	0.008
621. LP (1) O 4	/***. BD*(1) C 120 - $H^{o\text{-}Ar}$ 236	0.60	0.86	0.020
621. LP (1) O 4	/***. BD*(1) C 128 - $H^{o\text{-}Ar}$ 244	0.63	0.88	0.021
622. LP (2) O 4	/***. BD*(1) C 120 - $H^{o\text{-}Ar}$ 236	0.07	0.66	0.006
622. LP (2) O 4	/***. BD*(1) C 128 - $H^{o\text{-}Ar}$ 244	2.17	0.68	0.034

from unit 9 to unit 4

638. LP (1) N^{meso} 20	/***. BD*(1) O 4 - H 208	1.55	0.65	0.029
638. LP (1) N^{meso} 20	/***. BD*(1) O 4 - H 216	0.43	0.64	0.015
646. LP (1) N^{Dz} 28	/***. RY*(1) H 216	0.19	1.02	0.013
646. LP (1) N^{Dz} 28	/***. BD*(1) O 4 - H 216	16.28	0.65	0.095
654. LP (1) N^{Dz} 36	/***. BD*(1) O 4 - H 208	2.35	0.65	0.036

from unit 4 to unit 10

621. LP (1) O 4	/***. RY*(1) H^{ax} 200	0.06	1.24	0.008
621. LP (1) O 4	/***. BD*(1) C 80 - H^{ax} 200	0.10	0.83	0.008
622. LP (2) O 4	/***. RY*(1) H^{ax} 200	0.10	1.05	0.009
622. LP (2) O 4	/***. RY*(1) $H^{o\text{-}Ar}$ 260	0.15	0.71	0.009
622. LP (2) O 4	/***. BD*(1) C 80 - H^{eq} 224	0.41	0.65	0.014
622. LP (2) O 4	/***. BD*(1) C 144 - $H^{o\text{-}Ar}$ 260	0.12	0.65	0.008

from unit 5 to unit 9

623. LP (1) O 5	/***. RY*(1) $H^{o\text{-}Ar}$ 229	0.10	1.01	0.009
623. LP (1) O 5	/***. RY*(1) $H^{o\text{-}Ar}$ 239	0.23	0.85	0.013
623. LP (1) O 5	/***. BD*(1) C 113 - $H^{o\text{-}Ar}$ 229	0.64	0.88	0.021
623. LP (1) O 5	/***. BD*(1) C 123 - $H^{o\text{-}Ar}$ 239	0.67	0.85	0.021
624. LP (2) O 5	/***. BD*(1) C 113 - $H^{o\text{-}Ar}$ 229	2.18	0.68	0.035
624. LP (2) O 5	/***. BD*(1) C 123 - $H^{o\text{-}Ar}$ 239	0.06	0.66	0.006

from unit 9 to unit 5

639. LP (1) N^{meso} 21	/***. BD*(1) O 5 - H 211	0.42	0.64	0.015
639. LP (1) N^{meso} 21	/***. BD*(1) O 5 - H 217	1.65	0.65	0.030
647. LP (1) N^{Dz} 29	/***. BD*(1) O 5 - H 217	3.15	0.65	0.042
657. LP (1) N^{Dz} 39	/***. RY*(1) H 211	0.19	1.03	0.013
657. LP (1) N^{Dz} 39	/***. BD*(1) O 5 - H 211	14.32	0.66	0.089

from unit 5 to unit 10

623. LP (1) O 5	/***. BD*(1) C 75 - H^{ax} 203	0.09	0.84	0.008
624. LP (2) O 5	/***. RY*(1) H^{ax} 203	0.09	1.06	0.009
624. LP (2) O 5	/***. RY*(1) $H^{o\text{-}Ar}$ 251	0.16	0.72	0.010
624. LP (2) O 5	/***. BD*(1) C 75 - H^{eq} 227	0.39	0.65	0.014
624. LP (2) O 5	/***. BD*(1) C 131 - $H^{o\text{-}Ar}$ 251	0.14	0.65	0.009

from unit 8 to unit 9

629. LP (1) O 8	/***. RY*(1) $H^{o\text{-}Ar}$ 232	0.10	1.01	0.009
629. LP (1) O 8	/***. RY*(1) $H^{o\text{-}Ar}$ 238	0.23	0.85	0.013
629. LP (1) O 8	/***. BD*(1) C 116 - $H^{o\text{-}Ar}$ 232	0.64	0.88	0.021
629. LP (1) O 8	/***. BD*(1) C 122 - $H^{o\text{-}Ar}$ 238	0.67	0.85	0.021
630. LP (2) O 8	/***. BD*(1) C 116 - $H^{o\text{-}Ar}$ 232	2.20	0.68	0.035
630. LP (2) O 8	/***. BD*(1) C 122 - $H^{o\text{-}Ar}$ 238	0.06	0.66	0.006

from unit 9 to unit 8

642. LP (1) N^{meso} 24	/***. BD*(1) O 8 - H 210	0.42	0.64	0.015
642. LP (1) N^{meso} 24	/***. BD*(1) O 8 - H 220	1.67	0.65	0.030
650. LP (1) N^{Dz} 32	/***. BD*(1) O 8 - H 220	3.15	0.65	0.042
656. LP (1) N^{Dz} 38	/***. RY*(1) H 210	0.19	1.03	0.013
656. LP (1) N^{Dz} 38	/***. BD*(1) O 8 - H 210	14.32	0.66	0.089

from unit 8 to unit 10

629. LP (1) O 8	/***. RY*(1) H^{ax} 202	0.06	1.25	0.008
629. LP (1) O 8	/***. BD*(1) C 74 - H^{ax} 202	0.09	0.84	0.008
630. LP (2) O 8	/***. RY*(1) H^{ax} 202	0.09	1.06	0.009
630. LP (2) O 8	/***. RY*(1) $H^{o\text{-}Ar}$ 250	0.16	0.72	0.010
630. LP (2) O 8	/***. BD*(1) C 74 - H^{eq} 226	0.39	0.65	0.014
630. LP (2) O 8	/***. BD*(1) C 130 - $H^{o\text{-}Ar}$ 250	0.14	0.65	0.008

from unit 2 to unit 10

617. LP (1) O 2	/***. RY*(1) $H^{o\text{-}Ar}$ 234	0.16	0.87	0.011
617. LP (1) O 2	/***. RY*(1) $H^{o\text{-}Ar}$ 242	0.14	1.01	0.011
617. LP (1) O 2	/***. BD*(1) C 118 - $H^{o\text{-}Ar}$ 234	0.22	0.88	0.013
617. LP (1) O 2	/***. BD*(1) C 126 - $H^{o\text{-}Ar}$ 242	1.58	0.90	0.034
618. LP (2) O 2	/***. BD*(1) C 118 - $H^{o\text{-}Ar}$ 234	0.10	0.62	0.007
618. LP (2) O 2	/***. BD*(1) C 126 - $H^{o\text{-}Ar}$ 242	1.06	0.64	0.023

from unit 10 to unit 2

636. LP (1) N^{meso} 18	/***. BD*(1) O 2 - H 206	2.88	0.64	0.040
636. LP (1) N^{meso} 18	/***. BD*(1) O 2 - H 214	0.66	0.64	0.019
644. LP (1) N^{Dz} 26	/***. RY*(1) H 214	0.18	1.01	0.013
644. LP (1) N^{Dz} 26	/***. BD*(1) O 2 - H 214	16.10	0.65	0.094
652. LP (1) N^{Dz} 34	/***. BD*(1) O 2 - H 206	3.59	0.66	0.045

from unit 2 to unit 9

618. LP (2) O 2 /***. RY*(1) H^{ax} 198 0.13 0.88 0.010
618. LP (2) O 2 /***. BD*(1) C 78 - H^{ax} 198 2.79 0.59 0.036

from unit 3 to unit 10

619. LP (1) O 3 /***. RY*(1) $H^{o\text{-}Ar}$ 235 0.16 0.87 0.011
619. LP (1) O 3 /***. RY*(1) $H^{o\text{-}Ar}$ 243 0.14 1.01 0.011
619. LP (1) O 3 /***. BD*(1) C 119 - $H^{o\text{-}Ar}$ 235 0.22 0.88 0.013
619. LP (1) O 3 /***. BD*(1) C 127 - $H^{o\text{-}Ar}$ 243 1.57 0.90 0.034
620. LP (2) O 3 /***. BD*(1) C 119 - $H^{o\text{-}Ar}$ 235 0.10 0.62 0.007
620. LP (2) O 3 /***. BD*(1) C 127 - $H^{o\text{-}Ar}$ 243 1.05 0.64 0.023

from unit 10 to unit 3

637. LP (1) N^{meso} 19 /***. BD*(1) O 3 - H 207 2.89 0.64 0.040
637. LP (1) N^{meso} 19 /***. BD*(1) O 3 - H 215 0.66 0.64 0.019
645. LP (1) N^{Dz} 27 /***. RY*(1) H 215 0.18 1.01 0.013
645. LP (1) N^{Dz} 27 /***. BD*(1) O 3 - H 215 16.14 0.65 0.094
653. LP (1) N^{Dz} 35 /***. BD*(1) O 3 - H 207 3.57 0.66 0.045

from unit 3 to unit 9

620. LP (2) O 3 /***. RY*(1) H^{ax} 199 0.13 0.88 0.010
620. LP (2) O 3 /***. BD*(1) C 79 - H^{ax} 199 2.77 0.59 0.036

from unit 6 to unit 10

625. LP (1) O 6 /***. RY*(1) $H^{o\text{-}Ar}$ 230 0.14 1.01 0.011
625. LP (1) O 6 /***. RY*(1) $H^{o\text{-}Ar}$ 240 0.17 0.87 0.011
625. LP (1) O 6 /***. BD*(1) C 114 - $H^{o\text{-}Ar}$ 230 1.11 0.90 0.028
625. LP (1) O 6 /***. BD*(1) C 124 - $H^{o\text{-}Ar}$ 240 0.20 0.88 0.012
626. LP (2) O 6 /***. BD*(1) C 114 - $H^{o\text{-}Ar}$ 230 1.07 0.64 0.023
626. LP (2) O 6 /***. BD*(1) C 124 - $H^{o\text{-}Ar}$ 240 0.08 0.61 0.006

from unit 10 to unit 6

640. LP (1) N^{meso} 22 /***. RY*(1) H 218 0.06 0.97 0.007
640. LP (1) N^{meso} 22 /***. BD*(1) O 6 - H 212 0.53 0.65 0.017
640. LP (1) N^{meso} 22 /***. BD*(1) O 6 - H 218 2.81 0.65 0.039
648. LP (1) N^{Dz} 30 /***. BD*(1) O 6 - H 218 3.00 0.65 0.041
658. LP (1) N^{Dz} 40 /***. RY*(1) H 212 0.17 1.01 0.012
658. LP (1) N^{Dz} 40 /***. BD*(1) O 6 - H 212 14.10 0.66 0.089

from unit 6 to unit 9

626. LP (2) O 6 /***. RY*(1) H^{ax} 204 0.17 0.90 0.011
626. LP (2) O 6 /***. BD*(1) C 76 - H^{ax} 204 1.30 0.59 0.025

from unit 7 to unit 10

627. LP (1) O 7 /***. RY*(1) $H^{o\text{-}Ar}$ 231 0.14 1.01 0.011
627. LP (1) O 7 /***. RY*(1) $H^{o\text{-}Ar}$ 237 0.17 0.87 0.011
627. LP (1) O 7 /***. BD*(1) C 115 - $H^{o\text{-}Ar}$ 231 1.11 0.90 0.028
627. LP (1) O 7 /***. BD*(1) C 121 - $H^{o\text{-}Ar}$ 237 0.20 0.88 0.012
628. LP (2) O 7 /***. BD*(1) C 115 - $H^{o\text{-}Ar}$ 231 1.10 0.64 0.024
628. LP (2) O 7 /***. BD*(1) C 121 - $H^{o\text{-}Ar}$ 237 0.08 0.61 0.006

from unit 10 to unit 7

641. LP (1) N^{meso} 23	/***. RY*(1) H 219	0.06	0.97	0.007
641. LP (1) N^{meso} 23	/***. BD*(1) O 7 - H 209	0.52	0.65	0.017
641. LP (1) N^{meso} 23	/***. BD*(1) O 7 - H 219	2.80	0.65	0.039
649. LP (1) N^{Dz} 31	/***. BD*(1) O 7 - H 219	2.99	0.65	0.041
655. LP (1) N^{Dz} 37	/***. RY*(1) H 209	0.17	1.01	0.012
655. LP (1) N^{Dz} 37	/***. BD*(1) O 7 - H 209	14.06	0.66	0.089

from unit 7 to unit 9

627. LP (1) O 7	/***. BD*(1) C 73 - H^{ax} 201	0.06	0.86	0.006
628. LP (2) O 7	/***. RY*(1) H^{ax} 201	0.17	0.90	0.011
628. LP (2) O 7	/***. BD*(1) C 73 - H^{ax} 201	1.29	0.59	0.025

from unit 9 to unit 10

635. LP (1) N^{meso} 17	/***. RY*(1) H^{ax} 197	0.23	1.08	0.015
635. LP (1) N^{meso} 17	/***. BD*(1) C 77 - H^{ax} 197	5.38	0.67	0.055
638. LP (1) N^{meso} 20	/***. RY*(1) H^{ax} 200	0.23	1.08	0.015
638. LP (1) N^{meso} 20	/***. BD*(1) C 80 - H^{ax} 200	5.36	0.67	0.055
639. LP (1) N^{meso} 21	/***. RY*(1) H^{ax} 203	0.24	1.09	0.015
639. LP (1) N^{meso} 21	/***. BD*(1) C 75 - H^{ax} 203	5.26	0.67	0.055
642. LP (1) N^{meso} 24	/***. RY*(1) H^{ax} 202	0.24	1.09	0.015
642. LP (1) N^{meso} 24	/***. BD*(1) C 74 - H^{ax} 202	5.27	0.67	0.055
647. LP (1) N^{Dz} 29	/***. BD*(1) C 75 - H^{ax} 203	0.48	0.68	0.017
650. LP (1) N^{Dz} 32	/***. BD*(1) C 74 - H^{ax} 202	0.47	0.68	0.017
651. LP (1) N^{Dz} 33	/***. BD*(1) C 77 - H^{ax} 197	0.42	0.68	0.016
654. LP (1) N^{Dz} 36	/***. BD*(1) C 80 - H^{ax} 200	0.42	0.68	0.016

from unit 10 to unit 9

636. LP (1) N^{meso} 18	/***. BD*(1) C 78 - H^{ax} 198	0.30	0.66	0.013
637. LP (1) N^{meso} 19	/***. BD*(1) C 79 - H^{ax} 199	0.31	0.66	0.013
640. LP (1) N^{meso} 22	/***. BD*(1) C 76 - H^{ax} 204	0.60	0.66	0.018
641. LP (1) N^{meso} 23	/***. BD*(1) C 73 - H^{ax} 201	0.60	0.66	0.018
648. LP (1) N^{Dz} 30	/***. BD*(1) C 76 - H^{ax} 204	0.38	0.67	0.015
649. LP (1) N^{Dz} 31	/***. BD*(1) C 73 - H^{ax} 201	0.38	0.67	0.015
652. LP (1) N^{Dz} 34	/***. BD*(1) C 78 - H^{ax} 198	0.27	0.67	0.012
653. LP (1) N^{Dz} 35	/***. BD*(1) C 79 - H^{ax} 199	0.27	0.67	0.012

Notes to **S7-B**: units 1,4,5,8 denote H_2O near unit 9 ($^{tBuPh}DzPzH_2$ subunit in the ligand dimer **1**); units 2,3,6,7 – H_2O near unit 10 ($^{tBuPh}DzPzH_2$ subunit in the ligand dimer **1**).

References

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2. E. N. Tarakanova, O. A. Levitskiy, T. V. Magdesieva, P. A. Tarakanov, V. E. Pushkarev and L. G. Tomilova, *New J. Chem.*, 2015, **39**, 5797-5804.